simpeg

an open-source framework for simulation and parameter estimation in geophysics

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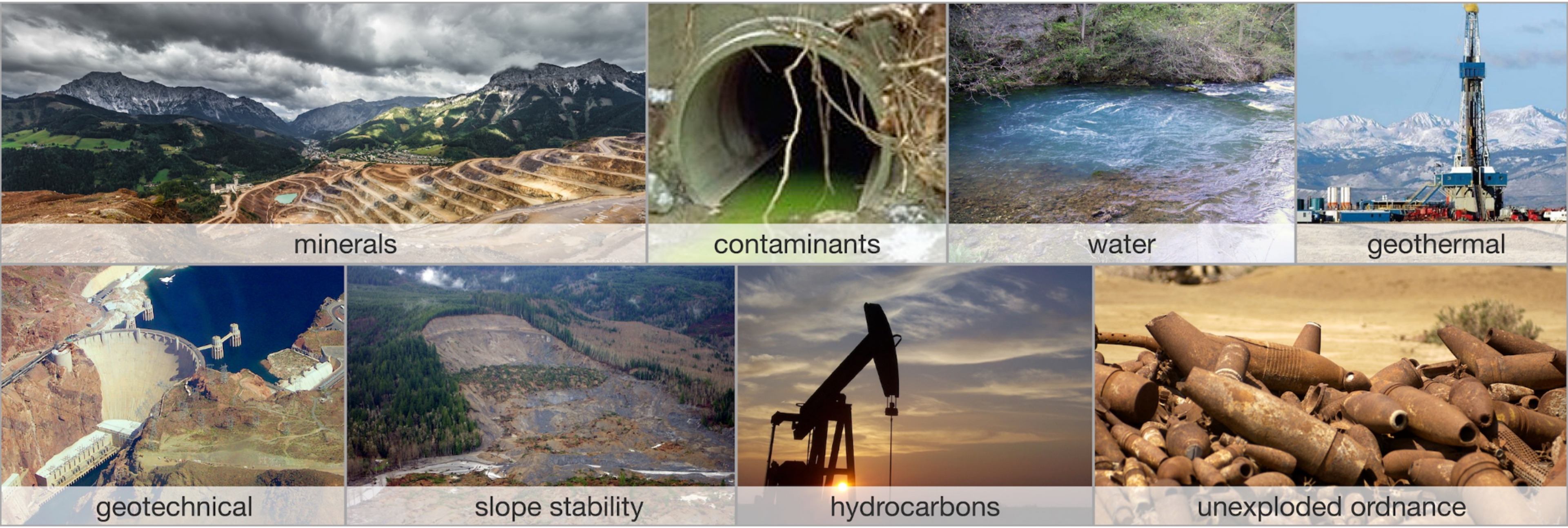
[3]Mira Geoscience
[4]University of Manitoba
[5]Curvenote Inc

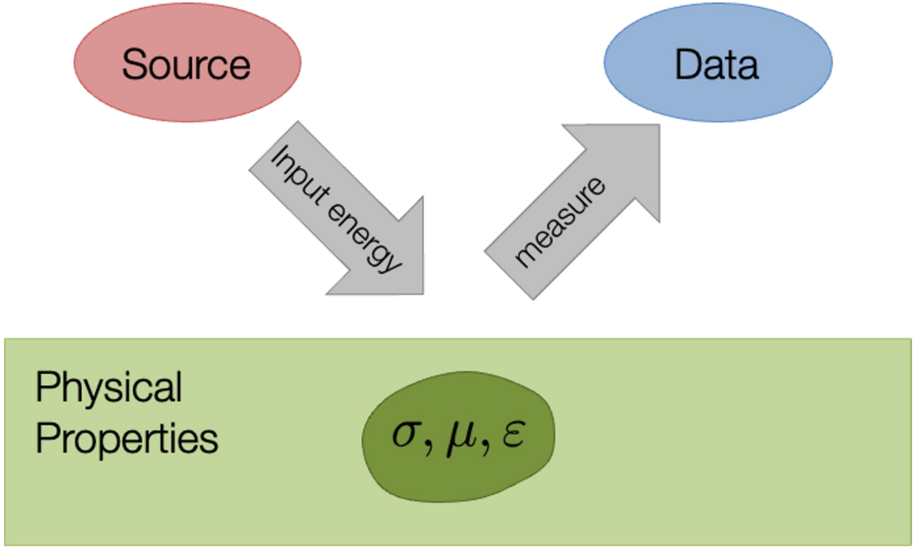
ICCOPT – 2025

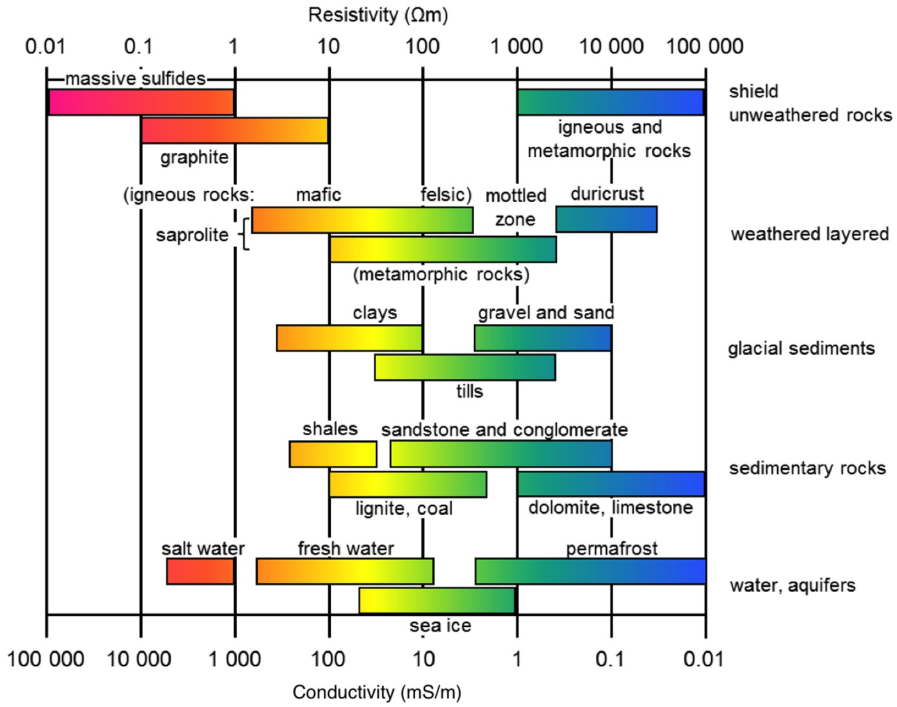
applications



in all… need to “image” the subsurface non-invasively

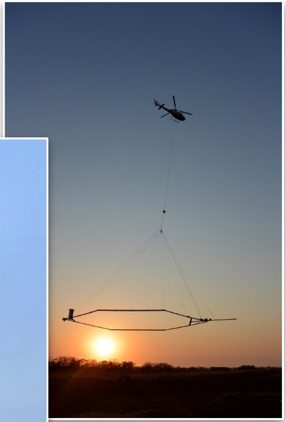
generic geophysical experiment





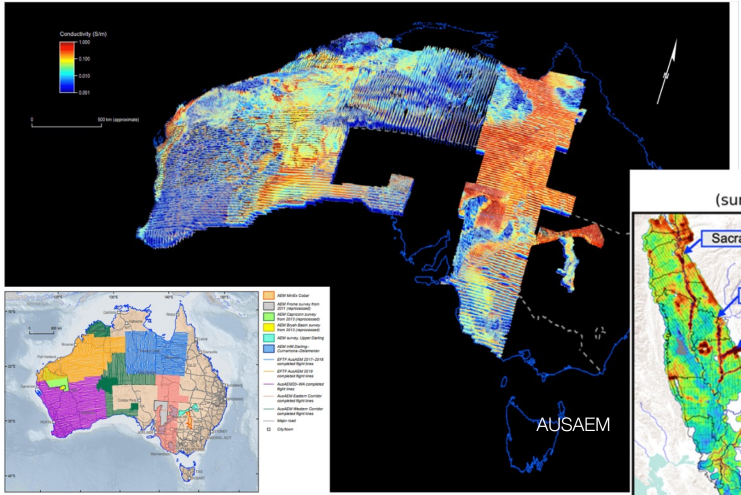
geophysical experiments

airborne

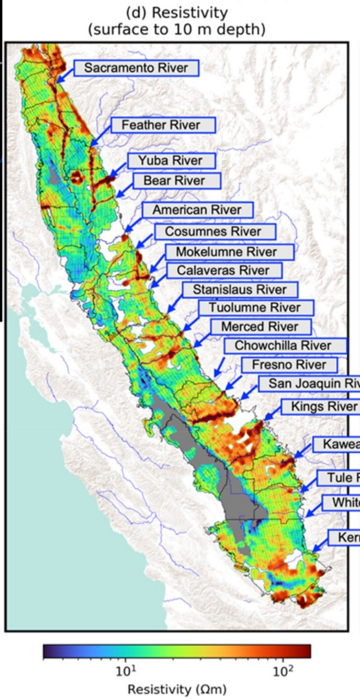


ground or borehole

often on large scales



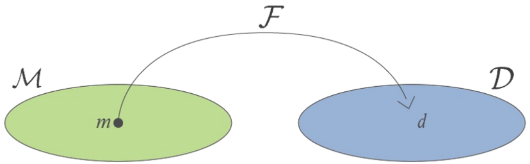
Central Valley, California
(Kang et al., 2025)

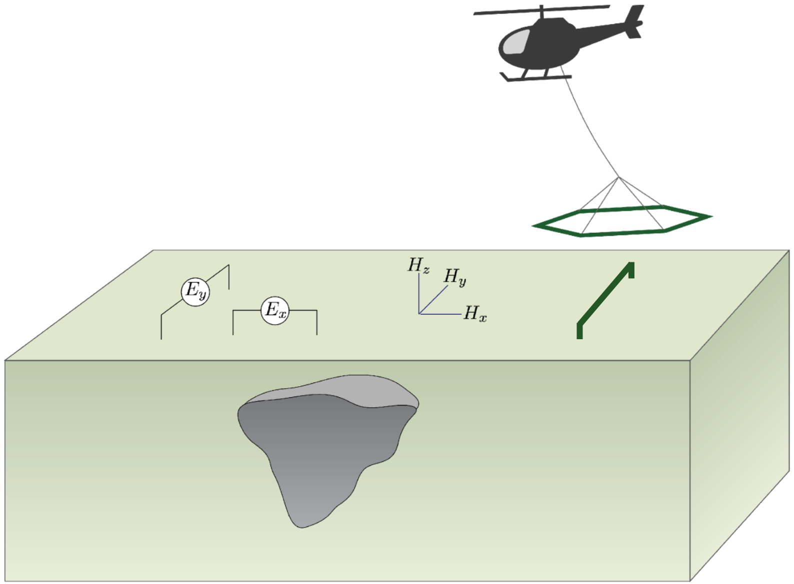


statement of the inverse problem

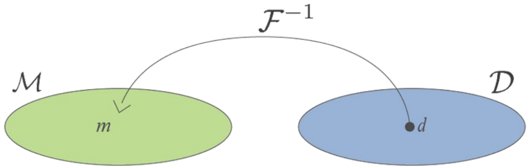
Given

- observations: $d_j^{obs}, \quad j = 1, \ldots, N$
- uncertainties: ϵ_j
- ability to forward model: $\mathcal{F}[m] = d$





