# capturing knowledge in code simpeg and geosci

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#### collaborators









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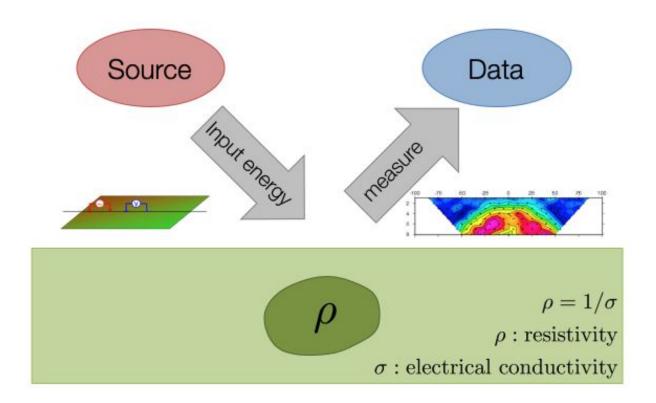




## Last week: Fundamentals of Inversion Doug Oldenburg

http://www.mtnet.info/EMinars/EMinars.html

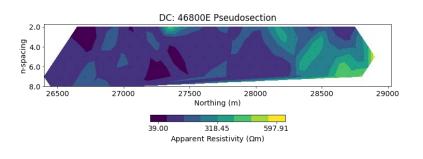
## Geophysical experiments & physical properties

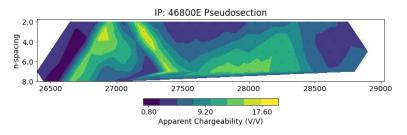


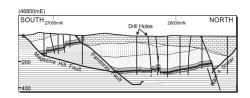
#### Last week: DC resistivity and IP at century

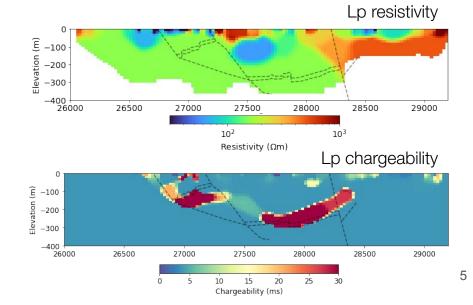
Last week: Century Deposit

- IP: linear inverse problem
- DC: non-linear inverse problem









# DC resistivity

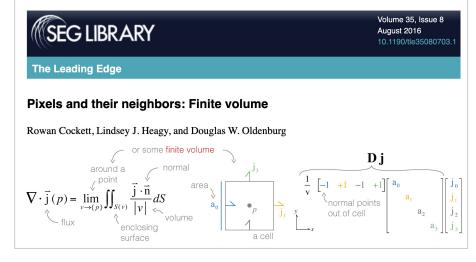
#### Governing PDE

$$\nabla \cdot \frac{1}{\rho} \nabla \phi = -I \delta(r)$$

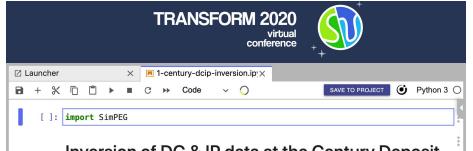
DC is an illustrative problem

- foundation for the physics of EM
- poisson equation, starting point: numerical simulations, finite volume
- inverse problem: non-linear, ideal example for showing impacts of: model norm, constraints, ...

#### Finite Volume Tutorial (Cockett et al, 2016)



#### Inversions with SimPEG (Heagy, 2020)

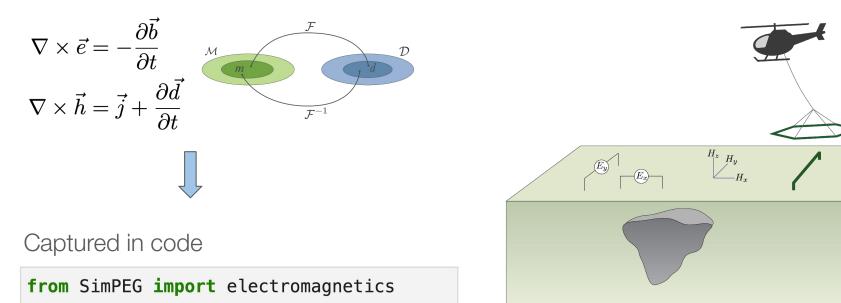


#### Inversion of DC & IP data at the Century Deposit

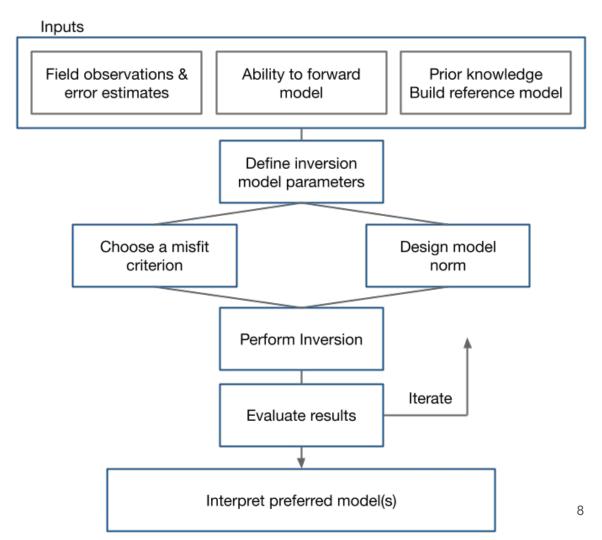
The Century Deposit is a Zinc-lead-silver deposit is located 250 km to the NNW of the Mt Isa region in Queensland Australia (Location: 18° 43' 15"S, 138° 35' 54"E).

