computational geophysics in a changing climate

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University of Tasmania | April 2022

UBC Vancouver is located on the traditional, ancestral, and unceded territory of the xʷməθkʷəy̓əm people

Hover Collective / UBC Brand & Marketing

climate crisis

solutions & mitigating impacts: opportunities for geophysics

critical minerals

geologic storage of CO_2

geotechnical
(e.g. permafrost)

groundwater

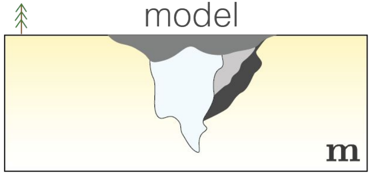
research interests: computational geoscience

physics-driven, inverse problems

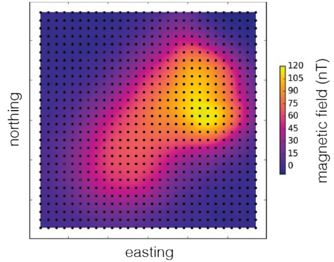
forward problem

$$\mathbf{d} = \mathcal{F}[\mathbf{m}]$$

physical property model



data



$$\tilde{\mathbf{m}} = \mathcal{F}^{-1}[\mathbf{d}]$$

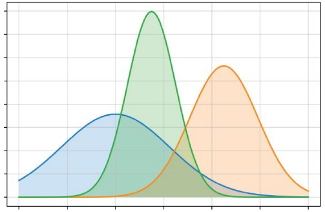
inverse problem

statistics, machine learning

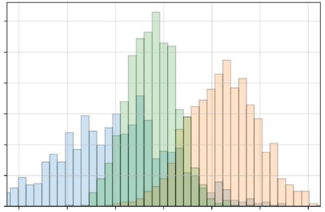
probability

$$X \sim \mathcal{N}(0, 1)$$

statistical model



observations



$$X \sim \mathcal{N}(\mu, \sigma)$$

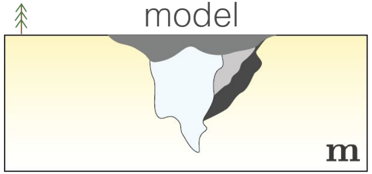
statistics
(inverse probability)

geophysical inversions

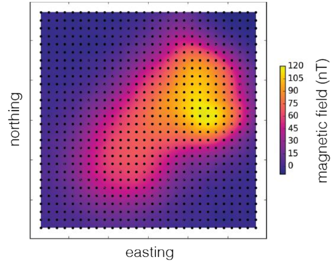
forward problem

$\mathbf{d} = \mathcal{F}[\mathbf{m}]$

physical property model



data



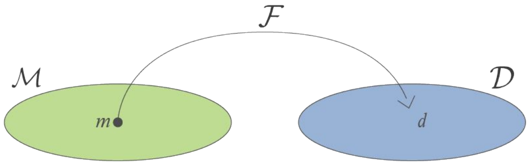
$\tilde{\mathbf{m}} = \mathcal{F}^{-1}[\mathbf{d}]$

inverse problem

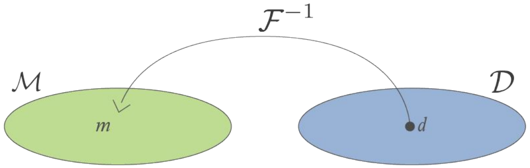
statement of the inverse problem

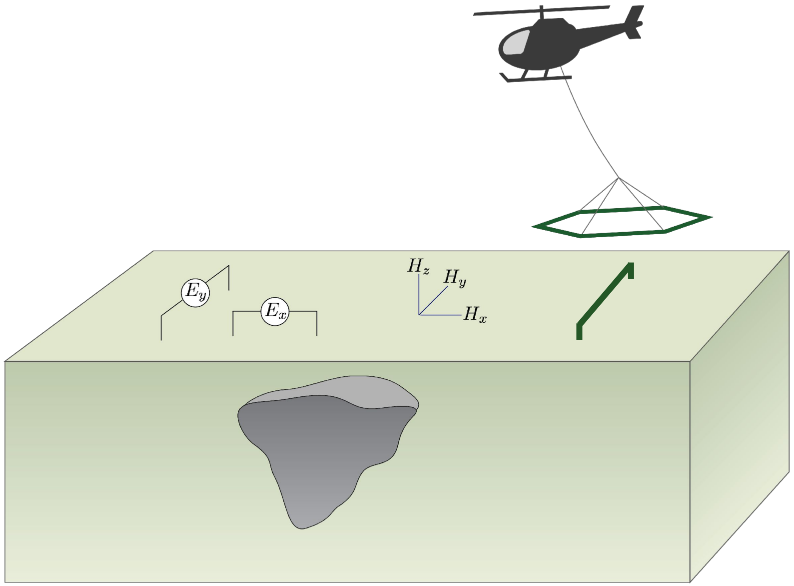
Given

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



Find the Earth model that gave rise to the data



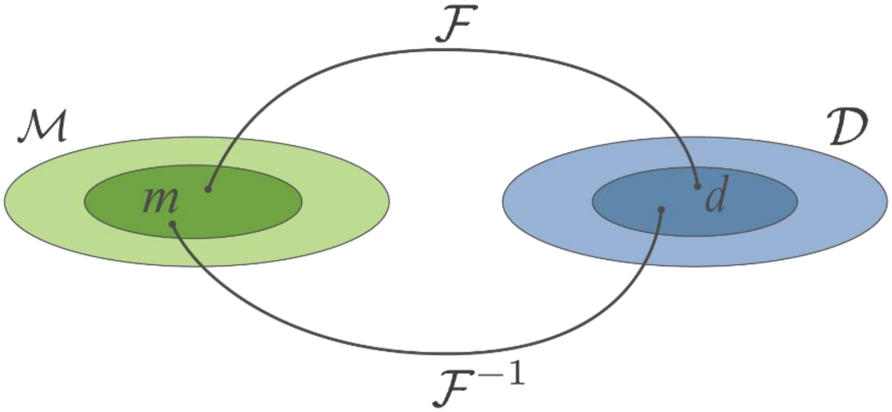


inverse problem

The inverse problem is ill-posed

- non-unique
- ill-conditioned

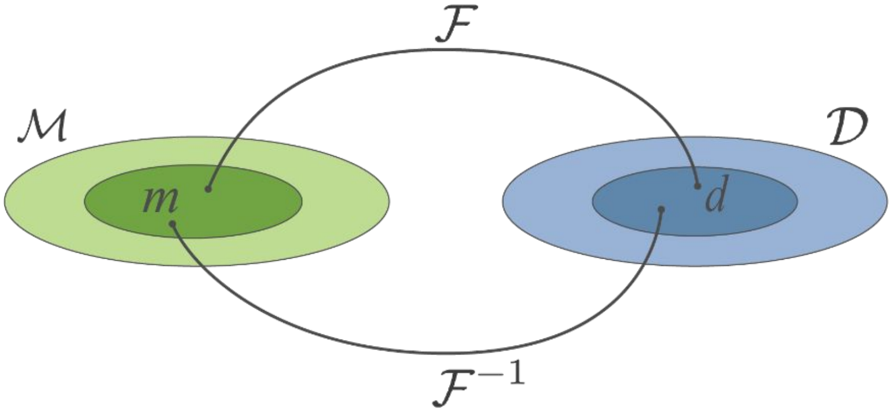
Any inversion approach must address these issues.



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:

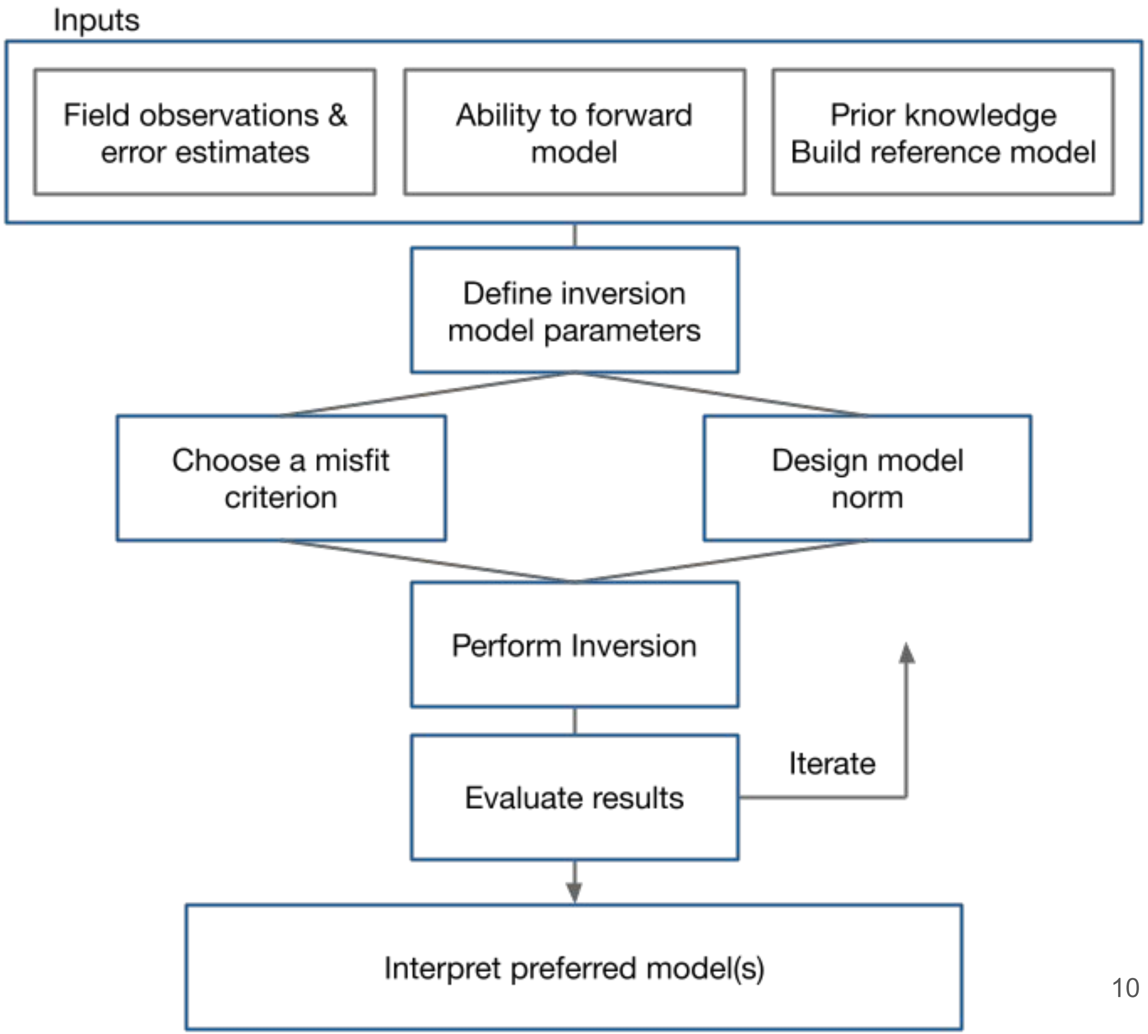
(a) Characterize $P(m|d^{obs})$

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

flow chart for the inverse problem

- many components
- iterative process to obtain solution
- each component requires evaluation, adjustment by user