Find an Earth model that fits those data and a-priori information

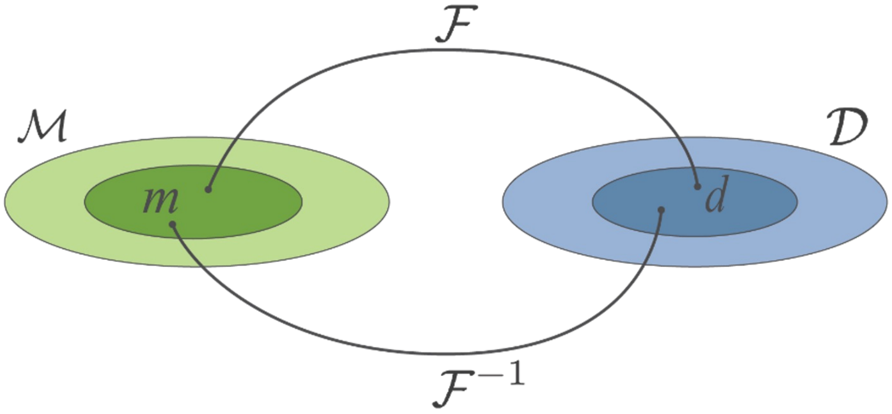


inverse problem

The inverse problem is ill-posed

- non-unique
- ill-conditioned

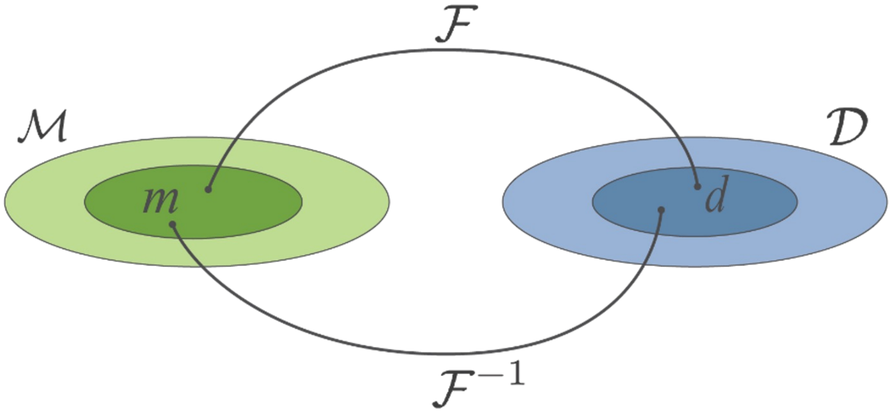
Any inversion approach must address these issues.



inverse problem

Prior information important to constrain the inversion

- geologic structures
- boreholes
- reference model
- bounds
- physical properties
- other geophysical data
- …



need a framework for inverse problem

Tikhonov (deterministic)

Find a single “best” solution by solving optimization

$$\text{minimize} \quad \phi = \phi_d + \beta\phi_m$$

$$\text{subject to} \quad m_L < m < m_H$$

$$\begin{cases} \phi_d\text{: data misfit} \\ \phi_m\text{: regularization} \\ \beta\text{: trade-off parameter} \\ m_L, m_H\text{: lower and upper bounds} \end{cases}$$

Bayesian (probabilistic)

Use Bayes’ theorem

$$P(m|d^{obs}) \propto P(d^{obs}|m)P(m)$$

$$\begin{cases} P(m)\text{: prior information about } m \\ P(d^{obs}|m)\text{: probability about the data errors (likelihood)} \\ P(m|d^{obs})\text{: posterior probability for the model} \end{cases}$$

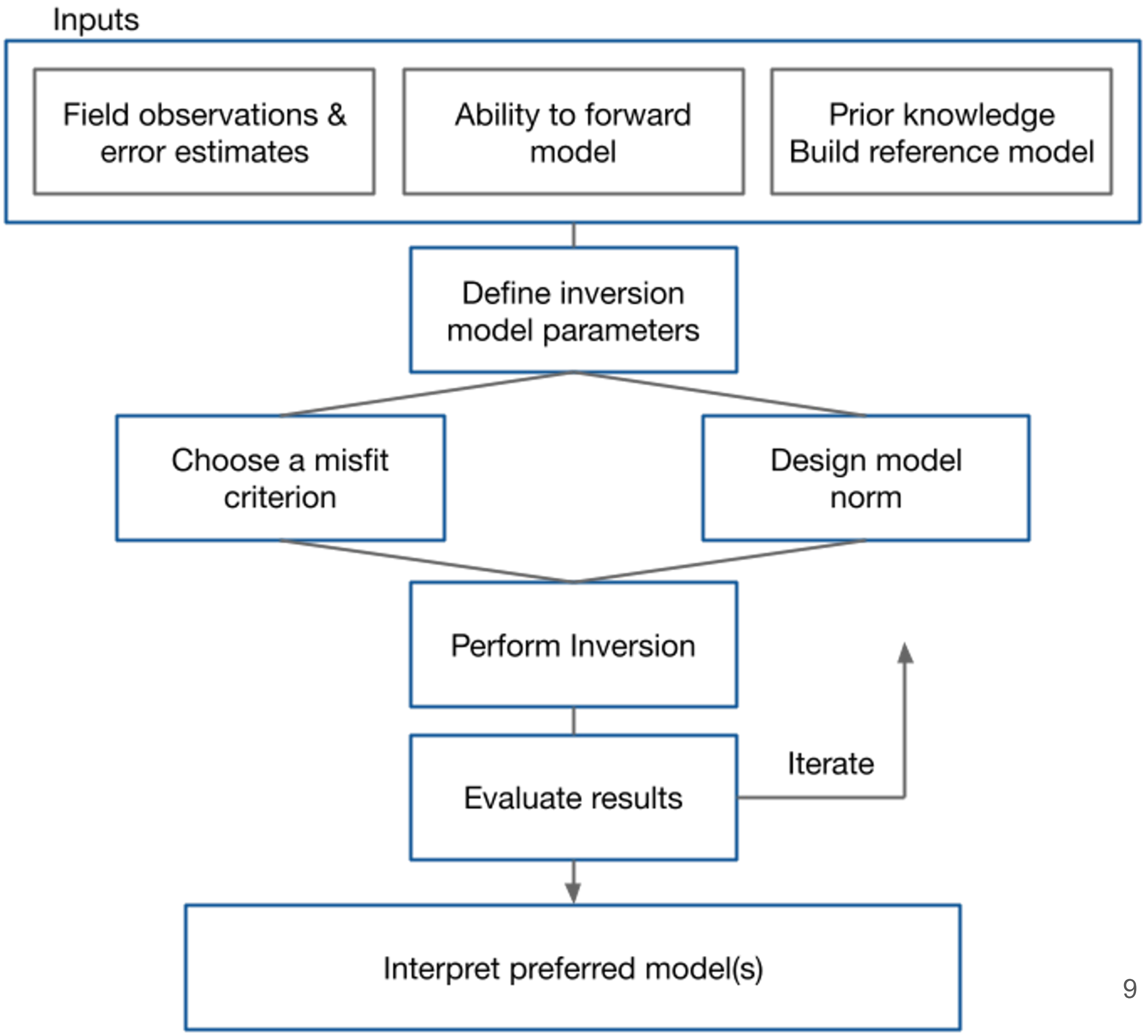
Two approaches:

(a) Characterize $P(m|d^{obs})$

(a) Find a particular solution that maximizes $P(m|d^{obs})$
MAP: (maximum a posteriori) estimate

flow chart for the inverse problem

- iterative process to obtain solution
- each component requires evaluation, adjustment by user
- opportunities for research within each component



simpeg

Simulation and parameter estimation in geophysics

common framework for simulations & inversions

accelerate research: build upon others work

facilitate reproducibility of results

build & deploy in python

open-source

WHY ABOUT CONTACT CONTRIBUTE

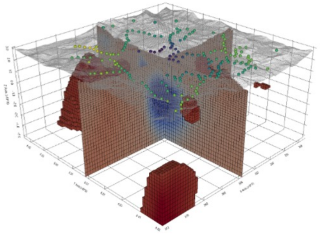
Simulation and Parameter Estimation in Geophysics

An open source python package for simulation and gradient based parameter estimation in geophysical applications.

Geophysical Methods

Contribute to a growing community of geoscientists building an open foundation for geophysics. SimPEG provides a collection of geophysical simulation and inversion tools that are built in a consistent framework.

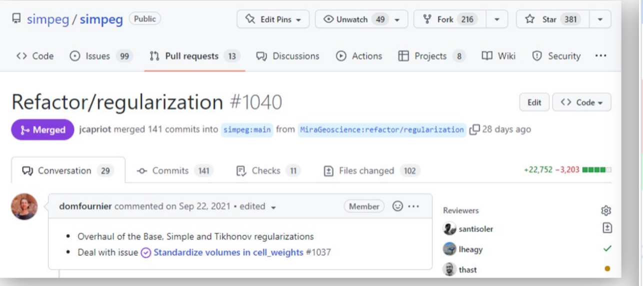
- Gravity
- Magnetics
- Direct current resistivity
- Induced polarization
- Electromagnetics
  - Time domain
  - Frequency domain
  - Natural source (e.g. Magnetotellurics)
  - Viscous remanent magnetization
- Richards Equation



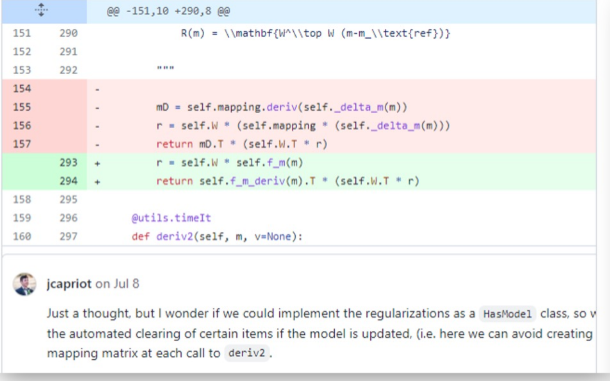
https://simpeg.xyz

open development: how contributions get included

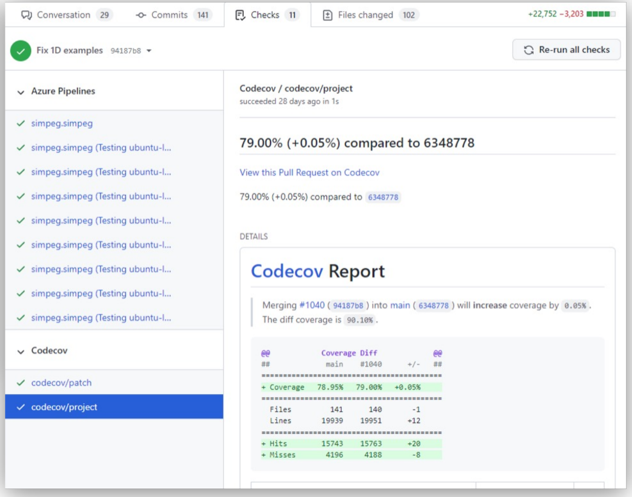
Submit proposed changes (Pull Request)



SimPEG community + maintainers review changes



Ensure existing unit tests pass and changes are also tested



codecov 86%

maintainers

S. Soler

J. Capriotti

https://github.com/simpeg/simpeg

testing

mathematical properties

analytic solutions, convergence criteria

code comparisons

confidence

Testing

11 jobs completed 31m 20s

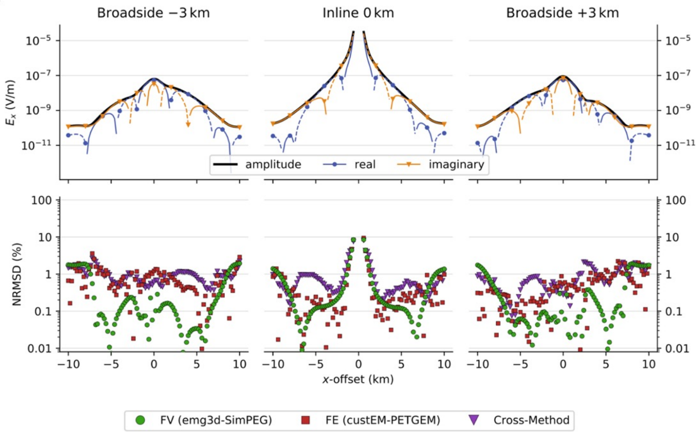
99.8% tests passed

12 artifacts

vector identity: $\nabla \cdot \nabla \times \vec{v} = 0$

```
[2]: v = np.random.rand(mesh.nE)
     np.all(mesh.faceDiv * mesh.edgeCurl * v == 0)

[2]: True
```

```
==================== check_derivative ====================
iter    h          |ft-f0|    |ft-f0-h*J0*dx|   Order
---------------------------------------------------------
 0    1.00e-01    1.690e-01     8.400e-03      nan
 1    1.00e-02    1.636e-02     8.703e-05      1.985
 2    1.00e-03    1.630e-03     8.732e-07      1.999
 3    1.00e-04    1.629e-04     8.735e-09      2.000
 4    1.00e-05    1.629e-05     8.736e-11      2.000
 5    1.00e-06    1.629e-06     8.736e-13      2.000
 6    1.00e-07    1.629e-07     8.822e-15      1.996
========================= PASS! =========================
Once upon a time, a happy little test passed.
```