# Focus for today: electromagnetics

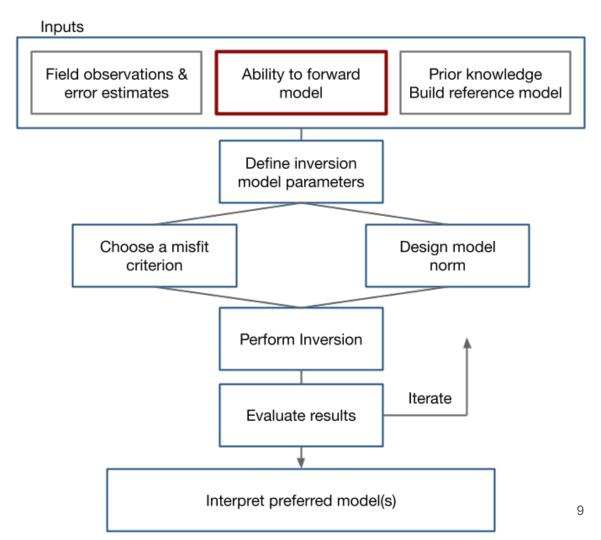
Theory: Maxwell's equations, inversion



# inversion flowchart



# inversion flowchart



## Electromagnetics: basic equations (quasi-static)

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

\* Solve with sources and boundary conditions

# Electromagnetics: frequency domain equations

Use constitutive relations, reduce to two equations, one field, one flux

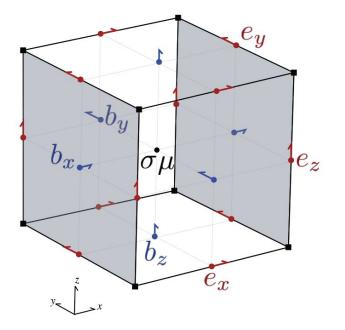
 $\nabla\times\vec{E}+i\omega\vec{B}=0$   $\nabla\times\mu^{-1}\vec{B}-\sigma\vec{E}=\vec{J_s}$ 

Boundary conditions

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

Staggered grid discretization

- Physical properties: cell centers
- Fields: edges
- Fluxes: faces



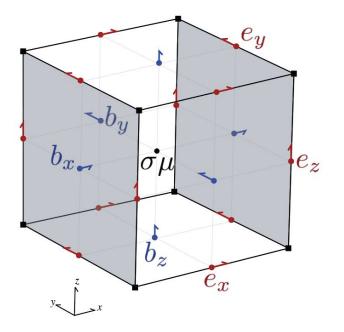
## Electromagnetics: frequency domain equations

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 (see: Haber, 2014; Cockett et al., 2016)

$$\mathbf{C}\mathbf{e} + i\omega\mathbf{b} = 0$$
$$\mathbf{C}^{\top}\mathbf{M}_{\mu^{-1}}^{f}\mathbf{b} - \mathbf{M}_{\sigma}^{e}\mathbf{e} = \mathbf{M}^{e}\mathbf{j}_{s}$$



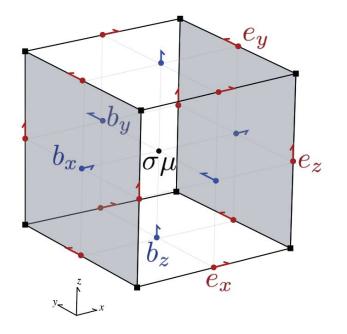
#### Electromagnetics: frequency domain equations

Discrete equations

$$\mathbf{C}\mathbf{e} + i\omega\mathbf{b} = 0$$
$$\mathbf{C}^{\top}\mathbf{M}_{\mu^{-1}}^{f}\mathbf{b} - \mathbf{M}_{\sigma}^{e}\mathbf{e} = \mathbf{M}^{e}\mathbf{j}_{s}$$

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

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



## Solving an FDEM problem

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

- Complex
- Symmetric

 $\mathbf{A}(\sigma,\omega)$ 

- Factor once for each frequency (solve for multiple sources)
  - Need to refactor on each model update
  - Separable over frequencies

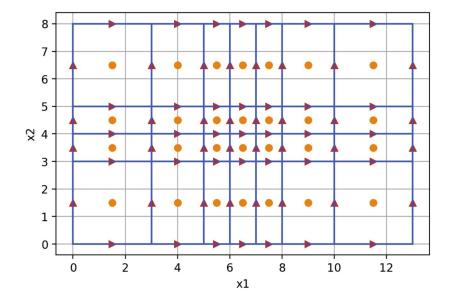
# Solving an FDEM problem

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

## Create a mesh: the discretize package

import discretize

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()
```

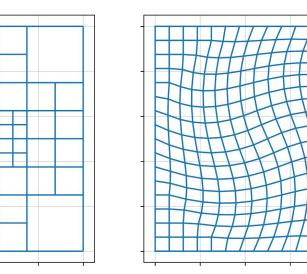
get interpolation matrix (location)

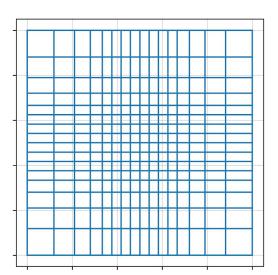
mesh types in simpeg

Tensor / Cylindrical



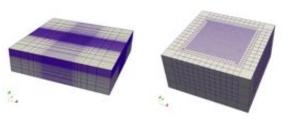












## Survey: sources and receivers

#### Sources

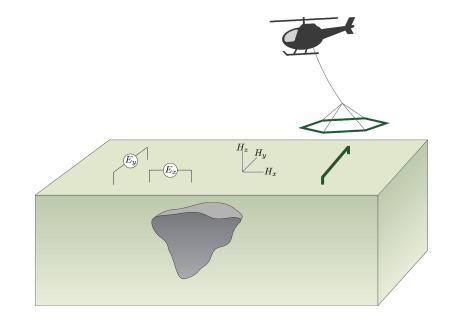
$$\underbrace{(\mathbf{C}^{\top}\mathbf{M}_{\mu^{-1}}^{f}\mathbf{C}+i\omega\mathbf{M}_{\sigma}^{e})}_{\mathbf{A}(\sigma,\omega)}\underbrace{\mathbf{e}}_{\mathbf{u}}=\underbrace{-i\omega\mathbf{M}_{\mathbf{j}\mathbf{s}}}_{\mathbf{q}(\omega)}$$

- inductive
- grounded

Receivers

- electric
- magnetic
- interpolate to locations

 $\mathbf{d}^{\mathrm{pred}} = \mathbf{P}(\mathbf{u}, \omega)$ 



# Bring it all together: simulation

from SimPEG.electromagnetics import frequency\_domain as fdem