Fundamentals of Inversion – D. Oldenburg
Capturing knowledge in code – L. Heagy
http://www.mtnet.info/EMinars/EMinars.html



choosing a software package

depends on needs / goals:

- production scale inversion
- methods oriented research
- education

influences priorities

- computational efficiency
- ease of use
- flexibility
- modularity
- license
- development style

a sampling of open tools in EM

MARE2DEM

pyGIMLi
Geophysical Inversion & Modelling Library

custEM

netgen

OSGeo

emgig

simpeg

. . .

simpeg

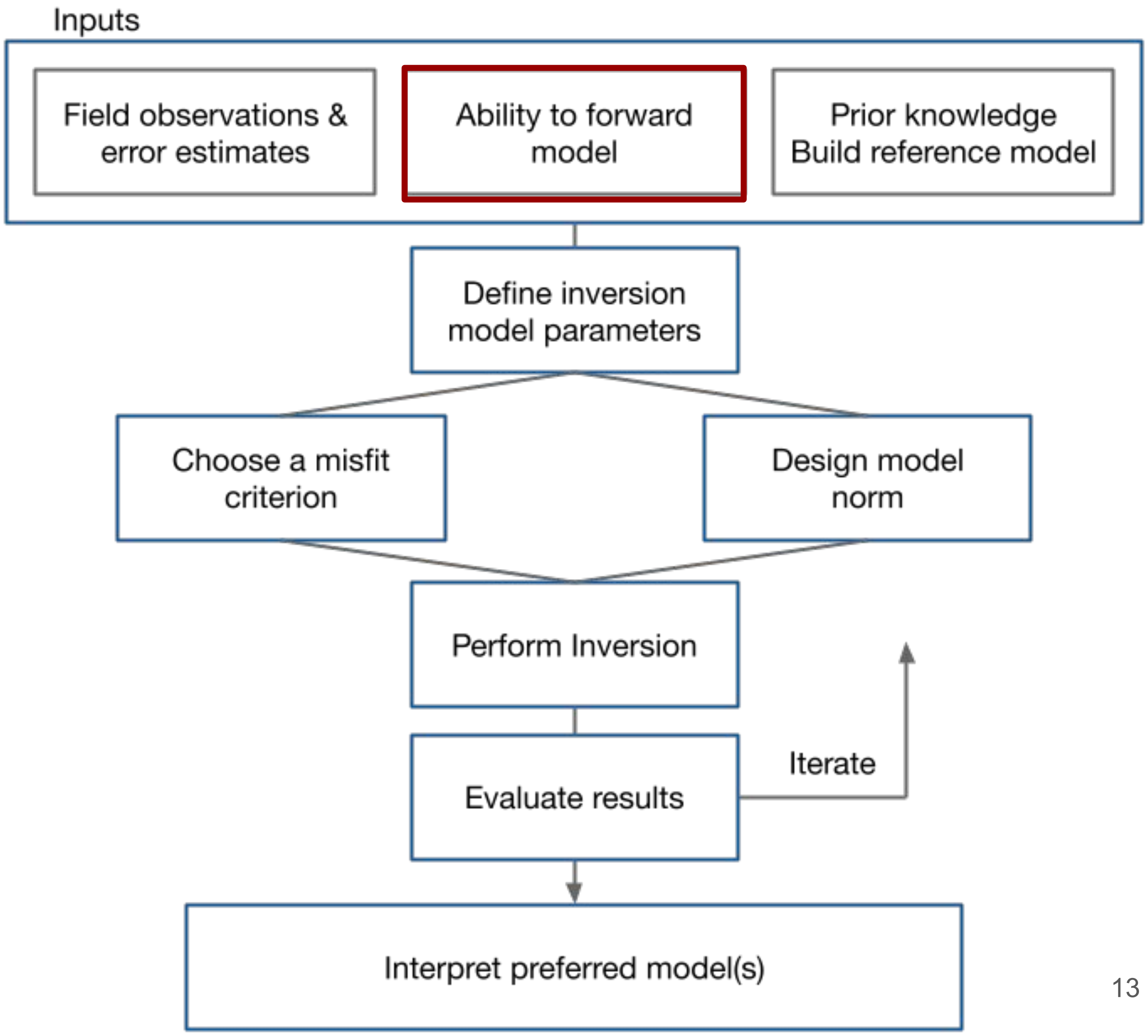
facilitate research in geophysics

prioritizes:

- **modularity:** building blocks, pieces available to manipulation
- **declarative code:** express intent, looks like the math
- **extensible:** integration of information
- **open community:** transparency, opportunities for collaboration

(Cockett et al, 2015; Heagy et al, 2017)

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)	$\vec{j} = \sigma \vec{e}$	$\vec{J} = \sigma \vec{E}$
	$\vec{b} = \mu \vec{h}$	$\vec{B} = \mu \vec{H}$
	$\vec{d} = \varepsilon \vec{e}$	$\vec{D} = \varepsilon \vec{E}$

* Solve with sources and boundary conditions

electromagnetics: frequency domain

Continuous equations

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

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

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

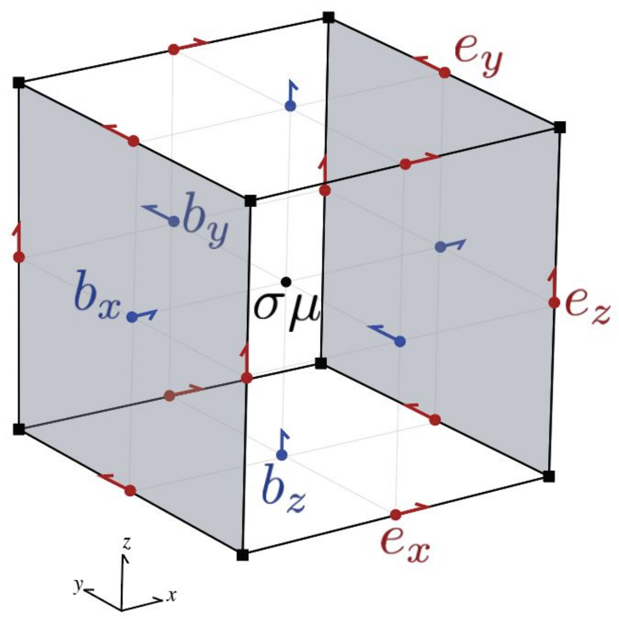
Finite volume discretization

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

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

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

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

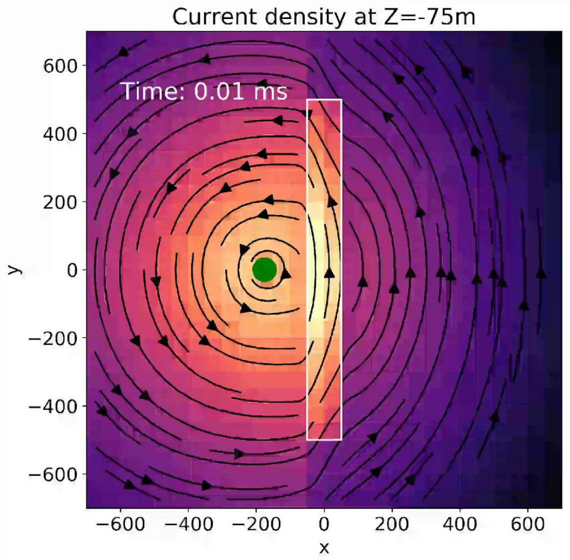


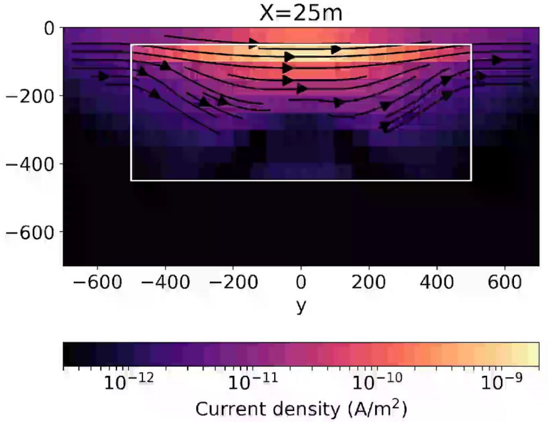
(Haber, 2014; Cockett et al, 2016)

solving a FDEM problem

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

```
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 + i * ω * Meσ
Ainv = Solver(A)  # acts like A inverse

Me = mesh.get_edge_inner_product()
q = -i * ω * Me * js

u = Ainv * q
```