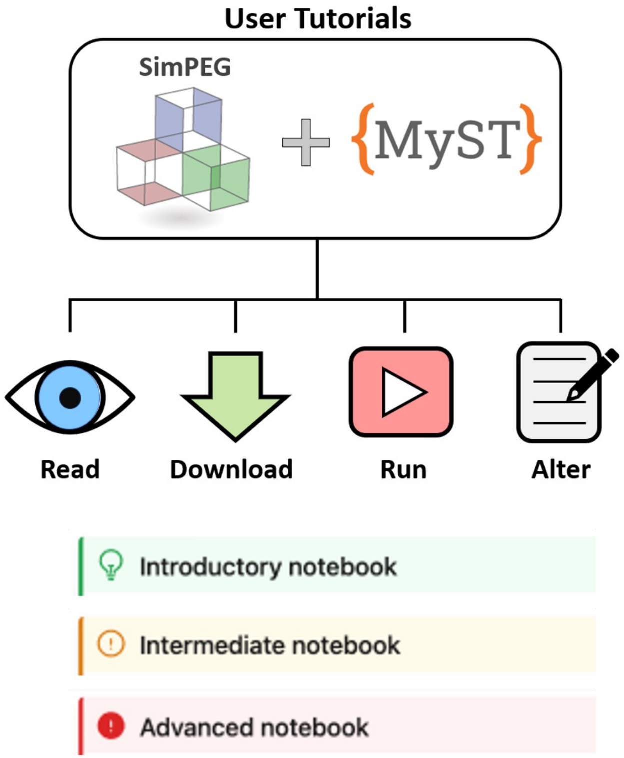


(Werthmüller et al., 2020)

user tutorials

growing library of training materials:

- parameter choices in setting up forward simulations, inversions, e.g.mesh design, regularization parameters
- basic, intermediate, and advanced forward simulation and inversion approaches
- understanding SimPEG objects

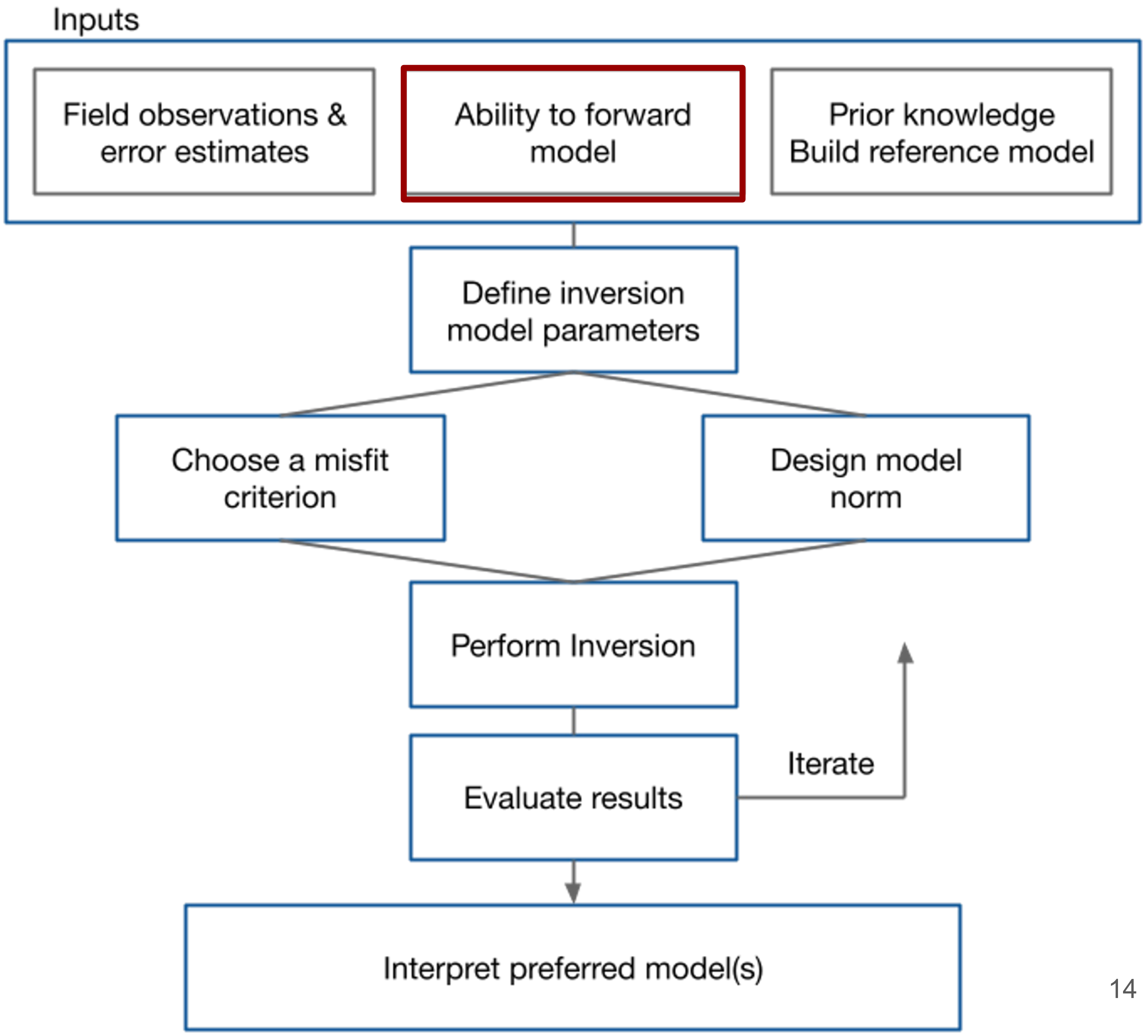



D. Cowan


S. Soler

https://simpeg.xyz/user-tutorials

flow chart for the inverse problem



electromagnetics: basic equations (quasi-static)

	Time	Frequency
Faraday's Law	$\nabla \times \vec{e} = -\frac{\partial \vec{b}}{\partial t}$	$\nabla \times \vec{E} = -i\omega \vec{B}$
Ampere's Law	$\nabla \times \vec{h} = \vec{j} + \frac{\partial \vec{d}}{\partial t}$	$\nabla \times \vec{H} = \vec{J} + i\omega \vec{D}$
No Magnetic Monopoles	$\nabla \cdot \vec{b} = 0$	$\nabla \cdot \vec{B} = 0$
Constitutive Relationships (non-dispersive)	$\vec{j} = \sigma \vec{e}$ $\vec{b} = \mu \vec{h}$ $\vec{d} = \varepsilon \vec{e}$	$\vec{J} = \sigma \vec{E}$ $\vec{B} = \mu \vec{H}$ $\vec{D} = \varepsilon \vec{E}$

* Solve with sources and boundary conditions

electromagnetics: frequency domain

Continuous equations

$$\nabla \times \vec{E} + i\omega \vec{B} = 0$$

$$\nabla \times \mu^{-1}\vec{B} - \sigma \vec{E} = \vec{J}_s$$

$$\hat{n} \times \vec{B}|_{\partial\Omega} = 0$$

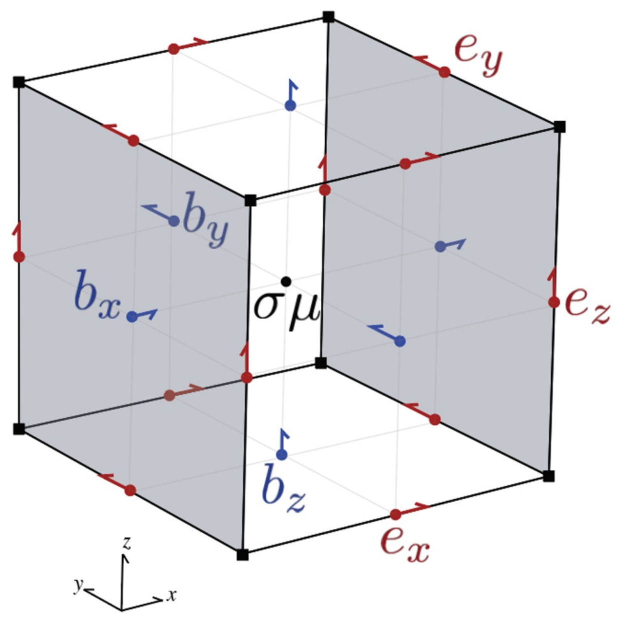
Finite volume discretization

$$\mathbf{C}\mathbf{e} + i\omega \mathbf{b} = 0$$

$$\mathbf{C}^\top \mathbf{M}^f_{\mu^{-1}}\mathbf{b} - \mathbf{M}^e_\sigma \mathbf{e} = \mathbf{M}^e \mathbf{j_s}$$

Eliminate **b** to obtain a second-order system in **e**

$$\underbrace{(\mathbf{C}^\top \mathbf{M}^f_{\mu^{-1}}\mathbf{C} + i\omega \mathbf{M}^e_\sigma)}_{\mathbf{A}(\sigma,\omega)} \underbrace{\mathbf{e}}_{\mathbf{u}} = \underbrace{-i\omega \mathbf{M}^e \mathbf{j_s}}_{\mathbf{q}(\omega)}$$



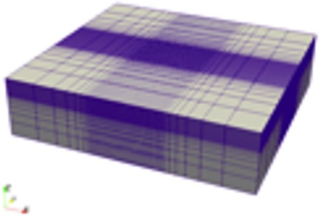
(Haber, 2014; Cockett et al, 2016)

solving a FDEM problem

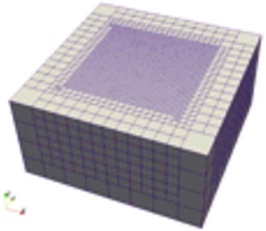
$$\underbrace{(\mathbf{C}^\top \mathbf{M}^f_{\mu^{-1}}\mathbf{C} + i\omega \mathbf{M}^e_\sigma)}_{\mathbf{A}(\sigma,\omega)} \underbrace{\mathbf{e}}_{\mathbf{u}} = \underbrace{-i\omega\mathbf{M}^e\mathbf{j_s}}_{\mathbf{q}(\omega)}$$

```
ω = 2 * pi * frequency

C = mesh.edge_curl
Mfμi = mesh.get_face_inner_product(1/mu_0)
Meσ = mesh.get_edge_inner_product(sigma)

A = C.T @ Mfμi @ C + 1j * ω * Meσ
Ainv = Solver(A)  # acts like A inverse

Me = mesh.get_edge_inner_product()
q = -1j * ω * Me @ js

u = Ainv @ q
```

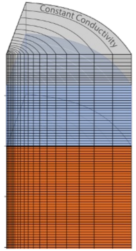
```
from simpeg import electromagnetics
```