```
simulation = fdem.Simulation3DElectricField(
    mesh=mesh, survey=survey, solver=Pardiso,
    sigmaMap=maps.IdentityMap()
```

For each frequency, solve

 $\mathbf{A}(\sigma,\omega)\mathbf{u} = \mathbf{q}(\omega)$ 

u = simulation.fields(model)

Project to receiver locations

$$\mathbf{d}^{\text{pred}} = \mathbf{P}(\mathbf{u}, \omega)$$

dpred = simulation.dpred(model, fields=u)

#### Sensitivities (we will need them later!)

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  $\rightarrow$  compute products with a vector if memory-limited

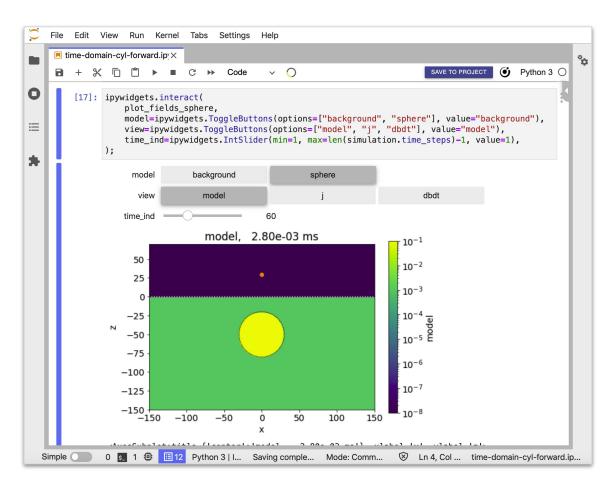
#### Demo

conductive sphere in a halfspace

cylindrical mesh

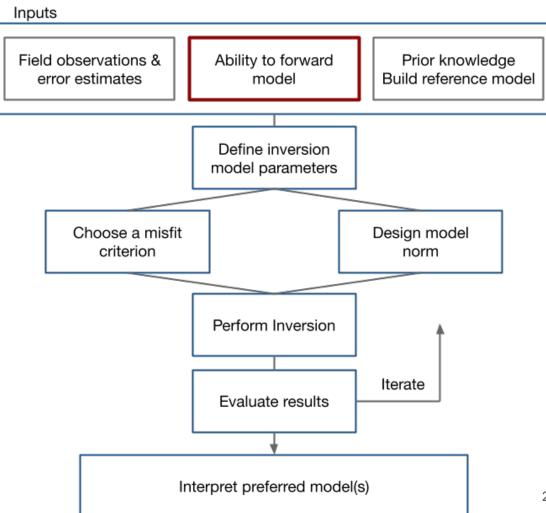
time-domain

$$abla imes \vec{e} = -rac{\partial \vec{b}}{\partial t}$$
 $abla imes \vec{h} = \vec{j}$ 

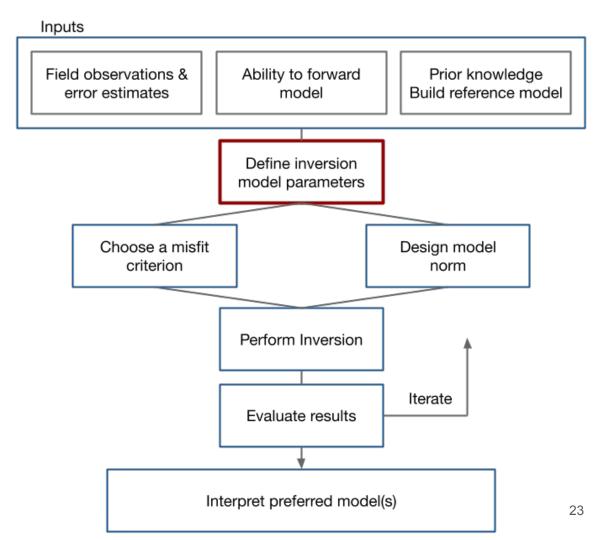


#### curvenote.com/@geosci/inversion-module

# inversion flowchart

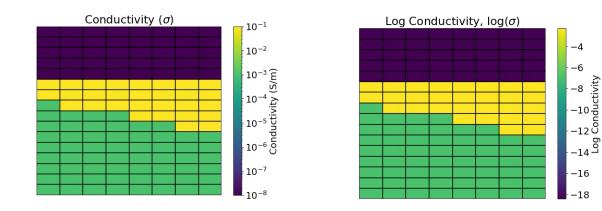


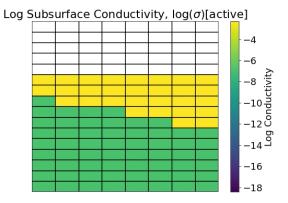
# inversion flowchart



# Inversion model parameters & mappings

What parameters are we inverting for?

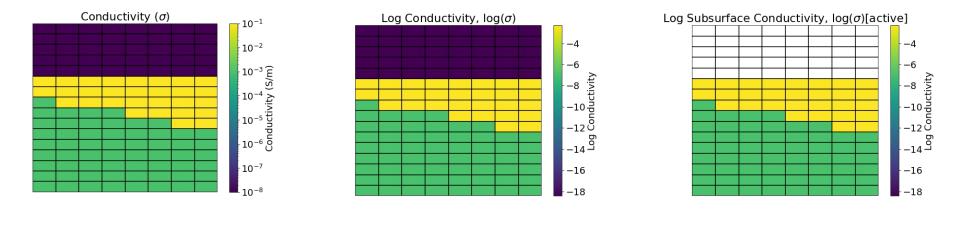




# Inversion model parameters & mappings

What parameters are we inverting for?

 $\sigma$ 



a mapping translates model parameters to physical properties on simulation mesh

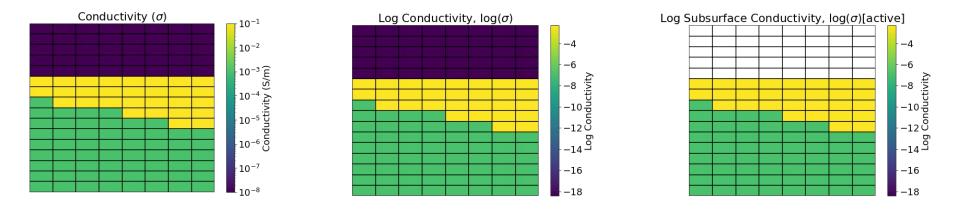
 $\sigma = \mathcal{M}(\mathbf{m})$ 

25

m

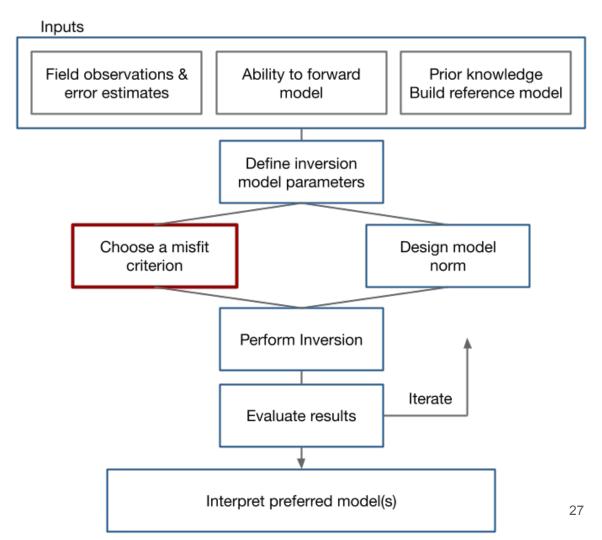
# Inversion model parameters & mappings

What parameters are we inverting for?



- Mappings can be composed
- $\sigma = \mathcal{M}(\mathbf{m})$  Includes parametric models
  - Keep track of derivatives (for sensitivities)

# inversion flowchart



#### observed data, uncertainties, and data misfit

Data misfit term

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

uncertainties captured in W matrix

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

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

#### observed data, uncertainties, and data misfit

Data misfit term

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

uncertainties captured in W matrix

$$\mathbf{W}_d = \operatorname{diag}\left(rac{1}{\epsilon}
ight)$$

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

Data class: survey geometry, observed data, assigned uncertainties

