accelerating research with community-driven open-source software for geophysical inversions

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IMAGE ‘23

accelerating research: important problems

opportunities for geophysics

critical minerals

geologic storage of CO_2

geothermal

groundwater

accelerating research: important problems




opportunities for geophysics

some common themes

- connecting physical properties & geology with geophysics
- combining multiple data types
- monitoring & time-lapse changes
- addressing questions about uncertainty
- collaboration between disciplines
- …

computational methods

- numerical simulations
- inversion
- machine learning
- optimization
- uncertainty quantification
- …

hypothesis: open-source software & open-science practices can accelerate research

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definition: open-source

1. Free Redistribution
2. Source Code
3. Derived Works
4. Integrity of The Author's Source Code
5. No Discrimination Against Persons or Groups
6. No Discrimination Against Fields of Endeavor
7. Distribution of License
8. License Must Not Be Specific to a Product
9. License Must Not Restrict Other Software
10. License Must Be Technology-Neutral

https://opensource.org/osd

license types

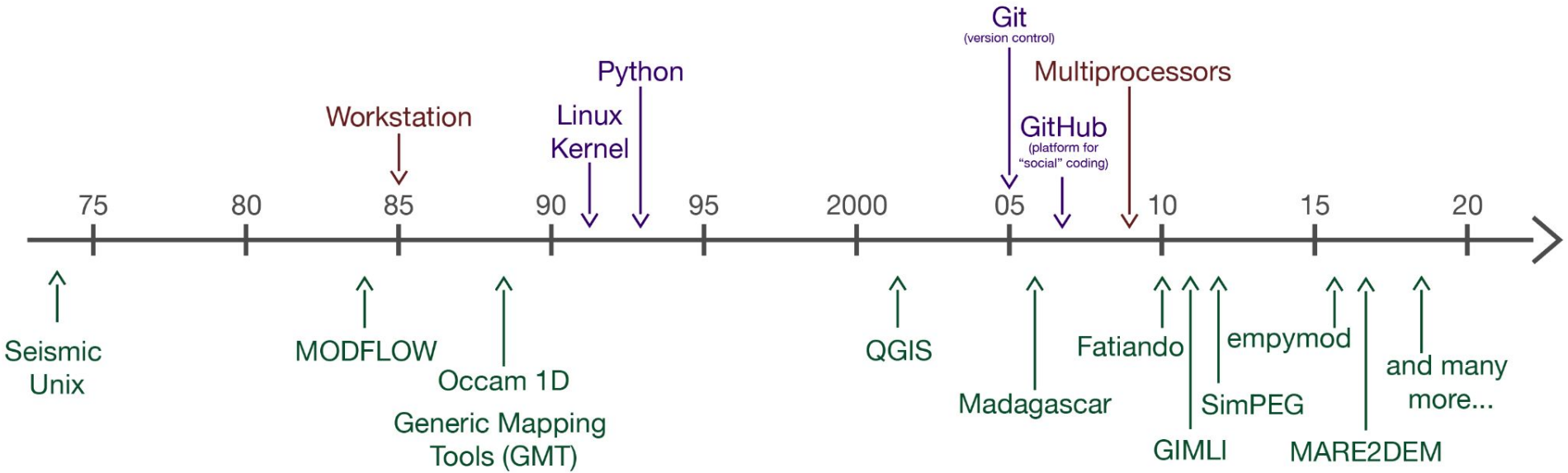
permissive
allows…

- reuse
- adaptation
- distribution of open or closed versions

copyleft
allows…

- reuse
- adaptation
- distribution must be open source

open source in applied geophysics: a loose timeline



today…

open source tools for

- data processing
- geologic modelling
- simulation
- inversion
- visualization
- data conversion
- gis
- …

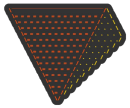
PyGMT

pyGIMLi

Geophysical Inversion & Modelling Library

Fatiando a Terra

GemPy



subsurface

And many more!