Tensor

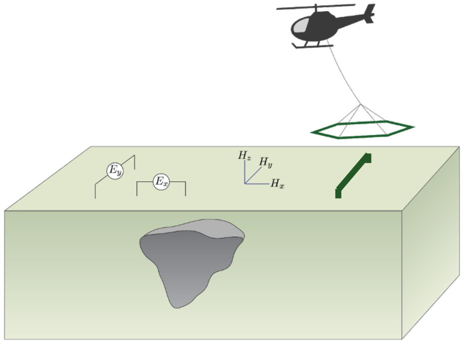


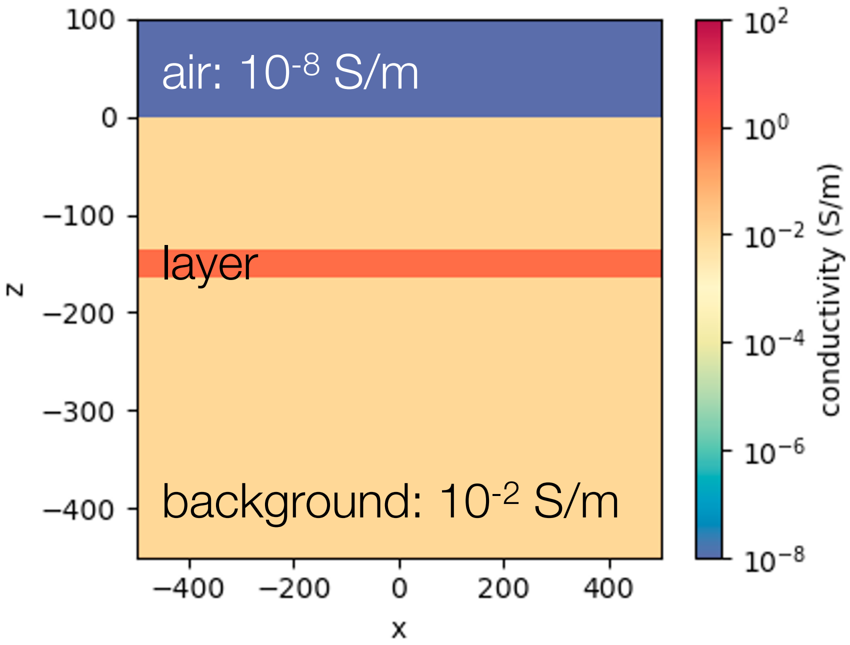
OcTree

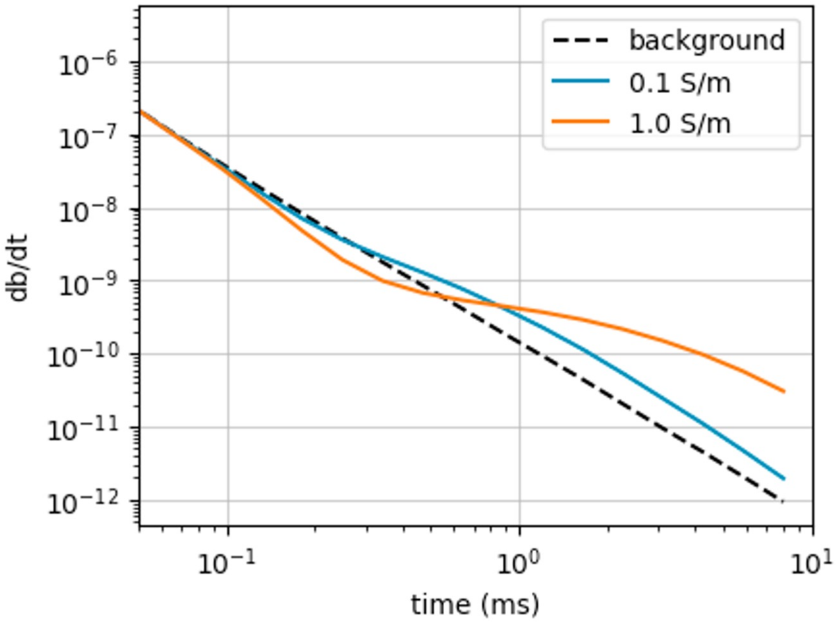


Cylindrical

example: airborne electromagnetics

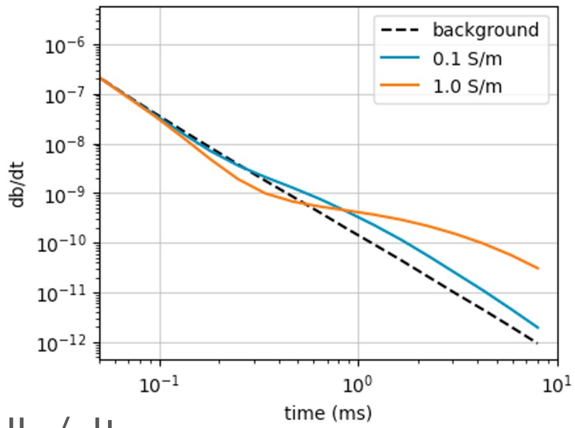




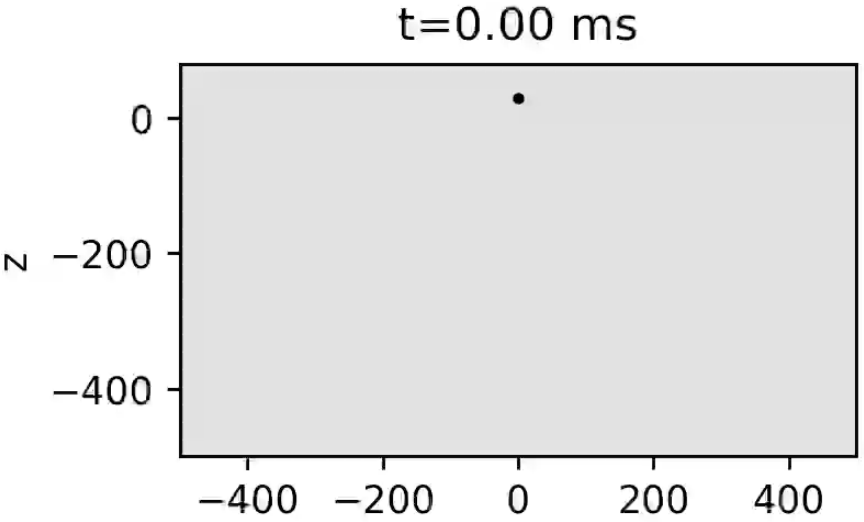


example: airborne electromagnetics

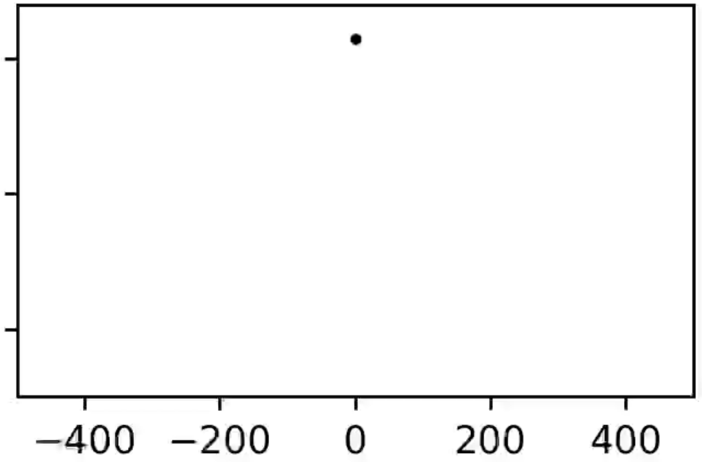
halfspace



current density

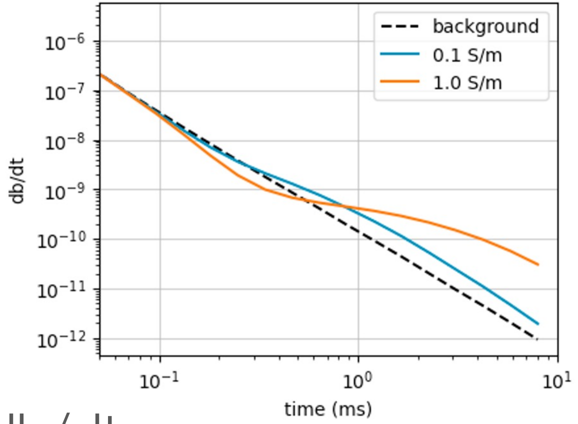


db/dt



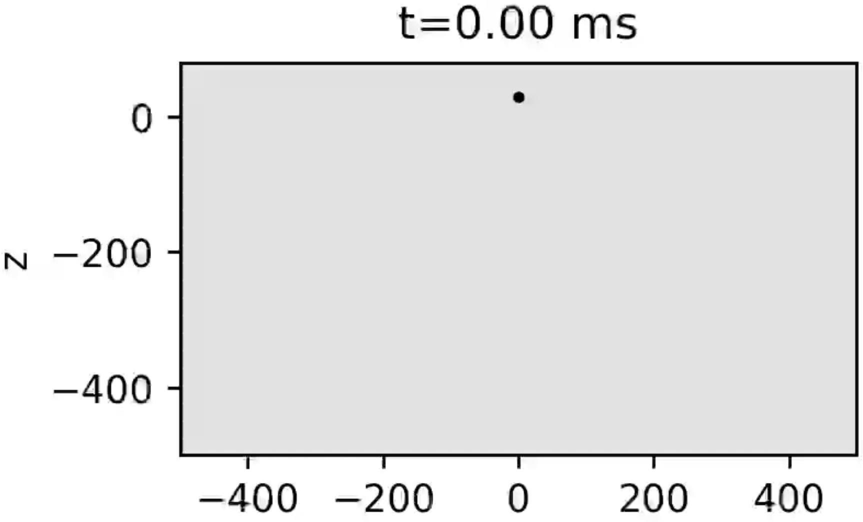
example: airborne electromagnetics

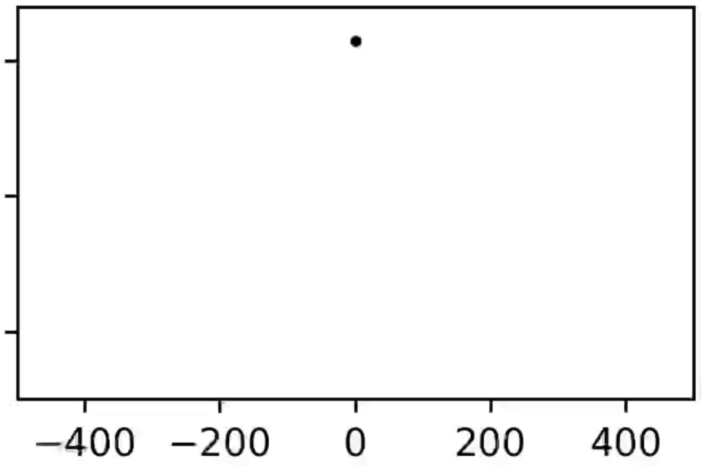
halfspace with a conductive layer



current density

db/dt





sensitivities

For inverse problem, need sensitivities (and adjoint)

$$\mathbf{J} = \frac{\partial \mathcal{F}[\mathbf{m}]}{\partial \mathbf{m}}$$

$$= \frac{\partial \mathbf{P}(\mathbf{u}, \omega)}{\partial \mathbf{u}} \frac{\partial \mathbf{u}}{\partial \mathbf{m}}$$

where the derivative of the fields (**u**) is computed implicitly (requires a solve)

$$\frac{\partial \mathbf{A}(\sigma, \omega)\mathbf{u}^{\text{fixed}}}{\partial \mathbf{m}} + \mathbf{A}(\sigma, \omega)\frac{\partial \mathbf{u}}{\partial \mathbf{m}} = 0$$

J is a large, dense matrix → compute products with a vector if memory-limited

flow chart for the inverse problem

What do we need for inversion?