```
from SimPEG import Data
data = Data(survey, dobs, relative_error, floor)
```

Data misfit instantiated with

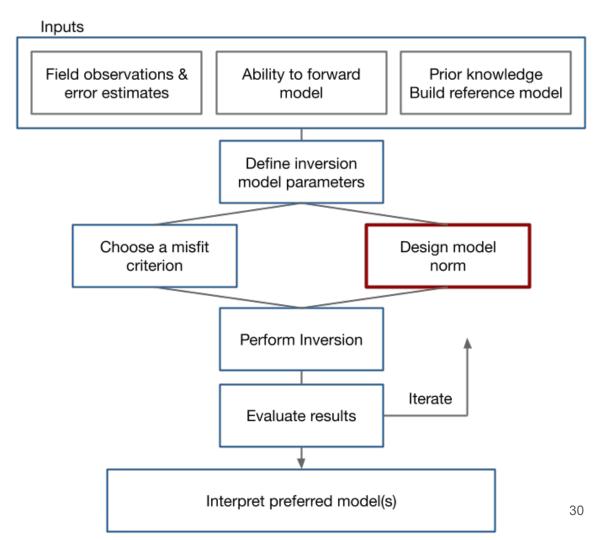
- simulation: to compute  $\mathcal{F}(\mathbf{m})$
- data: defines  $\mathbf{W}_d$ ,  $\mathbf{d}^{\mathrm{obs}}$

from SimPEG import data\_misfit
phi\_d = data\_misfit.L2DataMisfit(data, simulation)

can now evaluate data misfit + derivatives

phi\_d(m), phi\_d.deriv(m), phi\_d.deriv2(m, v)

# inversion flowchart



# Designing a model norm: regularization class

Basic Tikhonov regularization

$$\phi_{m} = \alpha_{s} \int_{V} w_{s} (m - m_{\text{ref}})^{2} dV + \alpha_{x} \int_{V} w_{x} \frac{d(m - m_{\text{ref}})^{2}}{dx} dV$$
smallness smoothness

discretize

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

Choices:

- α parameter values
- reference model
- mref in the smoothness terms
- norm applied on each term

# Designing a model norm: regularization class

Basic Tikhonov regularization

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

discretize

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

Choices:

- α parameter values
- reference model
- mref in the smoothness terms
- norm applied on each term

Regularization instantiated with

- mesh: to evaluate spatial derivs
- alphas, mref have default values, can be replaced with user values

from SimPEG import regularization

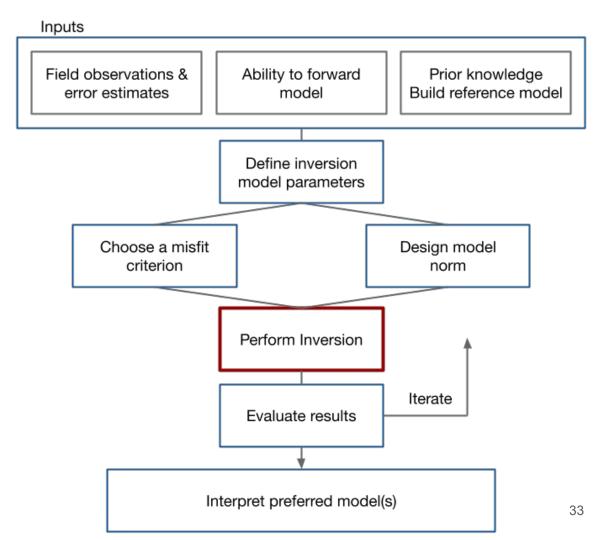
```
phi_m = regularization.Tikhonov(
    mesh, mref=mref, alpha_s=alpha_s, alpha_x=alpha_x
)
```