https://github.com/softwareunderground/awesome-open-geoscience

simpeg

what SimPEG solves…

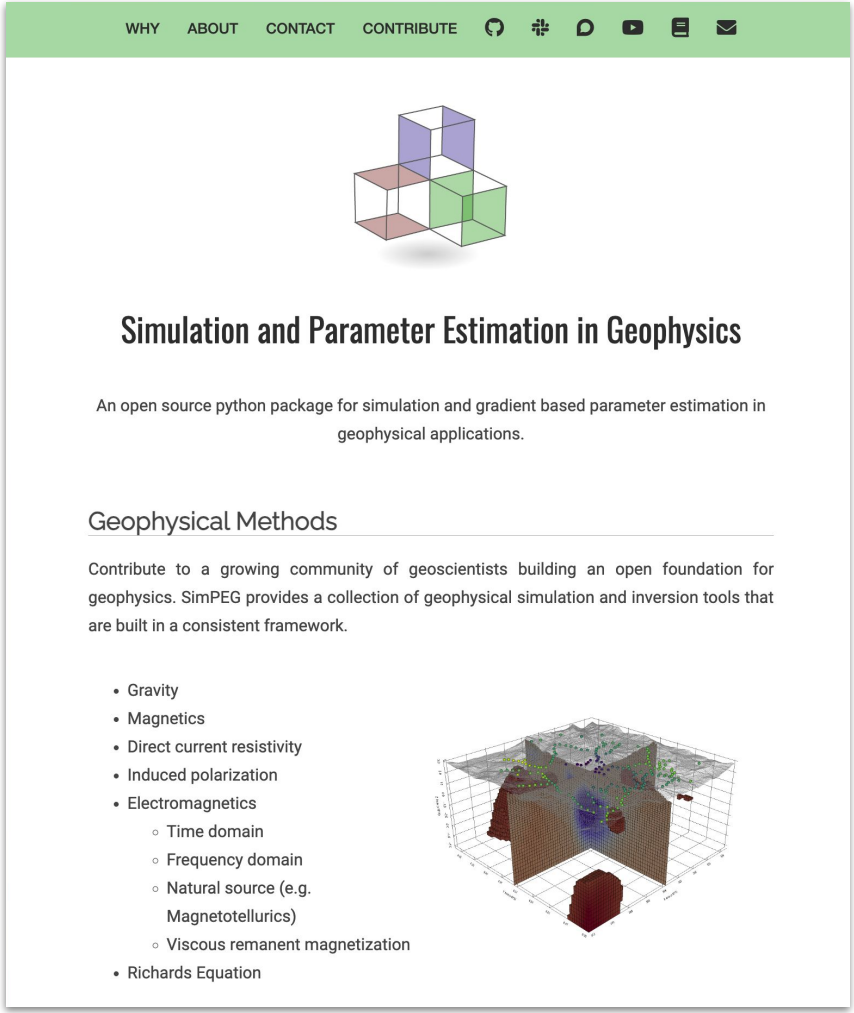
inversion as optimization

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

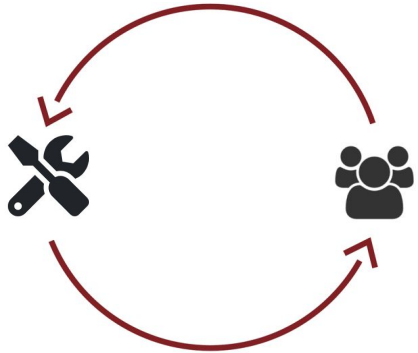
$$\text{s.t. } \phi_d \leq \phi_d^* \quad \mathbf{m}_L \leq \mathbf{m} \leq \mathbf{m}_U$$

requires:

- numerical simulation
- computation of sensitivities
- definition of regularization functional
- optimization machinery