$$\text{minimize} \quad \phi = \phi_d + \beta\phi_m$$

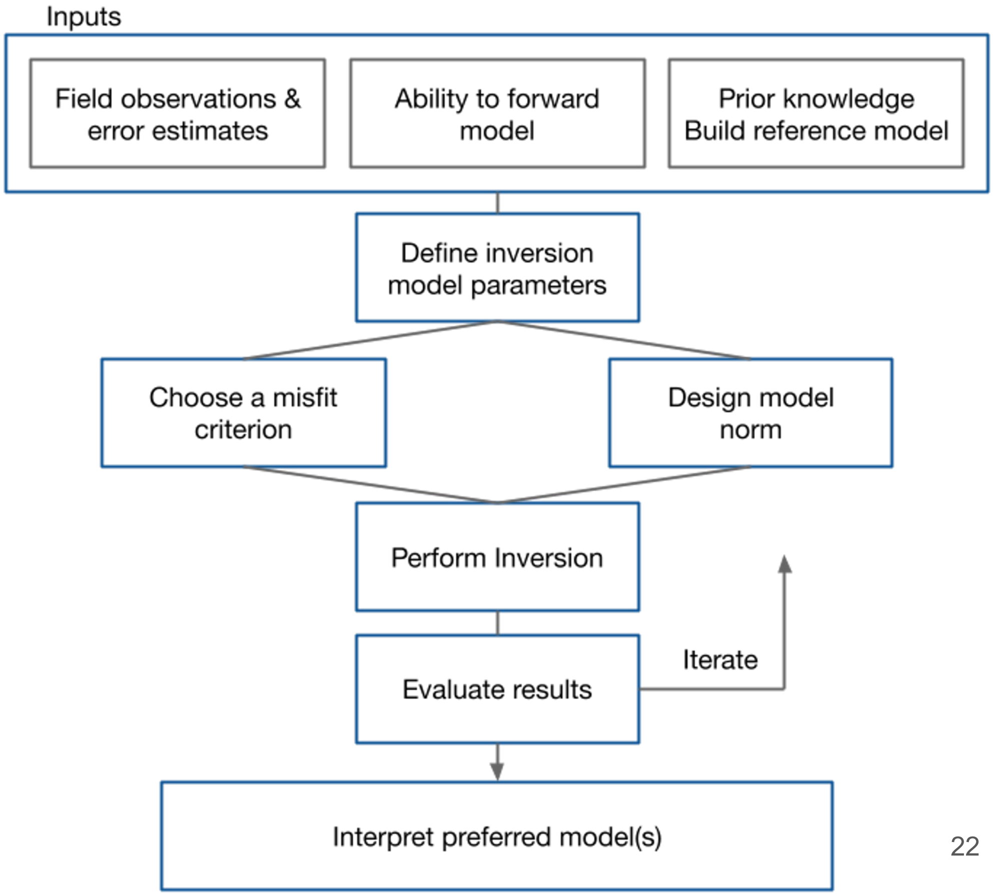
$$\text{subject to} \quad m_L < m < m_H$$

From the simulation

- adjoint sensitivity times a vector
- sensitivity times a vector

Inversion components:

- define a model norm
- perform optimization



inversion as an optimization problem

$$\min_{\mathbf{m}} \phi(\mathbf{m}) = \phi_d(\mathbf{m}) + \beta\phi_m(\mathbf{m})$$

$$\text{s.t. } \phi_d \leq \phi_d^* \quad \mathbf{m}_L \leq \mathbf{m} \leq \mathbf{m}_U$$

data misfit

$$\phi_d = \|\mathbf{W}_d(\mathcal{F}(\mathbf{m}) - \mathbf{d}^{\text{obs}})\|^2$$

uncertainties captured in **W**

$$\mathbf{W}_d = \text{diag}\left(\frac{1}{\boldsymbol{\epsilon}}\right)$$

$$\epsilon_j = \%|d_j^{\text{obs}}| + \text{floor}$$

typical model norm

$$\phi_m = \underbrace{\alpha_s \int_V w_s(m - m_{\text{ref}})^2 dV}_{\text{smallness}} + \underbrace{\alpha_x \int_V w_x \frac{d(m - m_{\text{ref}})}{dx}^2 dV}_{\text{first-order smoothness}}$$

discretize

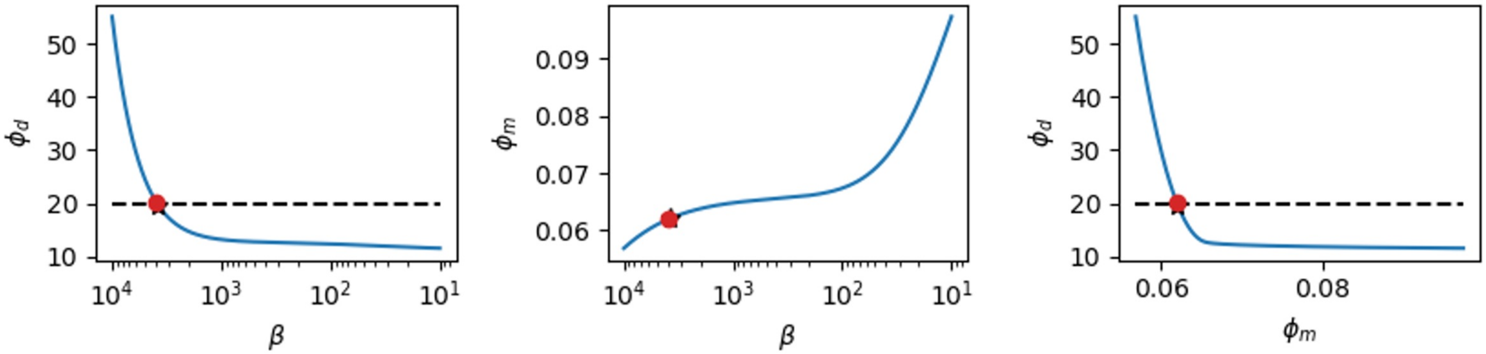
$$\phi_m = \alpha_s\|\mathbf{W}_s(\mathbf{m} - \mathbf{m}_{\text{ref}})\|^2 + \alpha_x\|\mathbf{W}_x(\mathbf{m} - \mathbf{m}_{\text{ref}})\|^2$$

solving the optimization problem

$$\min_{\mathbf{m}} \phi(\mathbf{m}) = \phi_d(\mathbf{m}) + \beta\phi_m(\mathbf{m})$$

$$\text{s.t. } \phi_d \leq \phi_d^* \quad \mathbf{m}_L \leq \mathbf{m} \leq \mathbf{m}_U$$

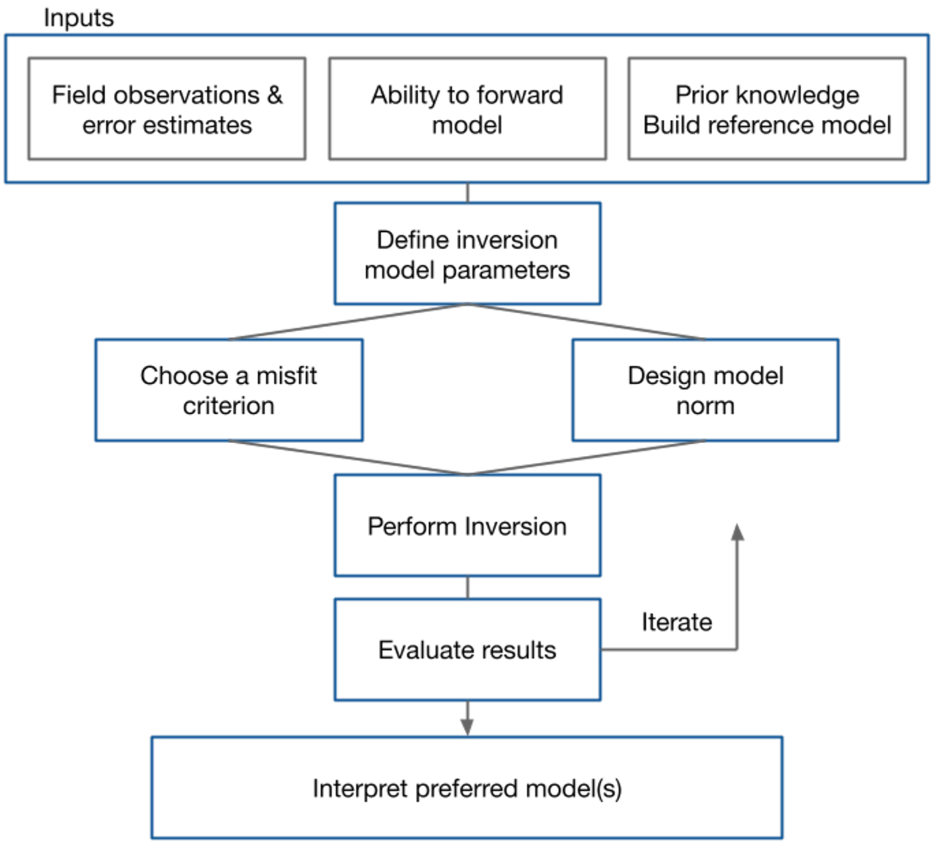
standard approach: Gauss Newton–CG + β-cooling strategy



different flavours of inversion & research opportunities

Two examples:

- Sparse & compact norms
- Using a GMM in the model norm



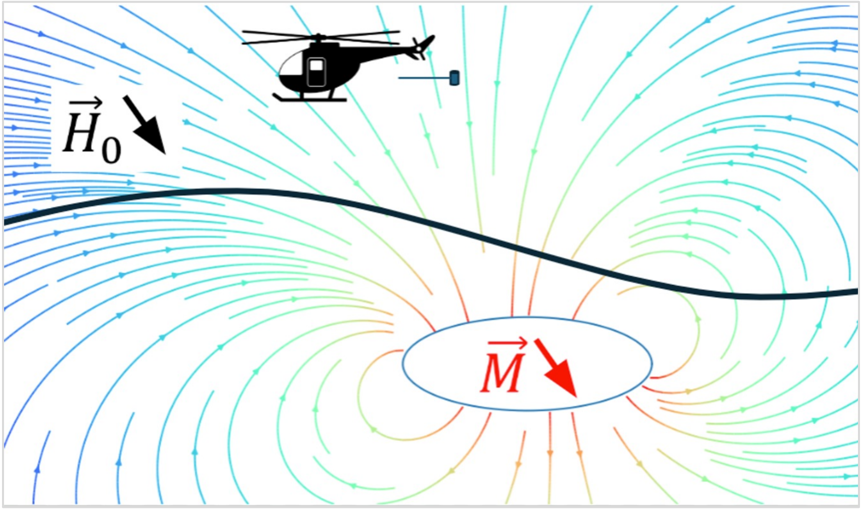
example 1: sparse / compact norms

sparse / compact norms with IRLS

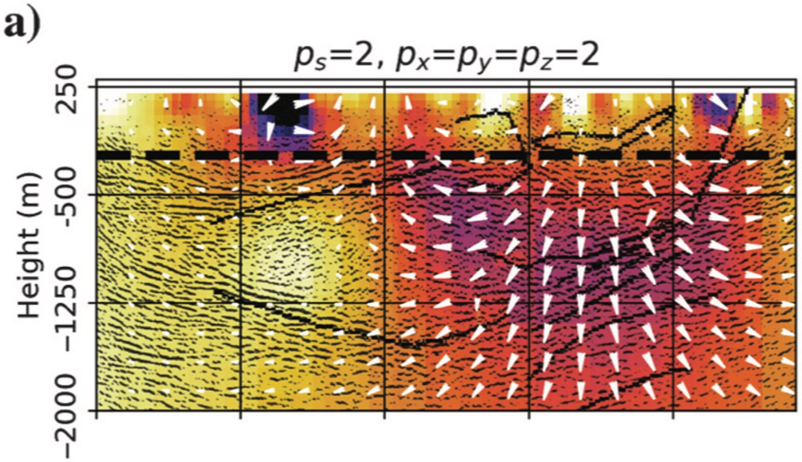
Fournier et al, 2019

$$\phi_m = \alpha_s \int_V w_s |m - m_{\text{ref}}|^{p_s} dV + \alpha_x \int_V w_x \left| \frac{d(m - m_{\text{ref}})}{dx} \right|^{p_x} dV$$