```
phi_m_sparse = regularization.Sparse(
        mesh, mref=mref, norms=[1, 1]
)
```

can now evaluate phi\_m + derivatives

phi\_m(m), phi\_m.deriv(m), phi\_m.deriv2(m, v)

# inversion flowchart



# Perform the inversion: stating the objective function

Inversion as an optimization problem (deterministic approach)

$$\min_{\mathbf{m}} \phi(\mathbf{m}) = \underline{\phi_d}(\mathbf{m}) + \beta \underline{\phi_m}(\mathbf{m})$$
  
s.t.  $\phi_d \le \phi_d^* \quad \mathbf{m}_L \le \mathbf{m} \le \mathbf{m}_U$ 

At this stage, we have specified

- parameters we are inverting for
- data misfit
- model norm

# Perform the inversion: stating the objective function

Inversion as an optimization problem (deterministic approach)

$$\underline{\min}_{\mathbf{m}} \phi(\underline{\mathbf{m}}) = \underline{\phi_d}(\mathbf{m}) + \underline{\beta}\underline{\phi_m}(\mathbf{m})$$
s.t.  $\phi_d \leq \underline{\phi_d^*}_d$   $\mathbf{m}_L \leq \mathbf{m} \leq \mathbf{m}_U$ 

Still to define

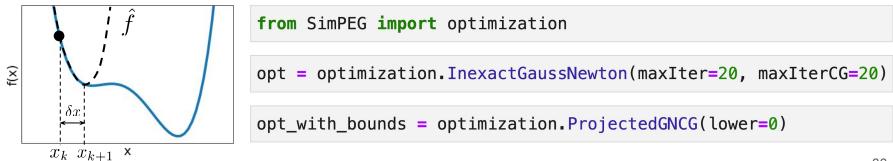
- optimization method
- upper and lower bounds
- choice of initial beta
- choice of beta-cooling schedule
- target misfit and stopping the inversion

## Perform the inversion: optimization approach

Inversion as an optimization problem (deterministic approach)

$$\min_{\mathbf{m}} \phi(\mathbf{m}) = \phi_d(\mathbf{m}) + \beta \phi_m(\mathbf{m})$$
s.t.  $\phi_d \le \phi_d^* \quad \mathbf{m}_L \le \mathbf{m} \le \mathbf{m}_U$ 

#### Second-order methods



Inversion as an optimization problem (deterministic approach)

$$\min_{\mathbf{m}} \phi(\mathbf{m}) = \phi_d(\mathbf{m}) + \beta \phi_m(\mathbf{m})$$
  
s.t.  $\phi_d \le \phi_d^* \quad \mathbf{m}_L \le \mathbf{m} \le \mathbf{m}_L$ 

We use **directives** to make parameter updates and orchestrate the inversion, e.g.

- estimating initial beta
- defining a beta-cooling schedule
- stopping the inversion when target misfit reached

Inversion as an optimization problem (deterministic approach)

$$\min_{\mathbf{m}} \phi(\mathbf{m}) = \phi_d(\mathbf{m}) + \beta \phi_m(\mathbf{m})$$
  
s.t.  $\phi_d \le \phi_d^* \quad \mathbf{m}_L \le \mathbf{m} \le \mathbf{m}_L$ 

Initial beta

• estimate "size" of data misfit and model norm by approximating eigenvalues of

$$\mathbf{J}^{\top}\mathbf{W}_{d}^{\top}\mathbf{W}_{d}\mathbf{J}, \ \mathbf{W}_{m}^{\top}\mathbf{W}_{m}$$

• take ratio, weight by a parameter controlling relative importance of each