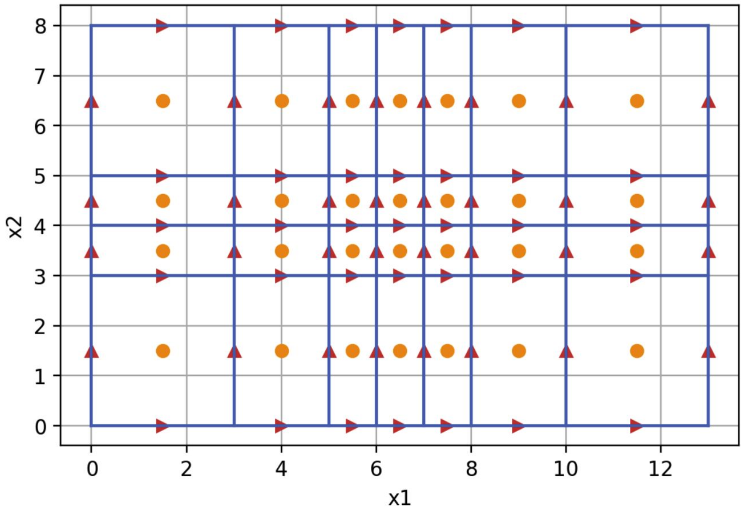




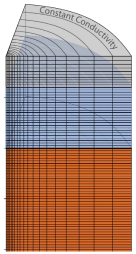
create a mesh: the discretize package

```python
import discretize
```

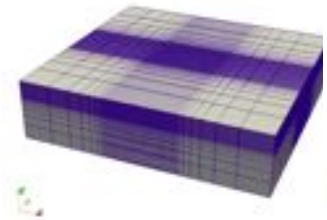
```python
hx = [3, 2, 1, 1, 1, 2, 3]
hy = [3, 1, 1, 3]
mesh = discretize.TensorMesh([hx, hy])
mesh.plot_grid(edges=True, centers=True);
```



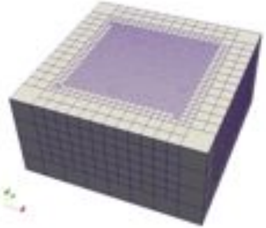
Properties or Methods
`dim, origin`
`n_cells, n_nodes, n_faces, n_edges`
`cell_volumes, face_areas, edge_lengths`
`cell_centers, nodes, edges, faces`
`nodal_gradient, face_divergence, edge_curl`
`average_edge_to_cell, average_node_to_cell, ...`
`get_edge_inner_product()`
`get_interpolation_matrix(location)`



Cylindrical



Tensor

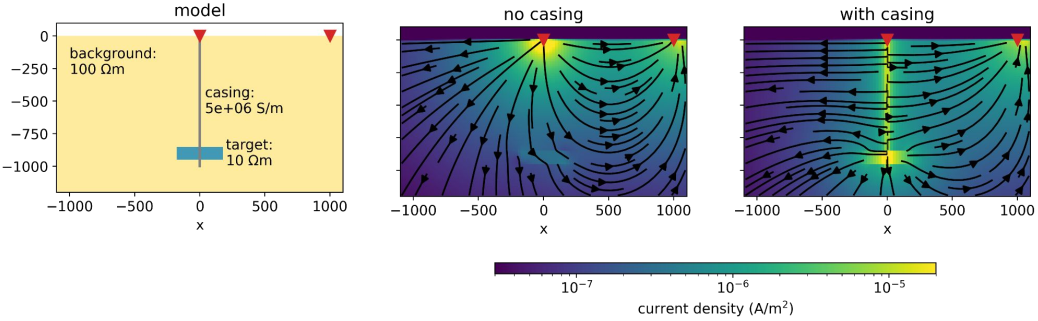


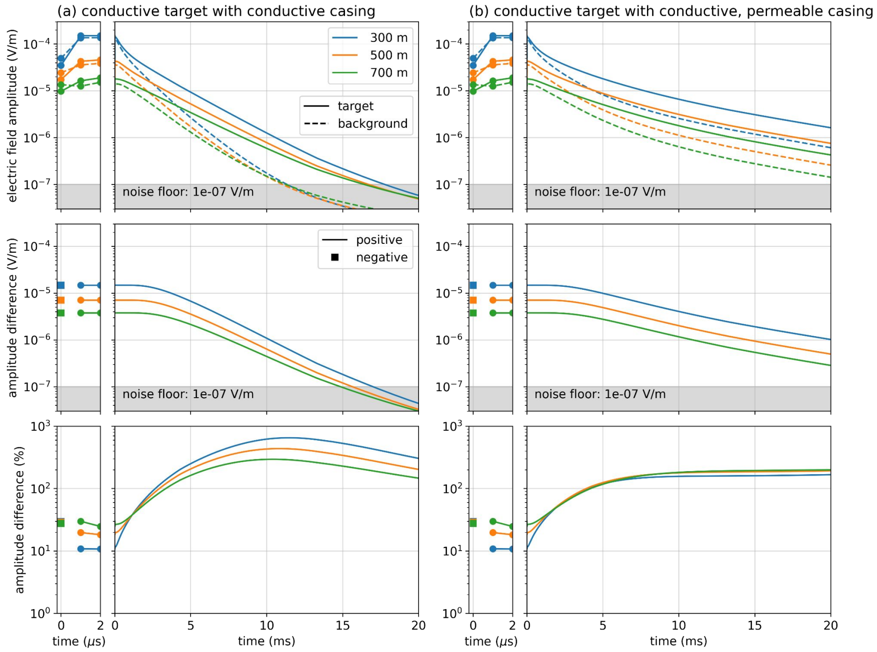
OcTree

J. Capriotti

an example: monitoring with steel-cased wells

- steel: highly conductive, also substantial magnetic permeability
- challenging geometry for numerical simulations
- but… advantageous for helping deliver current to depth





(Heagy & Oldenburg, 2022)

flow chart for the inverse problem

What do we need for inversion?

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

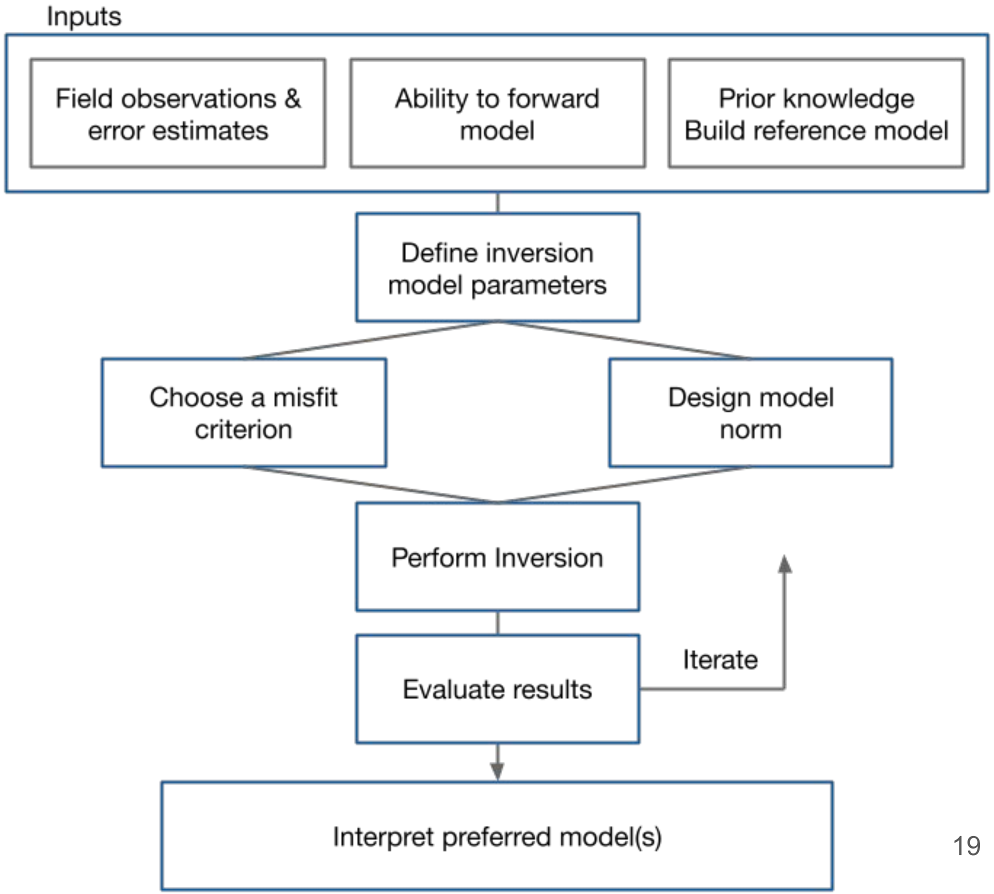
$$\text{subject to} \quad m_L < m < m_H$$

From the simulation

- adjoint sensitivity times a vector
- sensitivity times a vector

Inversion components:

- define a model norm
- perform optimization



sensitivities

For inverse problem, also need sensitivities (and adjoint)

$$\mathbf{J} = \frac{\partial \mathbf{d}^{\text{pred}}}{\partial \mathbf{m}}$$

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

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

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**

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

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

model norm

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

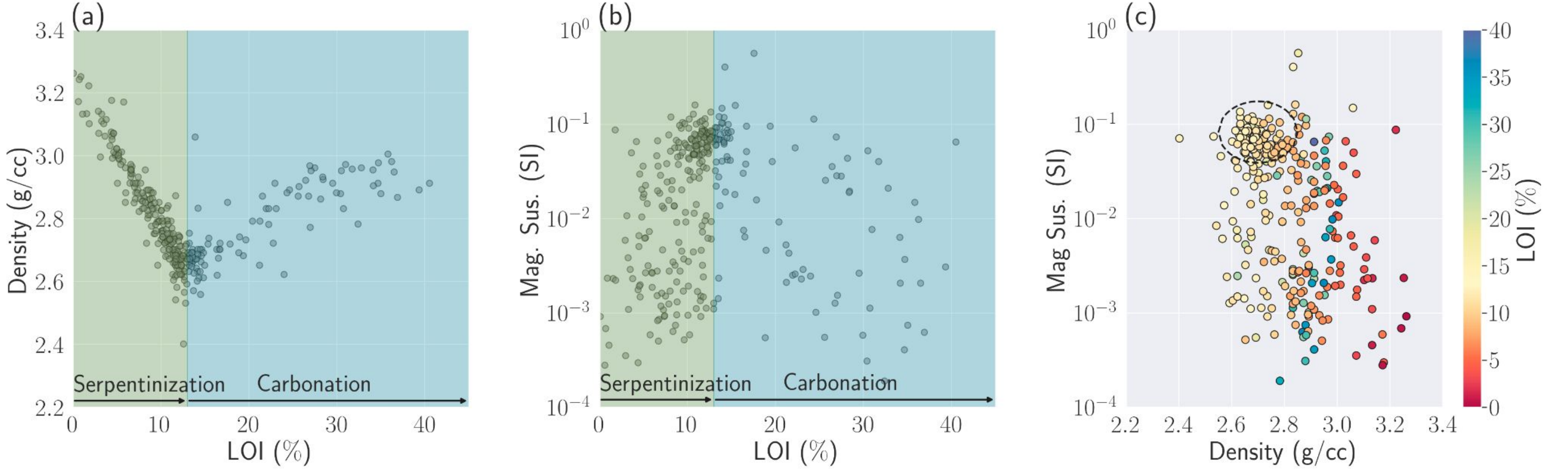
discretize

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

an example: carbon mineralization

- ultramafic rocks rich in Ca, Mg can react with CO_2 to form carbonated minerals

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



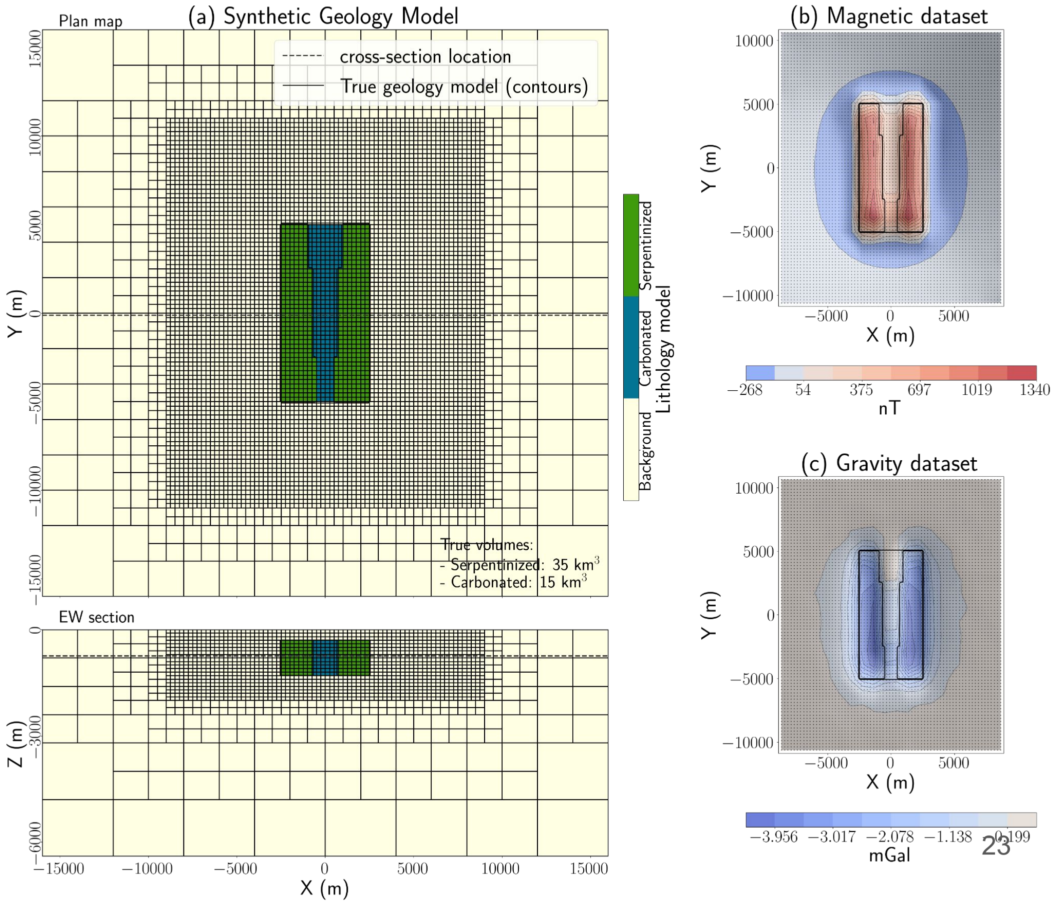
(Heagy et al, 2022)

an example: carbon mineralization

- motivated by Decar in BC
- serpentinized region with central carbonated region
- physical properties

	mag susc (SI)	density (g/cc)	dens. contrast (g/cc)
background	0	2.9	0.0
serpentinized	0.15	2.7	-0.2
carbonated	0.05	3.0	0.1

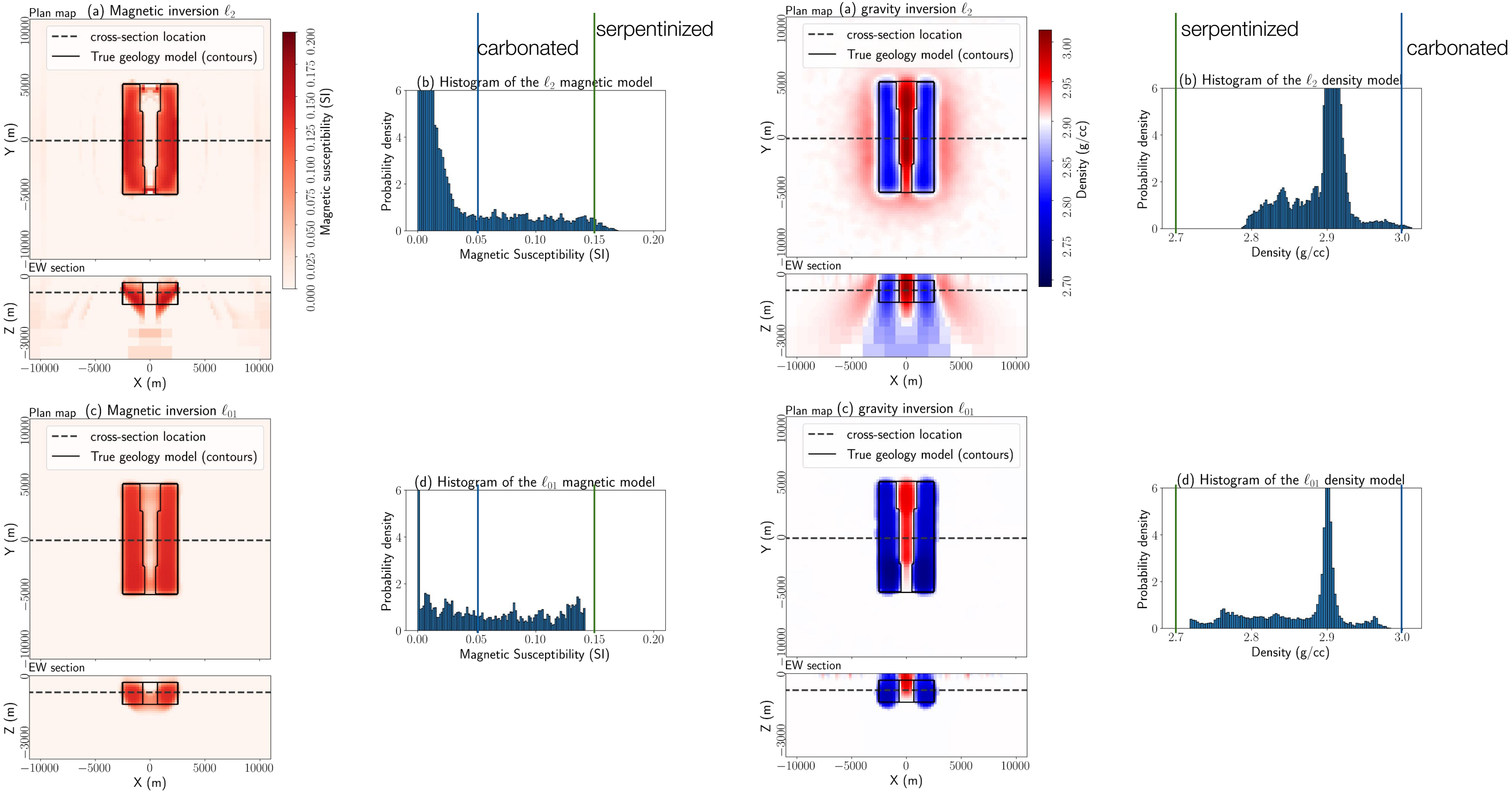
- goals: delineate, estimate volumes



an example: carbon mineralization

ℓ_2

ℓ_{01}



inverse problem

Given data, estimate a physical property model

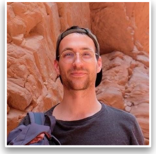
Pose as an optimization

$$\underset{m}{\text{minimize}}\ \phi(m) = \phi_d(m) + \beta\phi_m(m)$$

Model norm captures assumptions

$$\phi_m(m) = \alpha_s \int |m - m_{\text{ref}}|^p dV + \alpha_x \int \left|\frac{dm}{dx}\right|^q dV + \alpha_y \int \left|\frac{dm}{dy}\right|^q dV + \alpha_z \int \left|\frac{dm}{dz}\right|^q dV$$