Magnetic vector inversion (MVI)



inversion results: cross-section

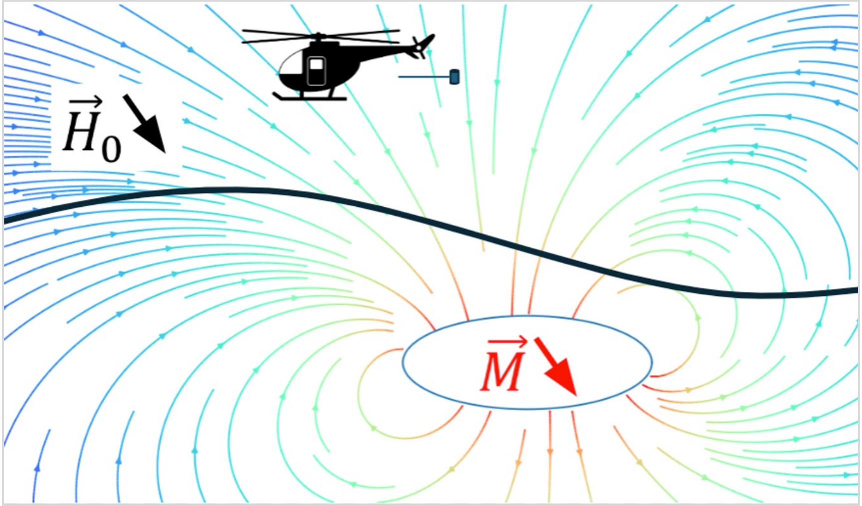


sparse / compact norms with IRLS

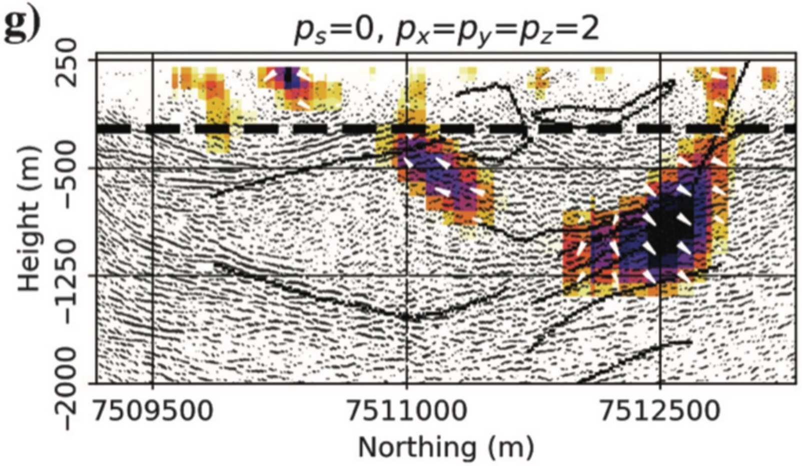
Fournier et al, 2019

$$\phi_m = \alpha_s \int_V w_s |m - m_{\text{ref}}|^{p_s} dV + \alpha_x \int_V w_x \left| \frac{d(m - m_{\text{ref}})}{dx} \right|^{p_x} dV$$

Magnetic vector inversion (MVI)



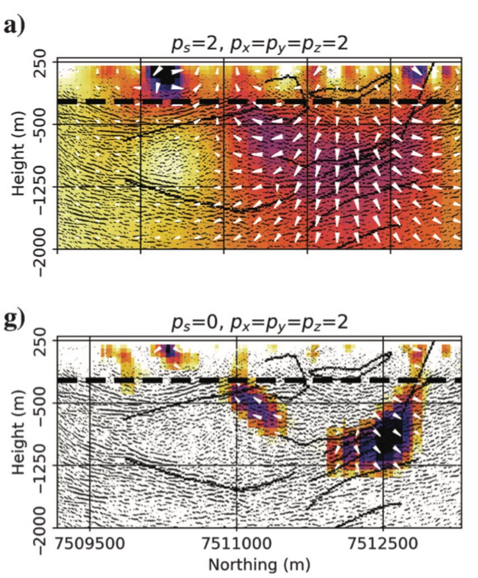
inversion results: cross-section



sparse / compact norms with IRLS

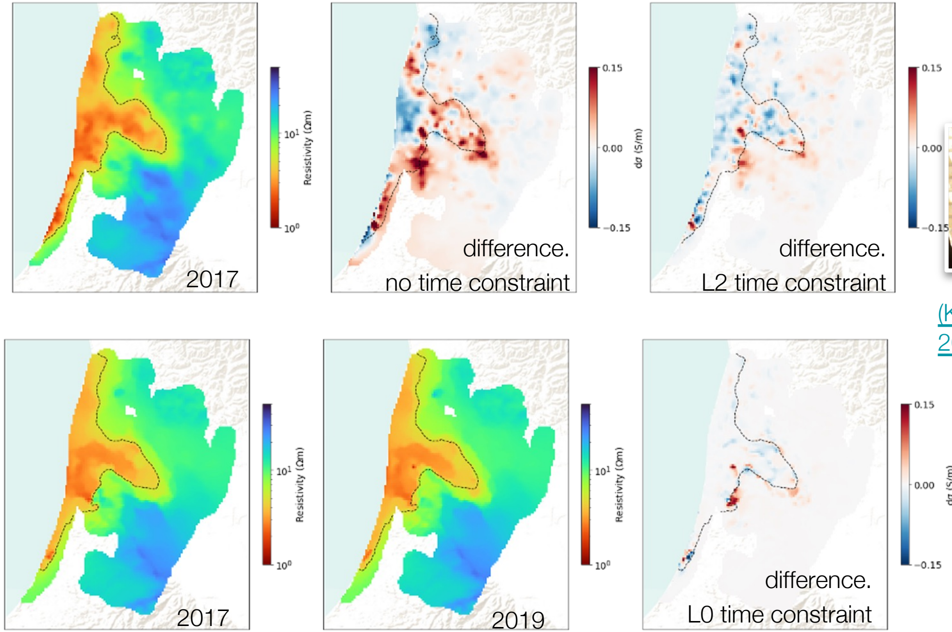
$$\phi_m = \alpha_s \int_V w_s |m - m_{\text{ref}}|^{p_s} dV + \alpha_x \int_V w_x \left| \frac{d(m - m_{\text{ref}})}{dx} \right|^{p_x} dV$$

developed in potential fields



(Fournier et al, 2019)

adapted to time-lapse electromagnetics: groundwater



(Kang & Knight, 2022)

example 2: using a gaussian mixture model in the inversion

Using a Gaussian Mixture Model in the model norm

Example: Carbon mineralization – Rocks that have been serpentinized (altered) can react with CO_2 to from carbonated minerals. Reactions change physical properties

serpentinization

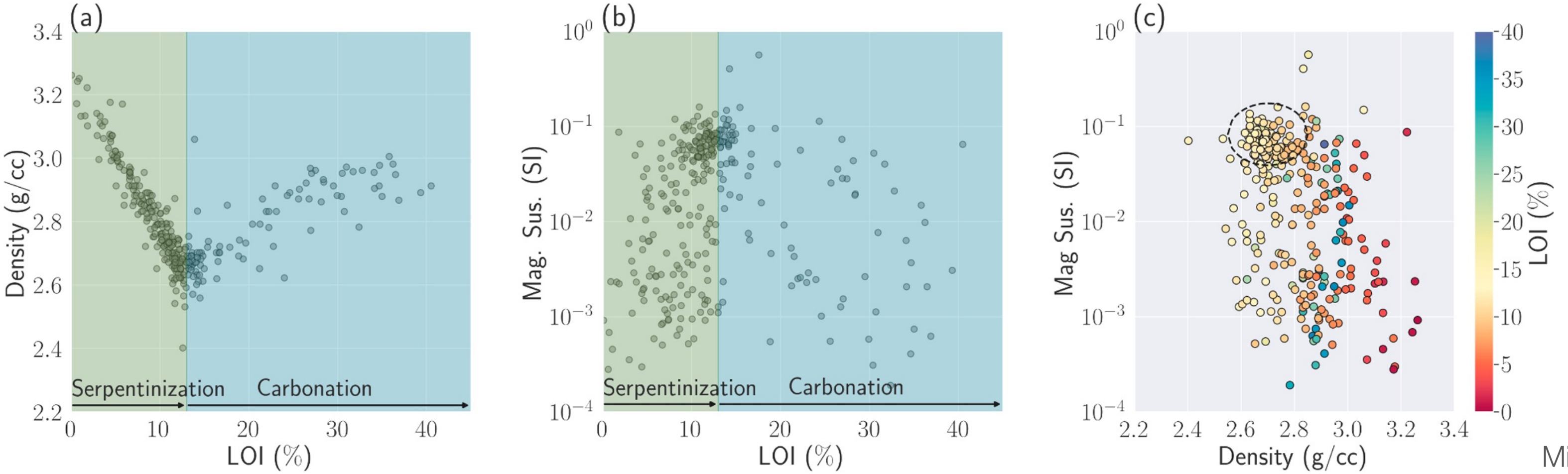
R1: olivine ± orthopyroxene + H_2O → serpentine ± brucite ± magnetite

carbonation

R2: olivine + brucite + CO_2 + H_2O → serpentine + magnesite + H_2O

R3: serpentine + CO_2 → magnesite + talc + H_2O

R4: talc + CO_2 → magnesite + quartz + H_2O



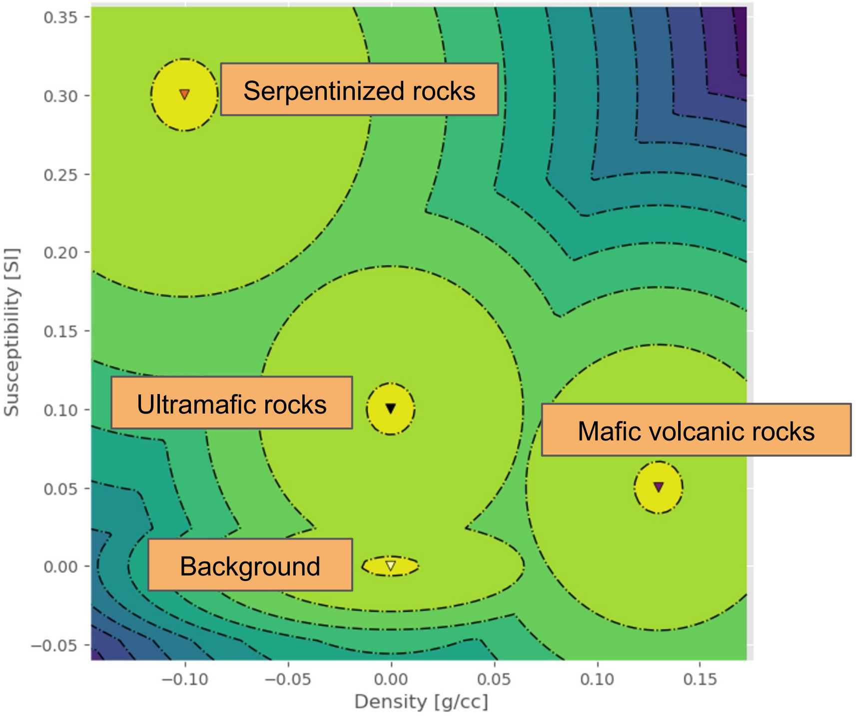
Cutts et al., 2021; Mitchinson et al., 2020

Using a Gaussian Mixture Model in the model norm

Astic & Oldenburg, 2020

Petrophysically and Geologically guided Inversion

GMM: carbon mineralization



$$\mathcal{P}_{\text{small}}(\mathbf{m}_i) = \sum_{j=1}^{c} \mathcal{P}(z_i = j)\, \mathcal{N}(\mathbf{m}_i | z_i = j)$$

c: Number of expected rock units

$\mathcal{P}(z_i = j)$: Proportions: geology information

$\mathcal{N}(\mathbf{m}_i | z_i = j)$: Petrophysical Information (+ geophy. weights)