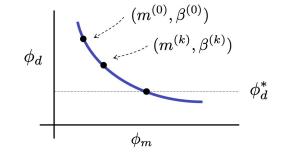
from SimPEG import directives
beta0 = directives.BetaEstimate\_ByEig(beta0\_ratio=100)

Inversion as an optimization problem (deterministic approach)

$$\min_{\mathbf{m}} \phi(\mathbf{m}) = \phi_d(\mathbf{m}) + \underline{\beta}\phi_m(\mathbf{m})$$
  
s.t.  $\phi_d \le \phi_d^* \quad \mathbf{m}_L \le \mathbf{m} \le \mathbf{m}_U$ 

Beta-cooling

- Define how often beta is reduced (every N iterations)
- Define how much beta is reduced by



beta\_cooling = directives.BetaSchedule(coolingRate=2, coolingFactor=4)

Inversion as an optimization problem (deterministic approach)

$$\min_{\mathbf{m}} \phi(\mathbf{m}) = \phi_d(\mathbf{m}) + \beta \phi_m(\mathbf{m})$$
  
s.t.  $\phi_d \le \phi_d^* \quad \mathbf{m}_L \le \mathbf{m} \le \mathbf{m}_U$ 

Target misfit

• Expected value of data misfit

$$E[\phi_d] \simeq N$$

• Define target misfit as (default  $\chi = 1$ )

$$\phi_d^* = \chi N$$



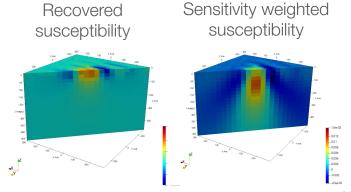
$\phi_d$	$(m^{(0)}, \beta^{(0)})$	- <i>d</i> *
		Ψa
	$\phi_m$	

Inversion as an optimization problem (deterministic approach)

$$\min_{\mathbf{m}} \phi(\mathbf{m}) = \phi_d(\mathbf{m}) + \beta \phi_m(\mathbf{m})$$
  
s.t.  $\phi_d \le \phi_d^* \quad \mathbf{m}_L \le \mathbf{m} \le \mathbf{m}_L$ 

Other uses for directives

- saving inversion model at each iteration
- saving inversion progress (beta, data misfit, ...)
- including / updating sensitivity weighting
- updating values for norms (L2  $\rightarrow$  Lp)



# Perform the inversion: bringing it all together

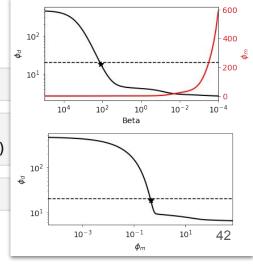
Inversion as an optimization problem (deterministic approach)

$$\min_{\mathbf{m}} \phi(\mathbf{m}) = \phi_d(\mathbf{m}) + \beta \phi_m(\mathbf{m})$$
  
s.t.  $\phi_d \le \phi_d^* \quad \mathbf{m}_L \le \mathbf{m} \le \mathbf{m}_L$ 

from SimPEG import inverse\_problem, inversion

inv\_prob = inverse\_problem.BaseInvProblem(phi\_d, phi\_m, opt)
inv = inversion.BaseInversion(inv\_prob, [beta0, beta\_cooling, target\_misfit])

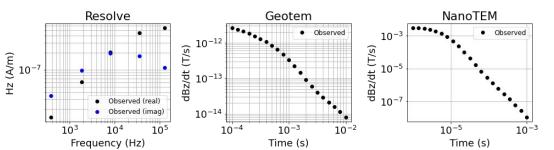
inv.run(m0)

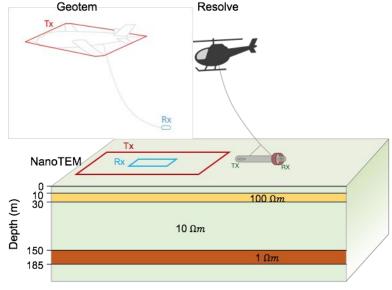


# An example: 1D inversions

Layered earth, 3 different EM systems

- Resolve (airborne, frequency)
- Geotem (airborne, time-domain)
- NanoTEM (ground, time-domain)





(Oldenburg et al, 2020)

#### Seogi Kang



- Efficient forward simulation, sensitivity calculation using digital filters