- ℓ_2 : p, q = 2: promotes smooth structures
- ℓ_{01} : p, q < 2: promotes sparse, compact structures

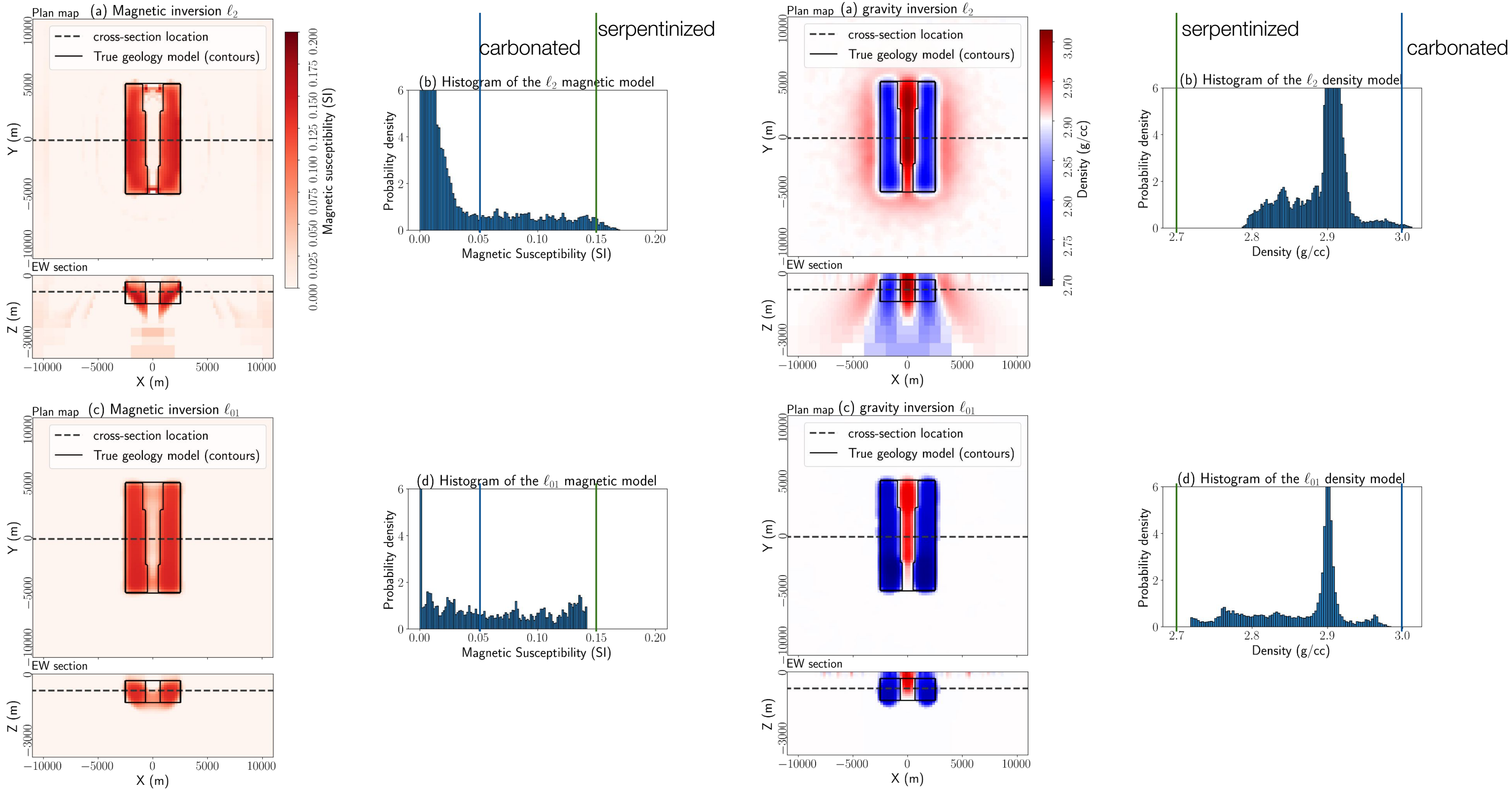


D. Fournier

an example: carbon mineralization

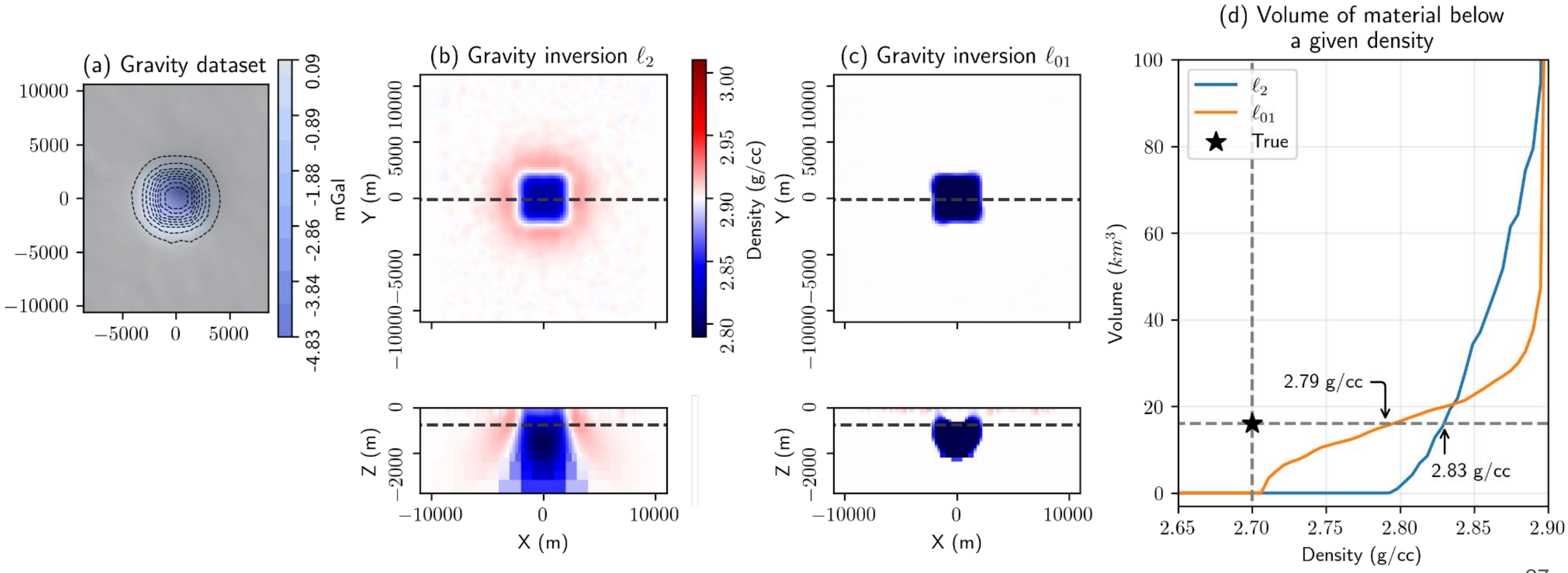
ℓ_2

ℓ_{01}



how do we choose a threshold?

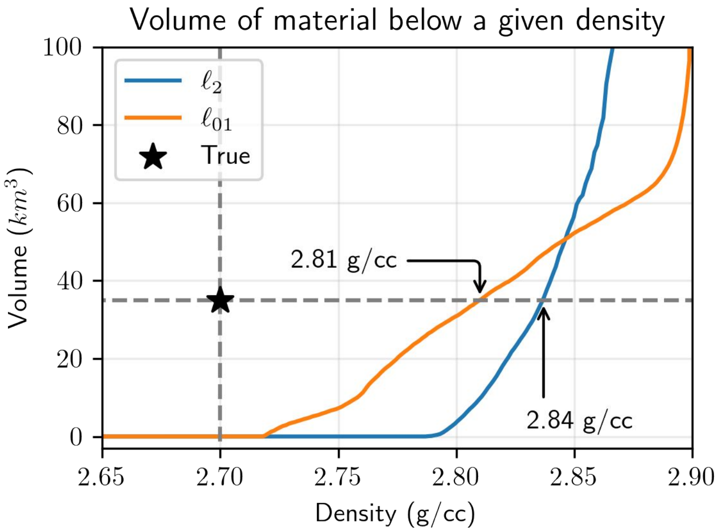
using: identical mesh, survey, inversion parameters, perform simulations and inversions with a representative block.

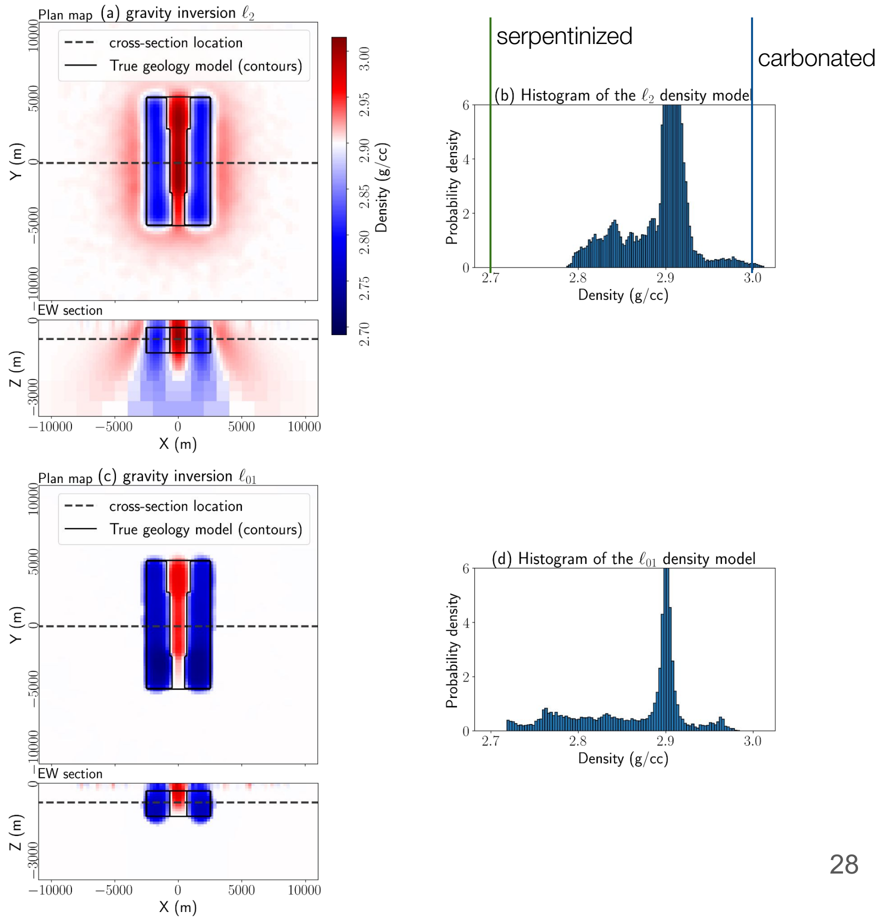


how do we choose a threshold?