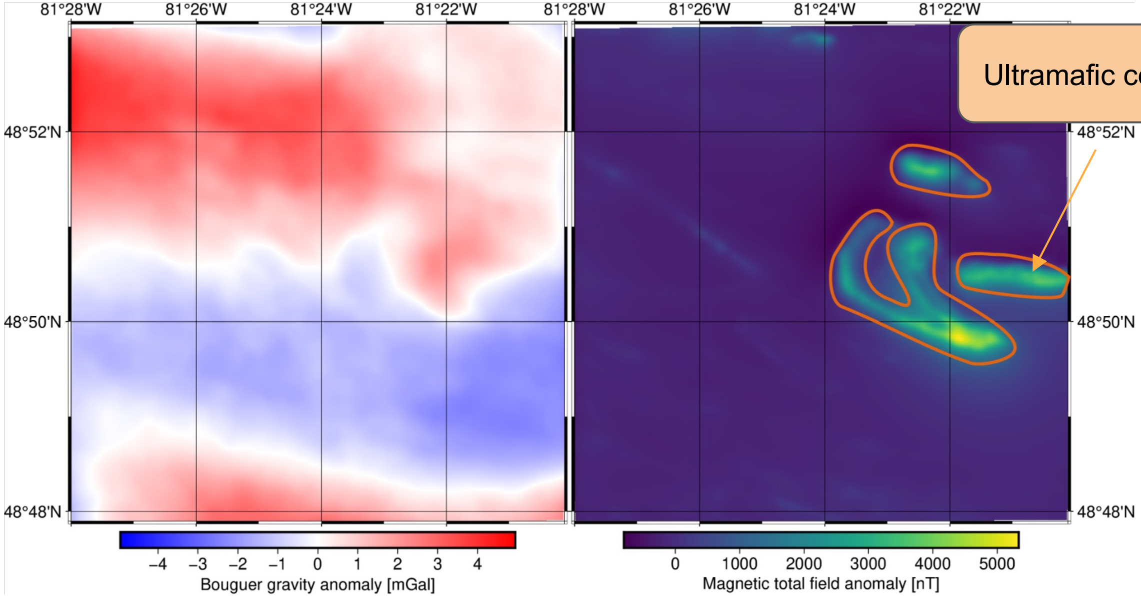
Define: $\Phi_{\text{small}}(\mathbf{m}) = -\log\left(\mathcal{P}_{\text{small}}(\mathbf{m})\right)$

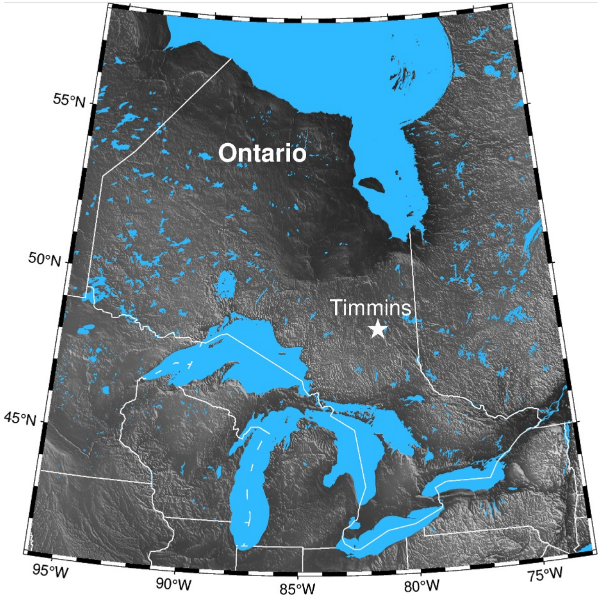
Using a Gaussian Mixture Model in the model norm

Soler et al., in prep

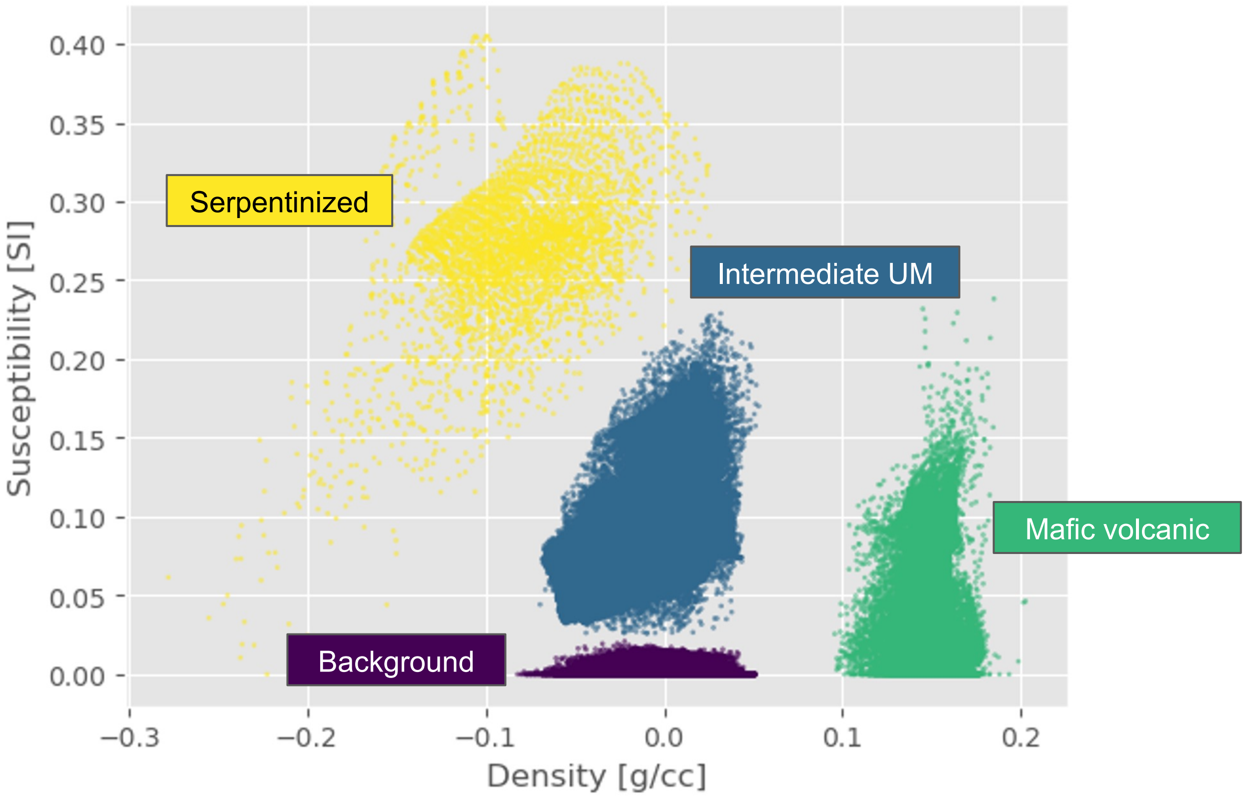
Petrophysically and Geologically guided Inversion