   relies on empymod (Werthmüller, 2017)
  - relies on empymod (Werthmüller, 2017)
- Parallelized over soundings
- Common FDEM, TDEM system parameters implemented

 NanoTEM
 Tx
 Tx

 0
 100 Ωm

 10
 10 Ωm

Resolve

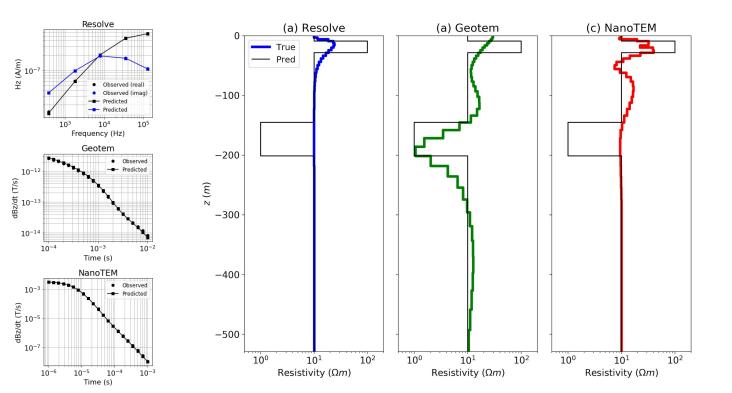
Geotem

Depth (m)



# Individual inversions

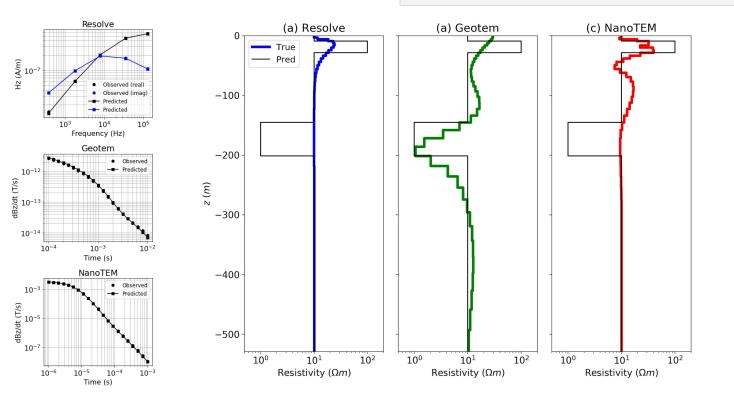
#### L2 regularization



$$\phi(\mathbf{m}) = \underbrace{\phi_d^{\text{Resolve}} + \phi_d^{\text{Geotem}} + \phi_d^{\text{NanoTEM}}}_{\phi_d(\mathbf{m})} + \beta \phi_m(\mathbf{m})$$

L2 regularization

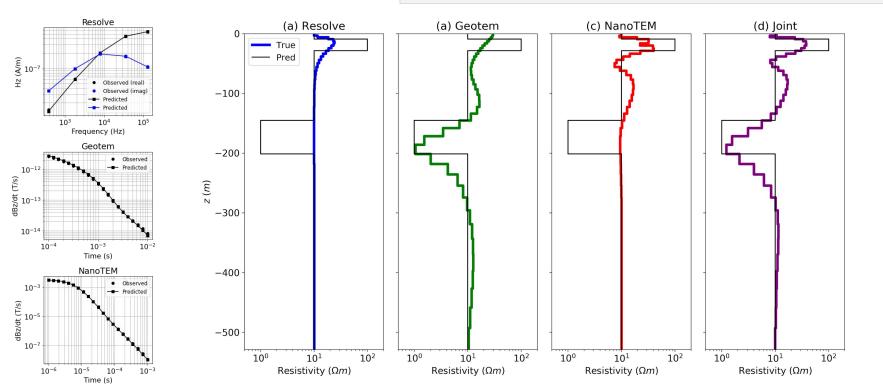
phi\_d = phi\_d\_resolve + phi\_d\_geotem + phi\_d\_nanotem



$$\phi(\mathbf{m}) = \underbrace{\phi_d^{\text{Resolve}} + \phi_d^{\text{Geotem}} + \phi_d^{\text{NanoTEM}}}_{\phi_d(\mathbf{m})} + \beta \phi_m(\mathbf{m})$$

L2 regularization

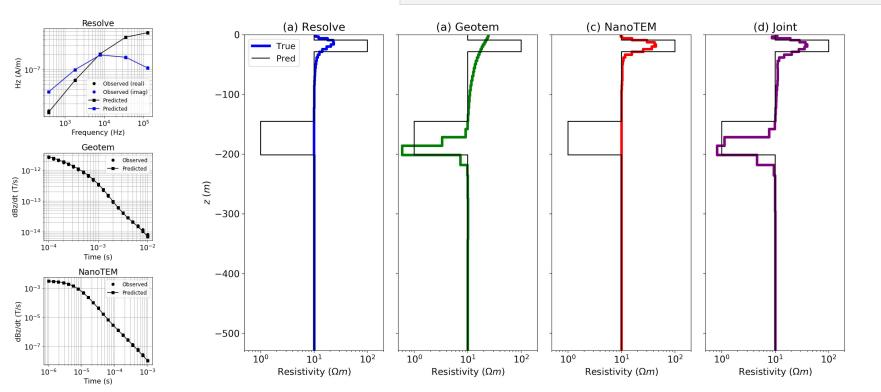
phi\_d = phi\_d\_resolve + phi\_d\_geotem + phi\_d\_nanotem



$$\phi(\mathbf{m}) = \underbrace{\phi_d^{\text{Resolve}} + \phi_d^{\text{Geotem}} + \phi_d^{\text{NanoTEM}}}_{\phi_d(\mathbf{m})} + \beta \phi_m(\mathbf{m})$$

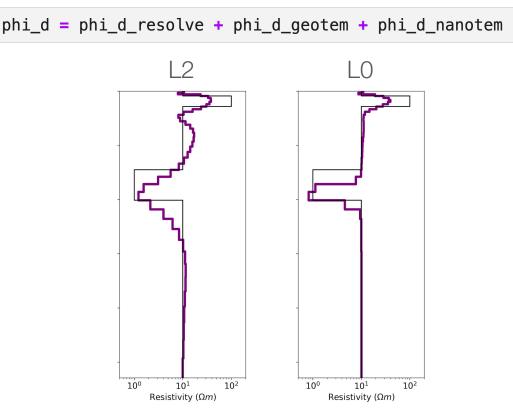
L0 regularization

phi\_d = phi\_d\_resolve + phi\_d\_geotem + phi\_d\_nanotem



Flexibility to handle:

- multiple surveys / physics
- different model parameterizations
- different simulation mesh for each datum
- separate forward simulation and inversion meshes



# Example: Bookpurnong

Murray River Floodplain

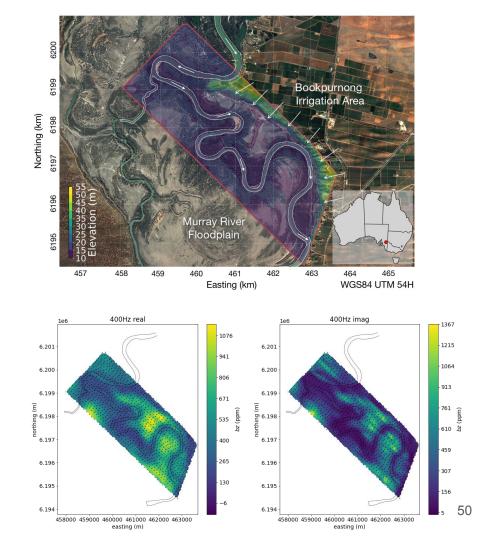
- over-irrigation and drought
- saline water recharges river
- floodplain salinization

#### Data

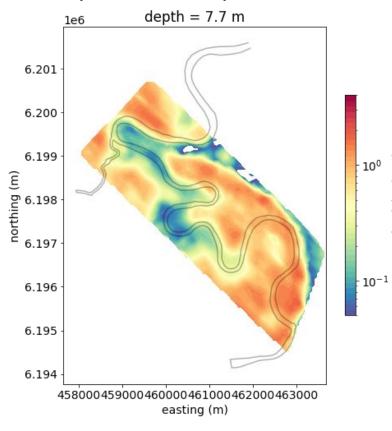
- 2006: SkyTEM (time-domain)
- 2008: RESOLVE (frequency-domain)

Inversion

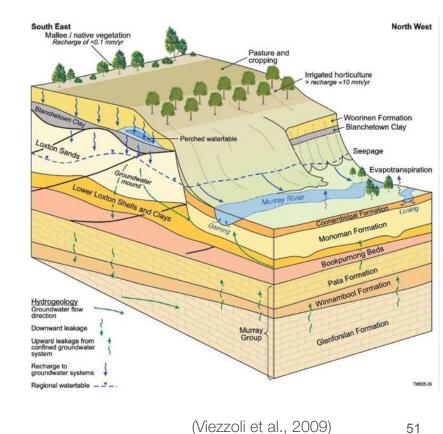
• Spatially constrained 1D



#### Example: Bookpurnong

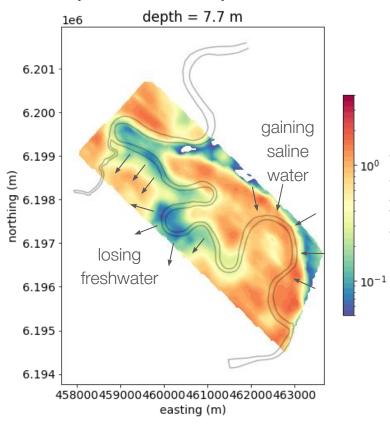


Conductivity (S/m)

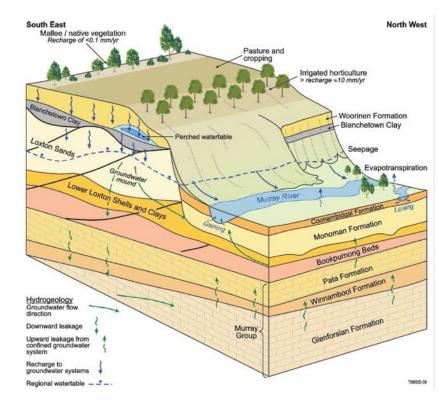


coming to the docs soon!

#### Example: Bookpurnong



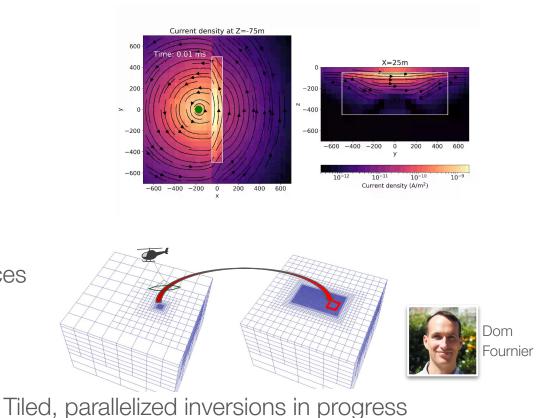
Conductivity (S/m)



coming to the <u>docs</u> soon!

# geophysical methods in SimPEG

- Gravity
- Magnetics
- Direct current resistivity
- Induced polarization
- Electromagnetics
  - Frequency Domain
  - Time Domain
  - Controlled + natural sources
- Fluid Flow
  - Richards Equation











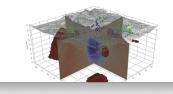
#### **Simulation and Parameter Estimation in Geophysics**

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.