Threshold from proxy: 2.83, 2.79 g/cc

- ℓ_2 : 27 km^3
- ℓ_{01}: 27 km^3



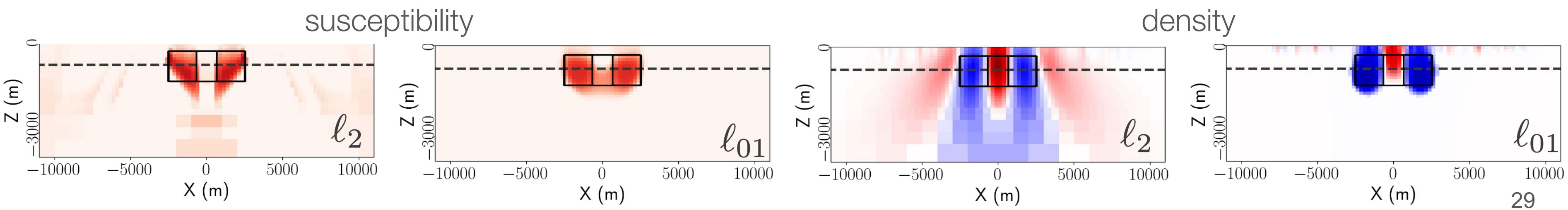


how do we choose a threshold?

- proxy model → tool for estimating an appropriate physical property threshold

Inversion	Threshold for correct volume	Threshold from proxy	Volume estimate with proxy threshold
ℓ_2 magnetics	0.08 SI	0.07 SI	40 km^3
ℓ_{01} magnetics	0.08 SI	0.07 SI	43 km^3
ℓ_2 gravity	2.84 g/cc	2.83 g/cc	27 km^3
ℓ_{01} gravity	2.81 g/cc	2.79 g/cc	27 km^3

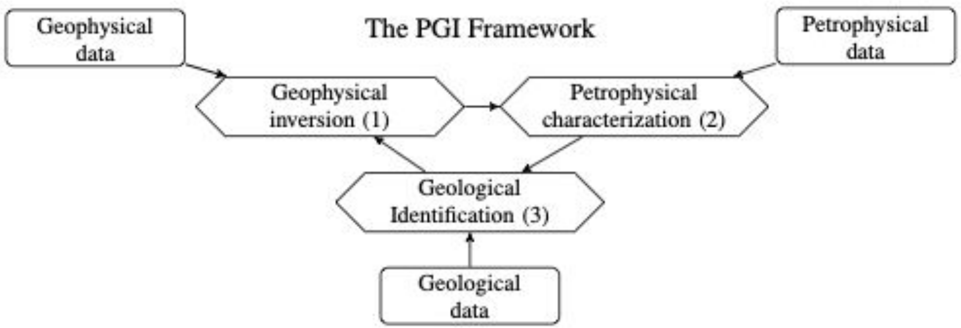
- Also of interest:
    - delineating the top → ex-situ vs. in-situ
    - joint inversion → consistent model?



Petrophysically and Geologically Guided Inversion

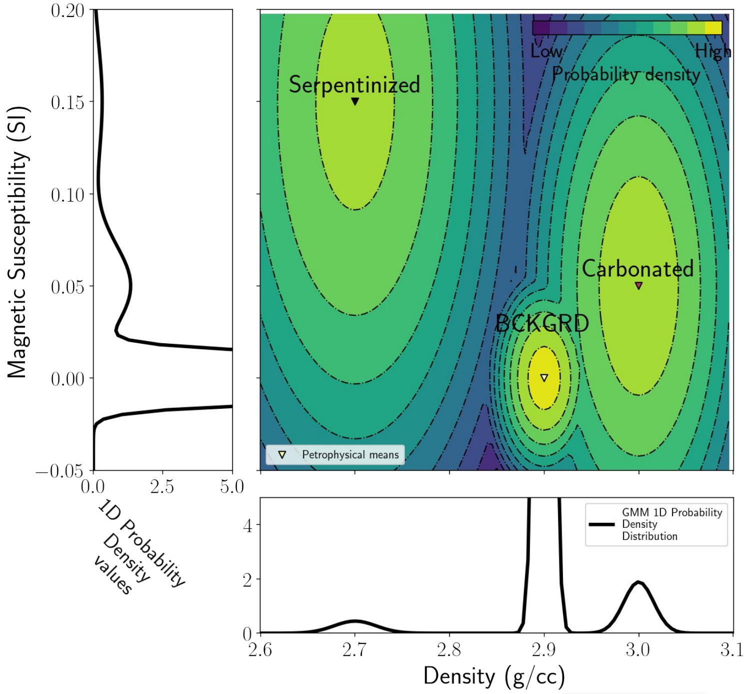
Alternative approach to the inverse problem

- brings in petrophysical information (GMM)
- builds a quasi-geology model



- important components in the inversion
  - multiple data misfits
  - including petrophysical information

Gaussian mixture model (GMM)



T. Astic

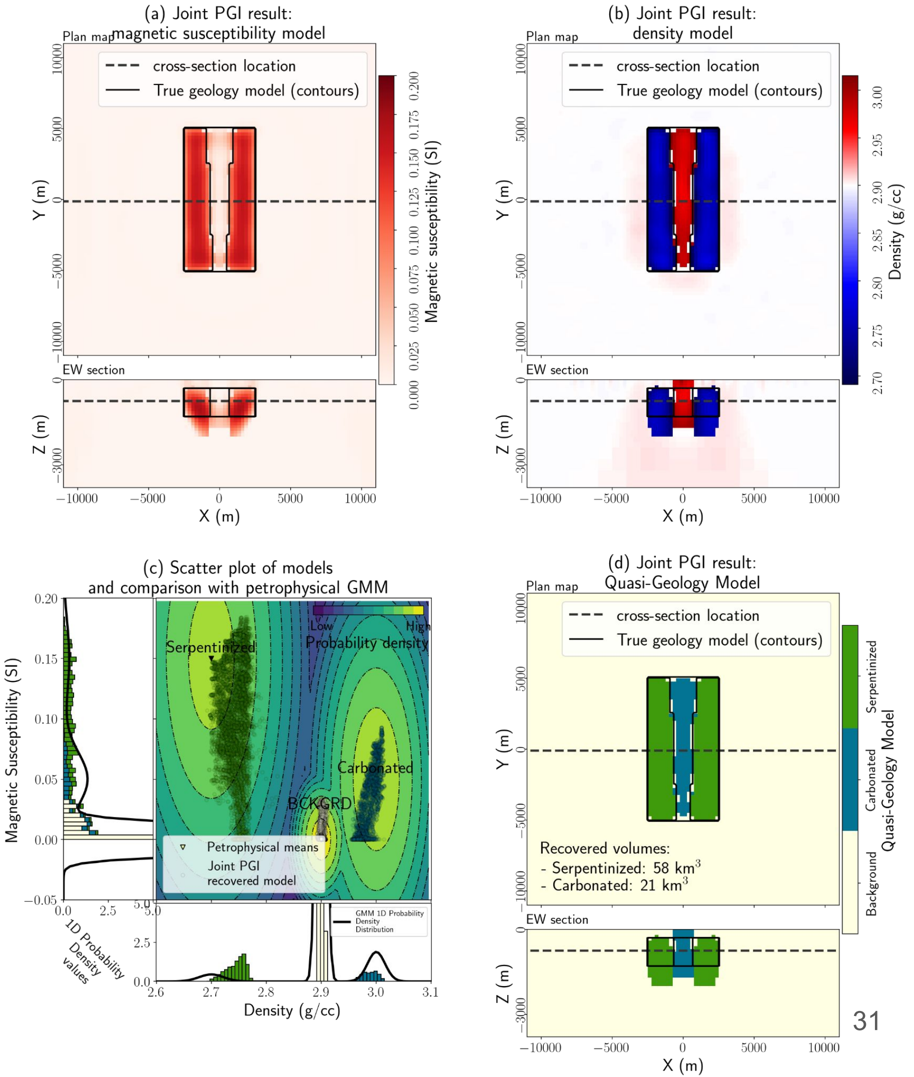
Joint PGI

- Inversion fits both geophysical data sets and petrophysical data

```
ϕ_data = ϕ_grav + ϕ_mag   # one earth?
```

  - Weighting strategies to balance contributions (Astic et al, 2021)

- One quasi geology model consistent with both data sets
- Good estimate to top of serpentinized rock volume