gravity gradiometry & magnetic data

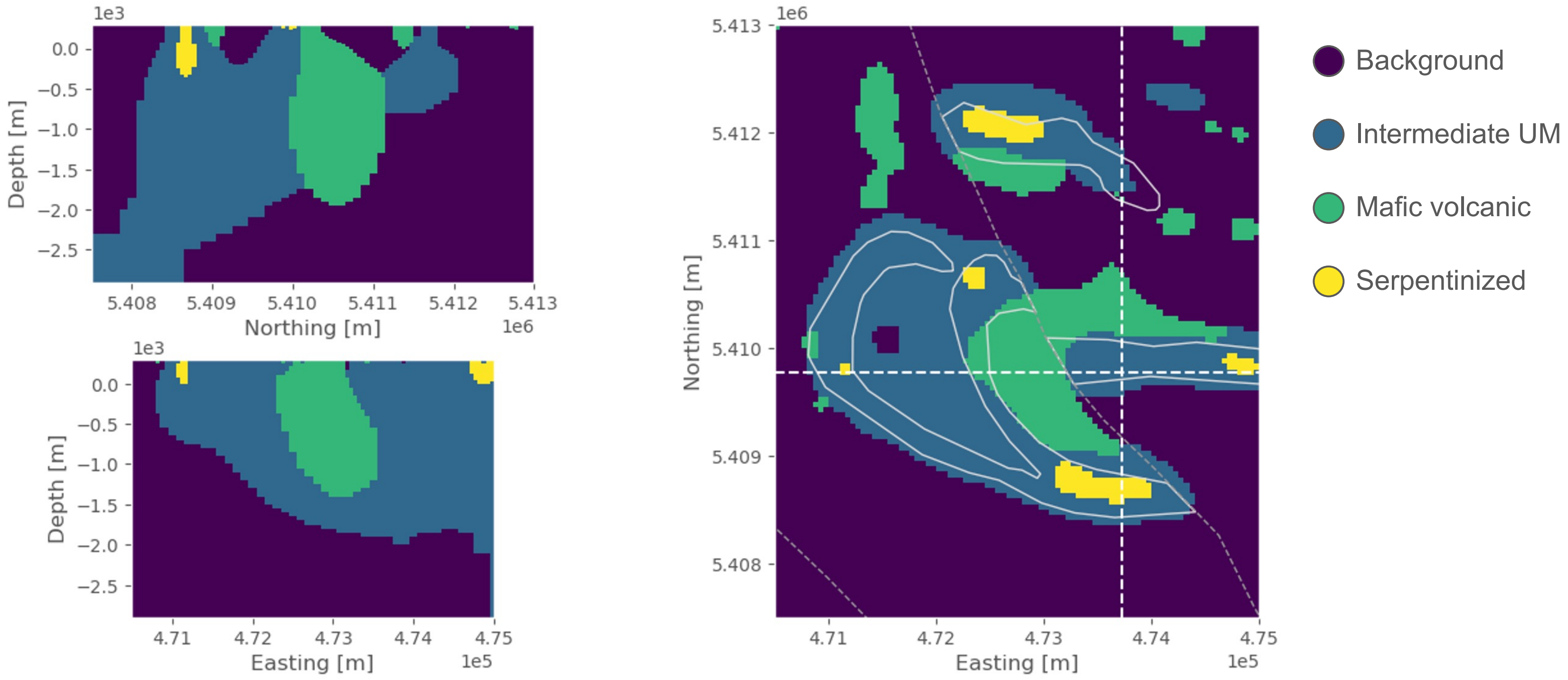




PGI Results

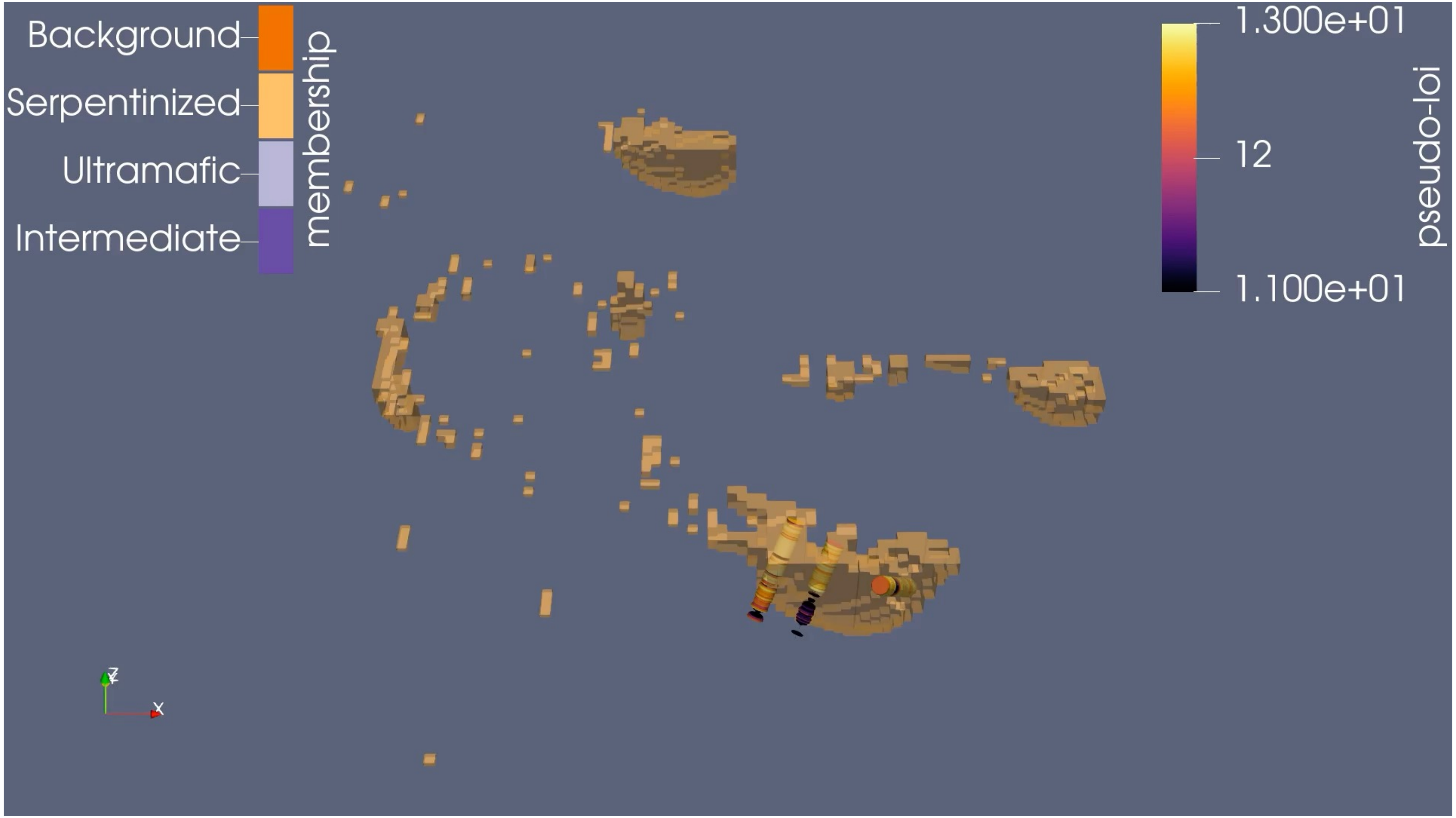

Serpentinized
Intermediate UM
Mafic volcanic
Background
Susceptibility [SI]
0.40
0.35
0.30
0.25
0.20
0.15
0.10
0.05
0.00
−0.3
−0.2
−0.1
0.0
0.1
0.2
Density [g/cc]

PGI Results



1e3
0.0
−0.5
−1.0
−1.5
−2.0
−2.5
Depth [m]
5.408
5.409
5.410
5.411
5.412
5.413
Northing [m]
1e6
1e3
Depth [m]
4.71
4.72
4.73
4.74
4.75
Easting [m]
1e5
1e6
5.413
5.412
5.411
5.410
5.409
5.408
Northing [m]
Easting [m]
1e5
Background
Intermediate UM
Mafic volcanic
Serpentinized

PGI Results


Background
Serpentinized
Ultramafic
Intermediate
membership
1.300e+01
12
1.100e+01
pseudo-loi
z
x

PGI Results

Soler et al., in prep

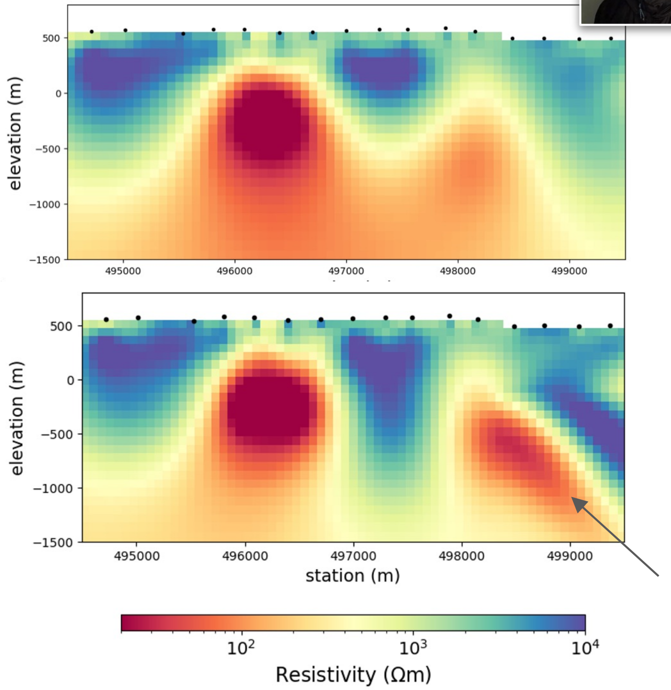
Prediction: regions with sequestration potential

Other examples

Leveraging image segmentation algorithms in the inversion (Kuttai & Heagy, submitted)

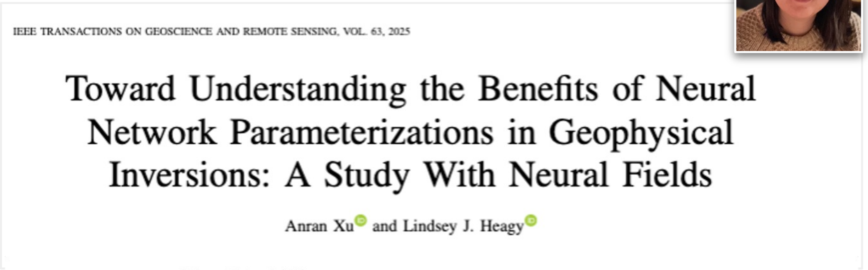
standard approach

incorporating image segmentation



better estimate of target dip!

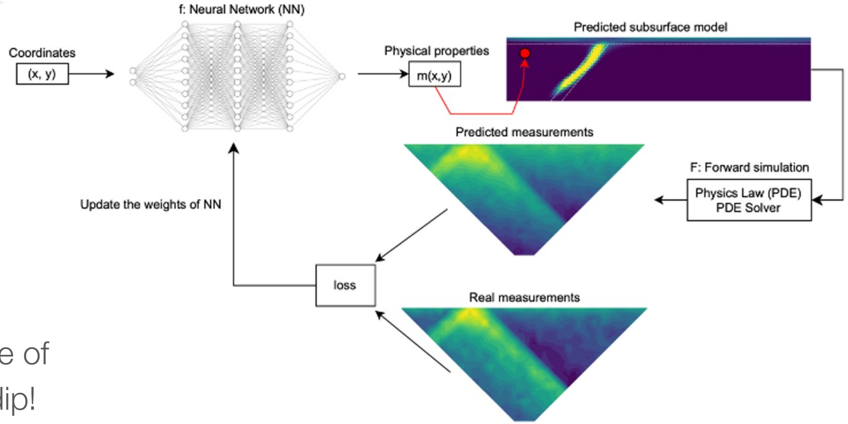
Parameterizing the inverse model by a neural network (Xu & Heagy, 2025)



IEEE TRANSACTIONS ON GEOSCIENCE AND REMOTE SENSING, VOL. 63, 2025

Toward Understanding the Benefits of Neural Network Parameterizations in Geophysical Inversions: A Study With Neural Fields

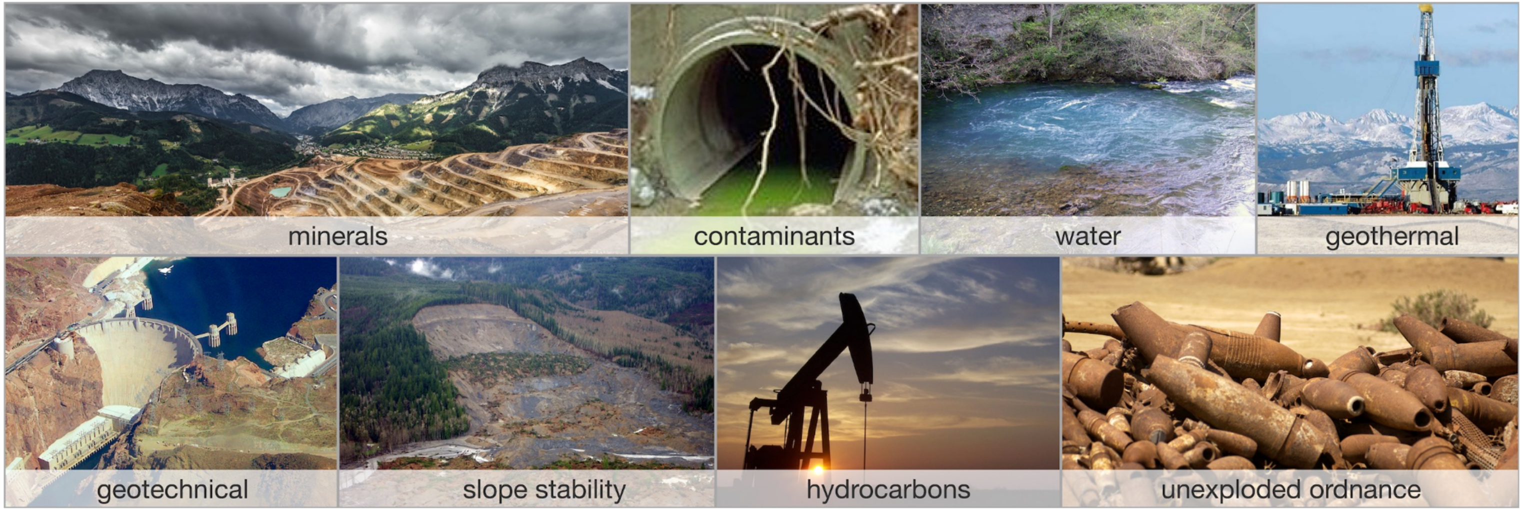
Anran Xu and Lindsey J. Heagy



Summary

modular, open-source framework provides a foundation for research

- accelerates on-boarding
- eases technology transfer
- opens collaboration opportunities



Thank you!

simpeg

simpeg.xyz

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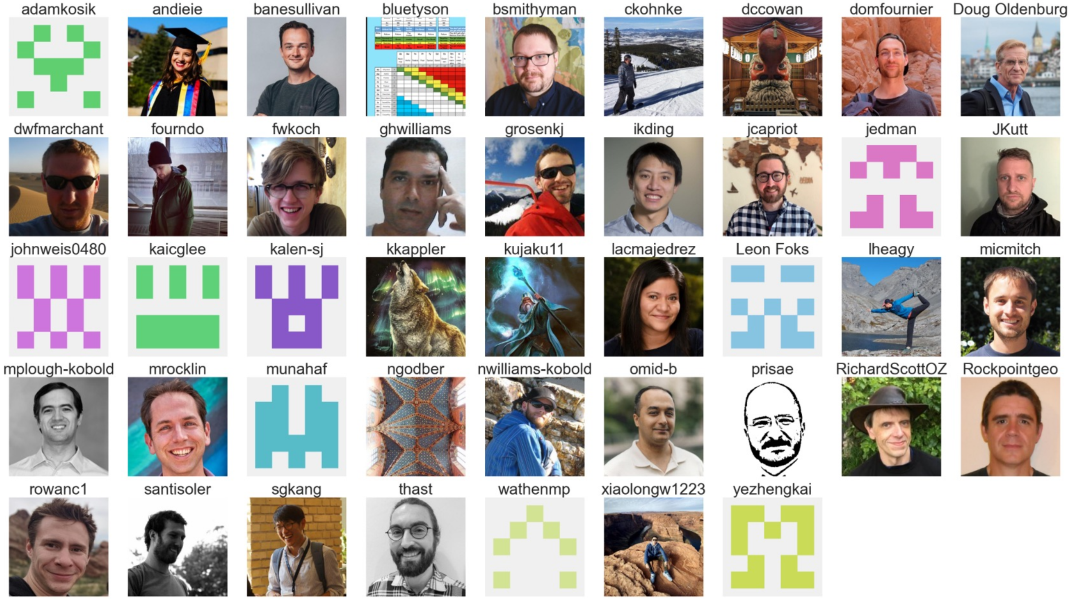
UBC GIF research consortium:

AngloAmerican, BHP, Condor Consulting Inc, Mitacs, BARRICK, Cameco, DIAS, GLENCORE, ideon, KoBold Metals, SJ GEOPHYSICS Science on Target, VALE



codebase contributions from:

UBC, Colorado School of Mines, University of Manitoba, TU Delft, GNS Science, Mira Geoscience ...modelling the earth, GIF, Stanford, UH, DIAS Geophysical, KoBold Metals, SJ GEOPHYSICS Science on Target ...