MINES.



icapriot







fourndo

lheagy

sakana



















#### https://simpeg.xyz





dougoldenburg

dwfmarchant

lacmajedrez

# code + community

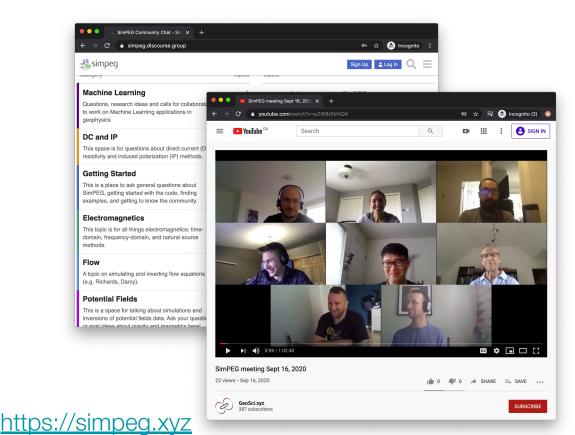


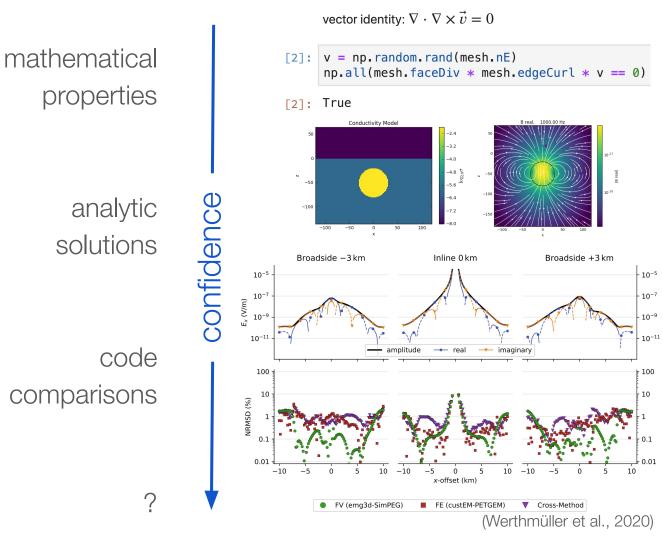
#### Software practices

- Versioning code
- Tracking issues
- Testing code
- Suggesting changes
- Peer-reviewing changes

#### Communication

- Weekly meetings (recorded)
- Discourse forum for Q&A
- Chat with slack

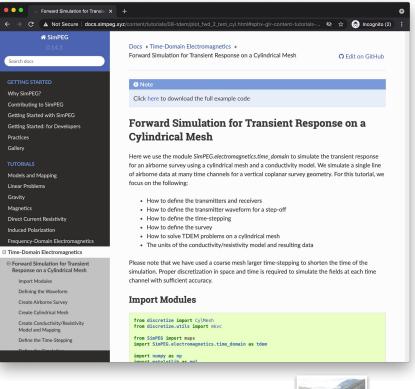




#### testing

#### community: connecting + resources

- documentation: <u>docs.simpeg.xyz</u>
- community forum: simpeg.discourse.group
- chat: <u>slack.simpeg.xyz</u>
- meeting notes + recordings:
   <u>curvenote.com/@simpeg/meeting-notes</u>



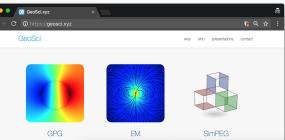


#### GeoSci.xyz



26 locations worldwide

#### https://geosci.xyz





Inverse Theory Overview Linear Tikhonov Inversio LinearInversion\_notebook.ipynb inearInversion-app.ipvnb inear L2-norm Inversion onlinear Inversior

Linear Tikhonov Inversion AUTHOR DATE Douglas Oldenburg Jan 18, 2021

geosci / inversion-module / linear-tikhonov-inversion - v21

In this chapter we present the basic elements for how an inverse problem can be formulated and solved using optimization theory. The quantity to be minimized is a weighted sum of misfit and regularization terms with their relative importance controlled by an adjustable Tikhonov parameter.

😭 🏾 🗂 Incognito

SIGN UP

The inverse problem has many elements and a solution is best achieved by adhering to the workflow shown below. Throughout this chapter we investigate each of these steps and illustrate the concepts with a simple linear problem. Jupyter notebooks are provided so that the concepts can be explored and all figures can be reproduced. The formative material for this chapter is extracted from the tutorial paper by Oldenburg and Li (Oldenburg & Li, 2005).

Field observations & error estimates	Ability to forward model	Prior knowledge Build reference mod

# 6.088 undergrad at UBC

Users

30K

t 28%

vs last year

Sessions

48K

t 30%

curvenote.com/@geosci/inversion-module

thank you!



dccowan

jcapriot





fwkoch



micmitch









dougoldenburg

JKutt



dwfmarchant

lacmajedrez

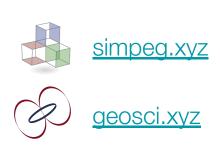




fourndo

lheagy











grosenkj





Max Moorkamp



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