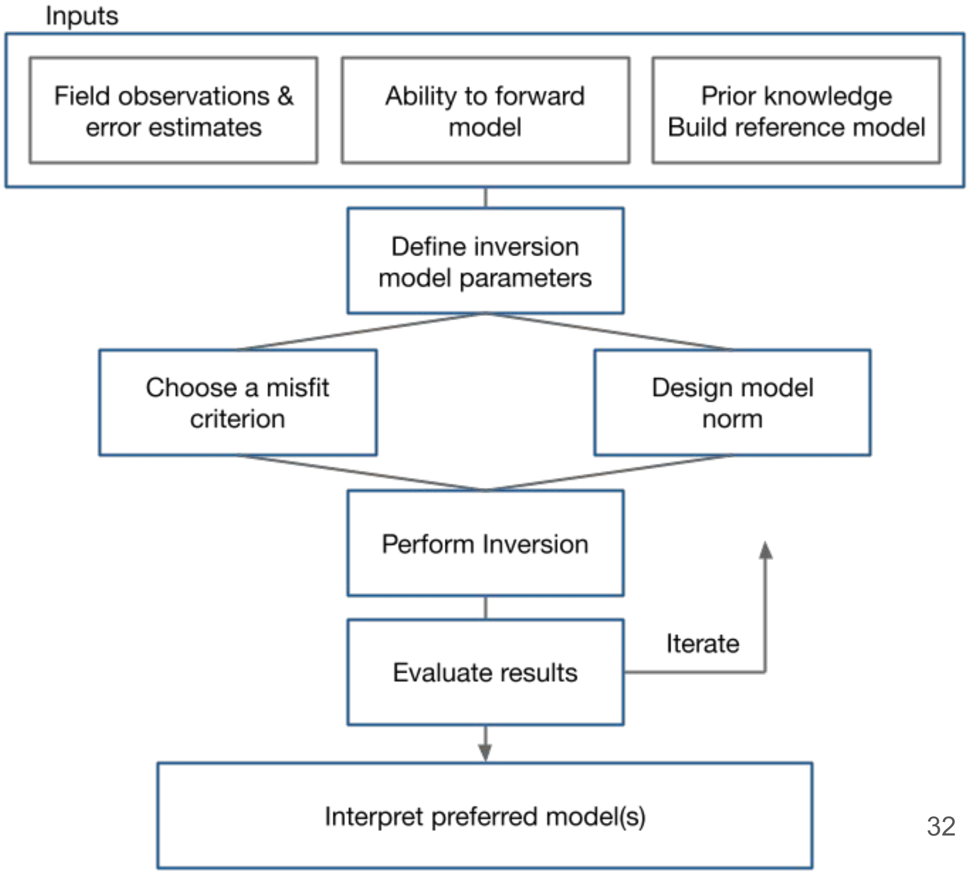
geophysics and multidisciplinary problems

critical minerals

geologic storage of CO_2

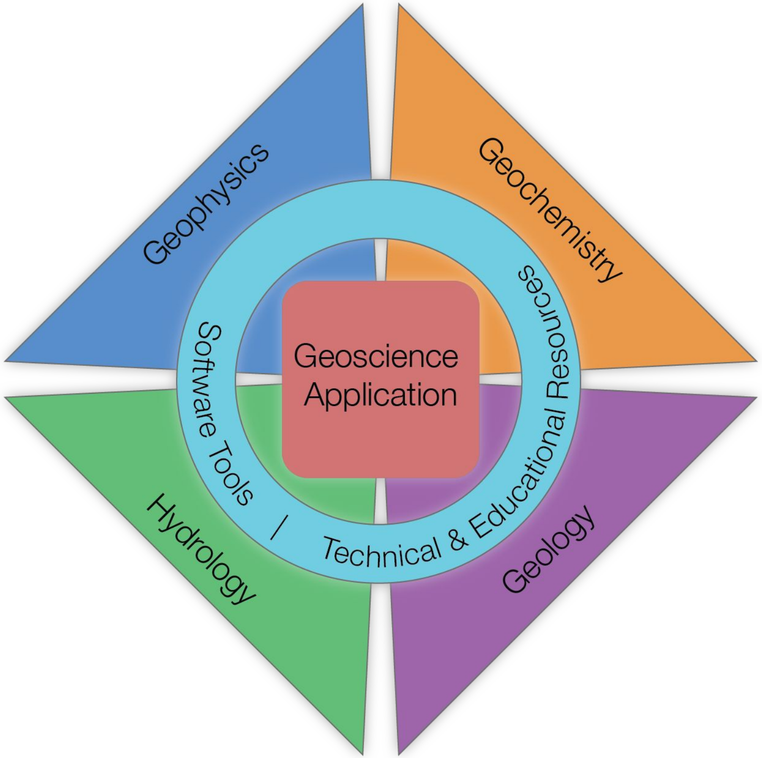
geotechnical
(e.g. permafrost)

groundwater



geophysics and multidisciplinary problems

- geophysics one piece
- need for
  - Technical advances: machine learning + inversion for combining data
  - Collaboration: between disciplines
- role of open science, educational resources

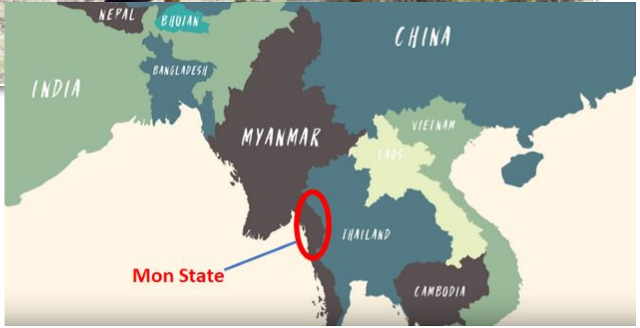


research + education: an example in humanitarian geophysics

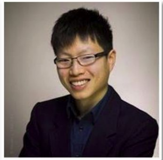
GEOSCIENTISTS without BORDERS®

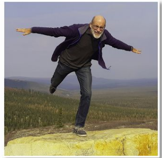
Improving Water Security in Mon state, Myanmar via Geophysical Capacity Building

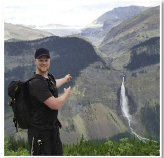
- Bring geophysical equipment to Mon state Myanmar
- Train local stakeholders
- Provide open-source software & educational resources




Doug Oldenburg


Kevin Fan


Michael Maxwell


Devin Cowan


Lindsey Heagy


Seogi Kang


Joe Capriotti

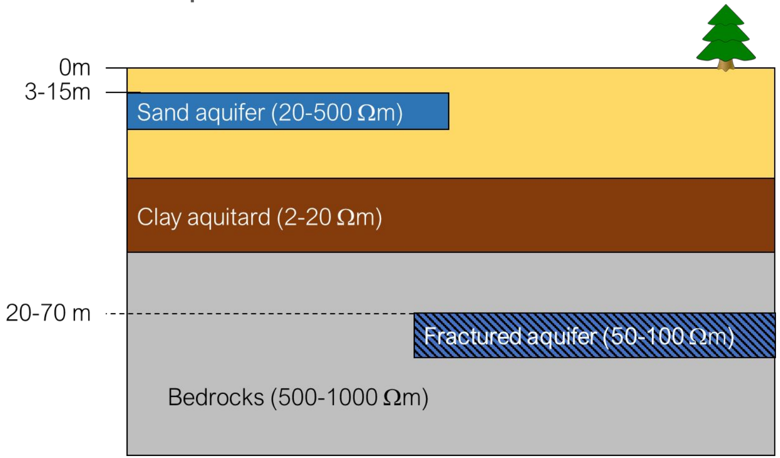
GOLDER

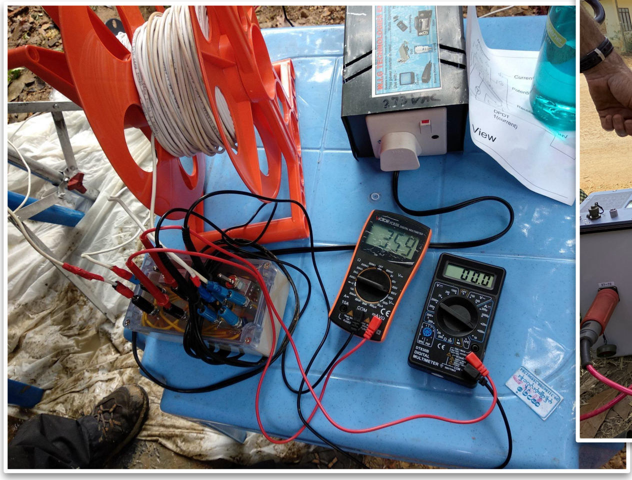
research + education:
an example in humanitarian geophysics

GEOSCIENTISTS without BORDERS®

Capabilities needed by local stakeholders:

- Understand the hydrogeologic problem and relationship to electrical resistivity
- Design field surveys
- Collect and process data
- Interpret those data





research + education:
an example in humanitarian geophysics

GEOSCIENTISTS without BORDERS®

Project stages

- Course instruction: fundamentals of DC resistivity & inversion
- Field surveying and processing
- Post-project sustainability

research + education:
an example in humanitarian geophysics

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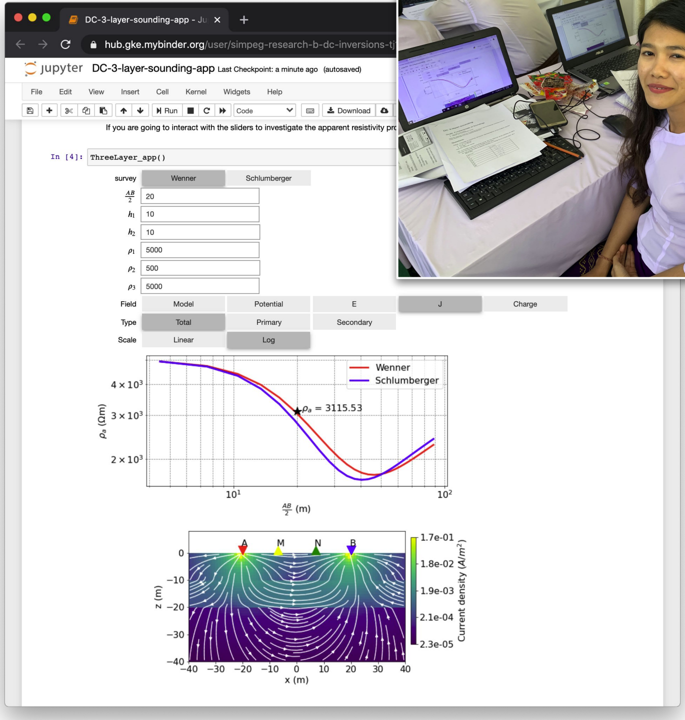
simpeg

Project resources

- Website for slides, videos and data
- Jupyter notebooks for teaching, working with data
- SimPEG software for processing
- Case History documents for collaboration and reproducibility
- Social media for collaboration



jupyter

research + education:
an example in humanitarian geophysics

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5 wells (>1000 gph)

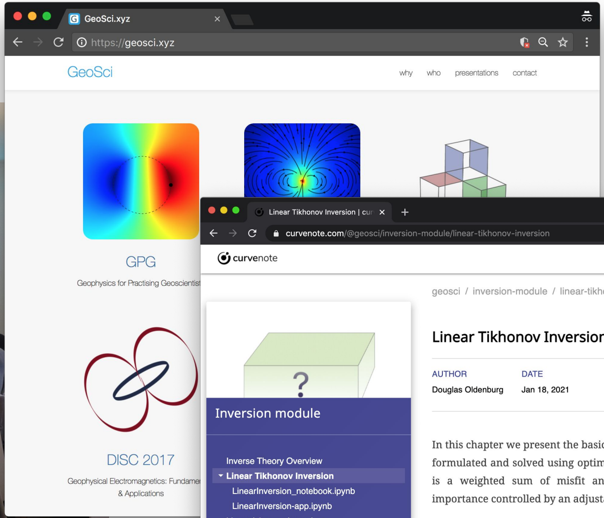
Benefits of using & developing open source resources

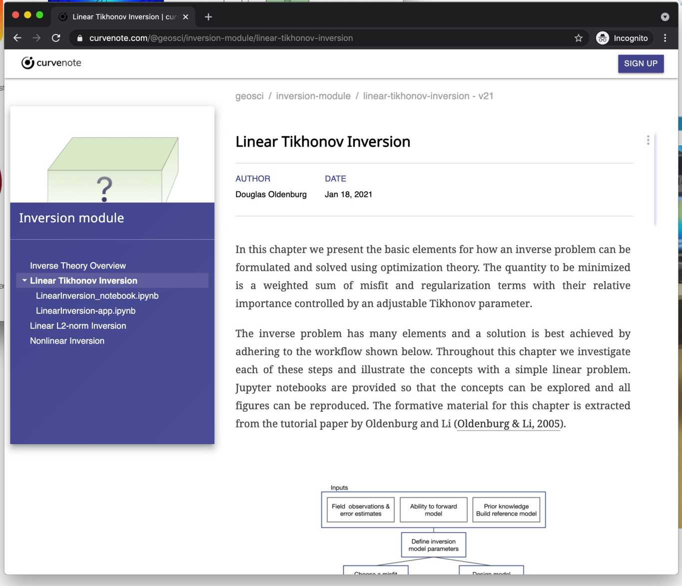
- No licensing or time-out concerns on software
- Easily design fit-for-purpose interactive tools for learning
- Readily update software, documentation based on user needs
- Encourage collaborative, reproducible practices

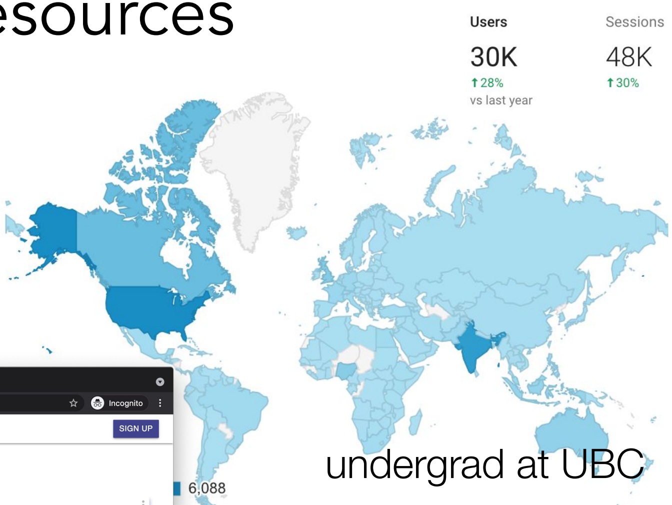
GeoSci .xyz open educational resources

https://geosci.xyz

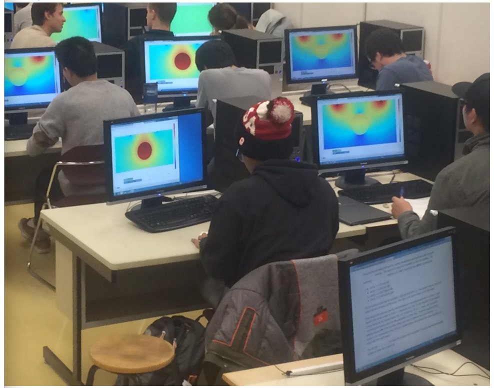
electromagnetics course:
26 locations worldwide







undergrad at UBC



opportunities for open science

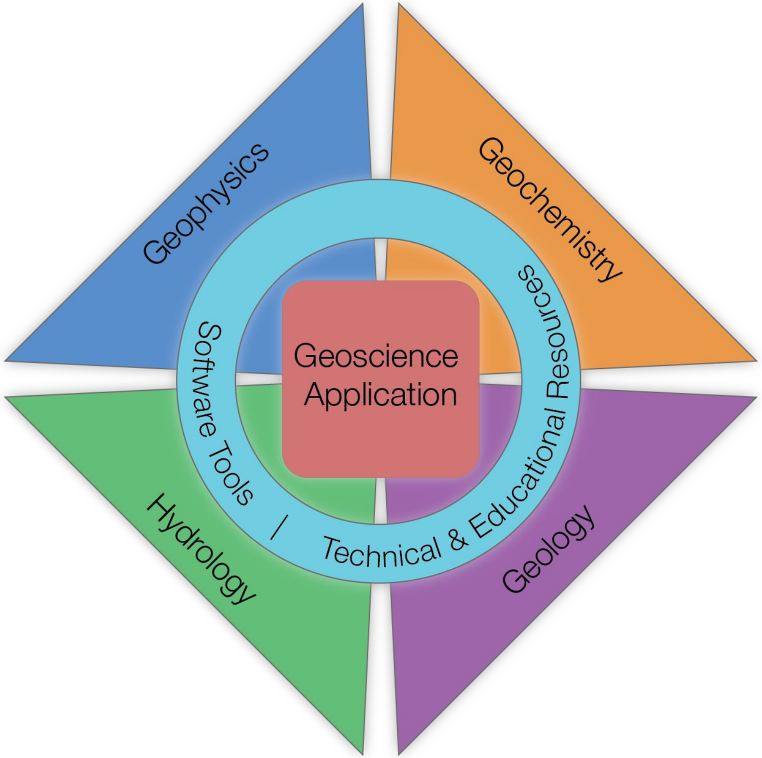
- **accelerate science:** collaboration & leveraging expertise, experience of others
- **broader impact:** enable others to build upon your work

critical minerals

geologic storage of CO_2

geotechnical (e.g. permafrost)

groundwater



thank you!

Tobias Stål

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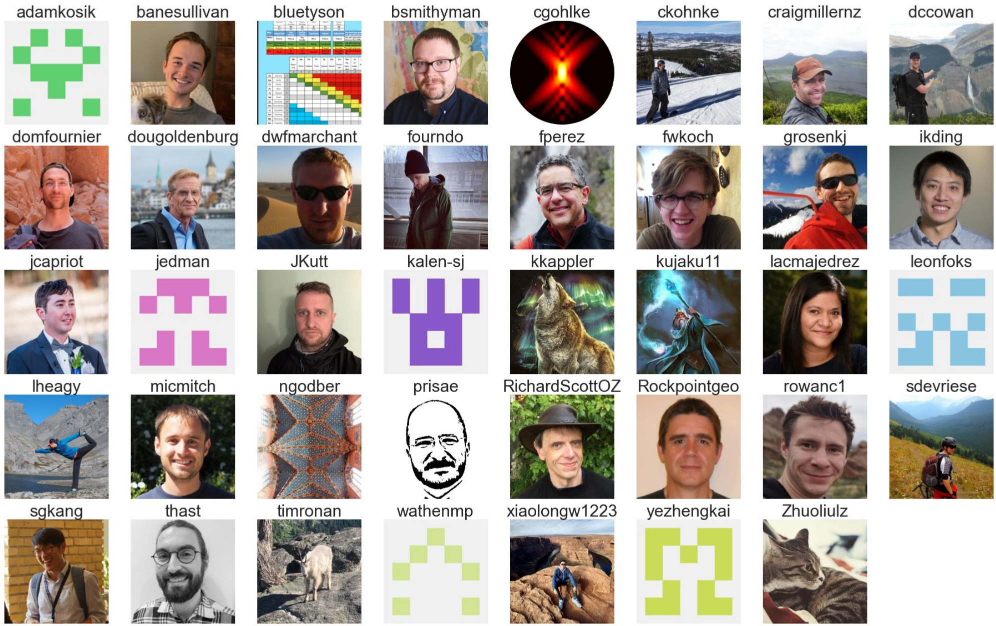
simpeg



UBC · Colorado School of Mines · University of California · TU Delft · Mira Geoscience ...modelling the earth · GIF · Stanford · UH · DIAS Geophysical

https://simpeg.xyz