advantages of open-source…



accelerates re-use and extension of ideas

enables combination of methods

facilitates collaboration

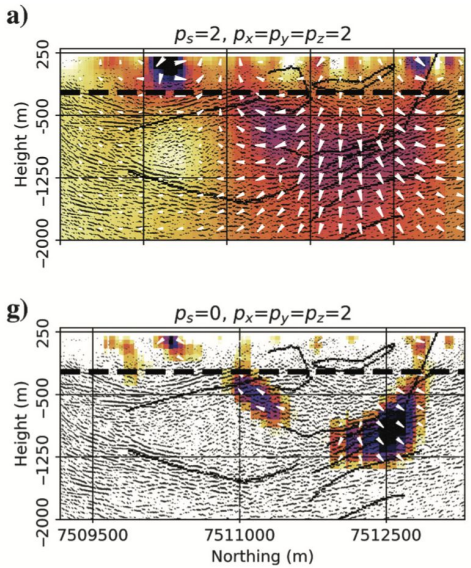
broadens impact

re-use and extension: sparse norms

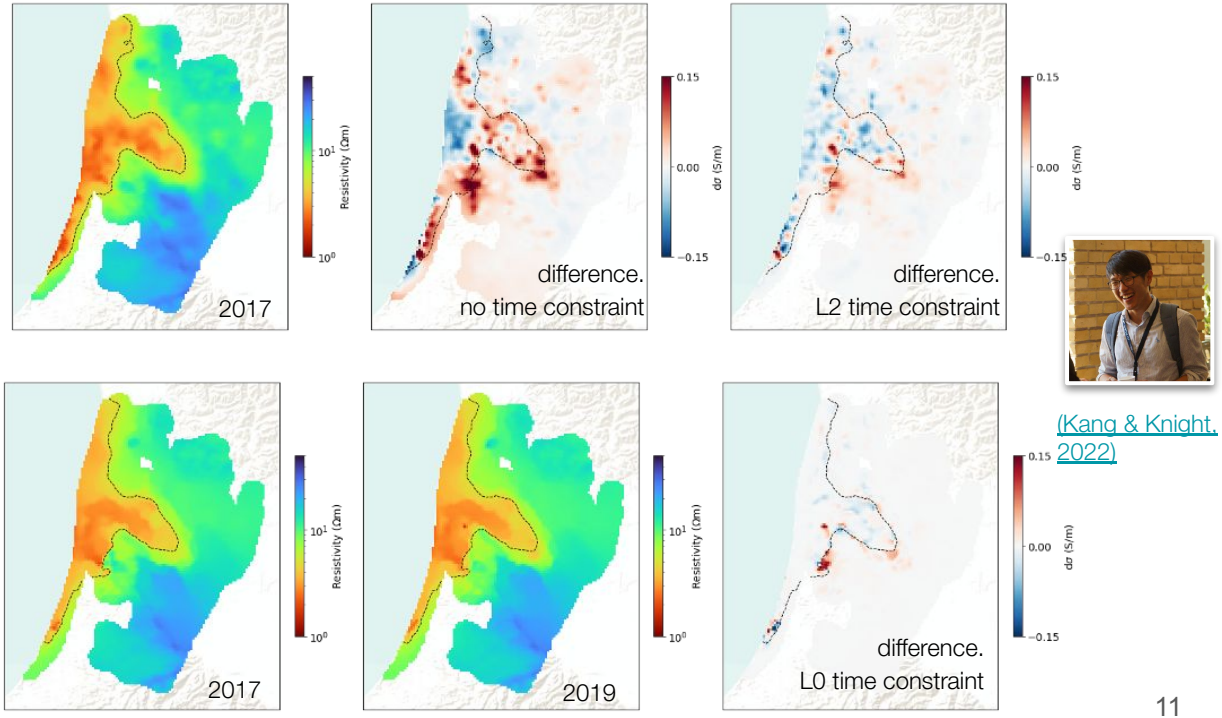
$$\phi_m = \alpha_s \int_V w_s |m - m_{\text{ref}}|^{p_s} dV + \alpha_x \int_V w_x \left| \frac{d(m - m_{\text{ref}})}{dx} \right|^{p_x} dV$$

developed in potential fields

(Fournier et al. 2019)



adapted to time-lapse AEM

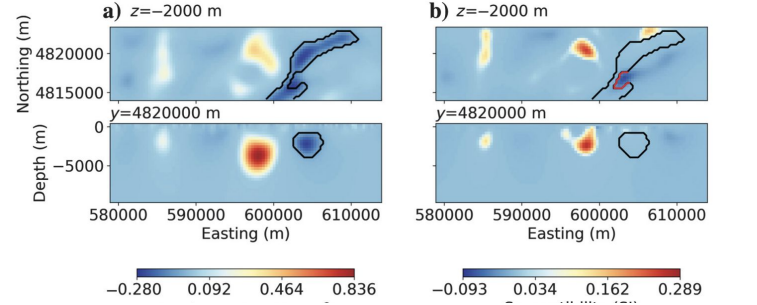


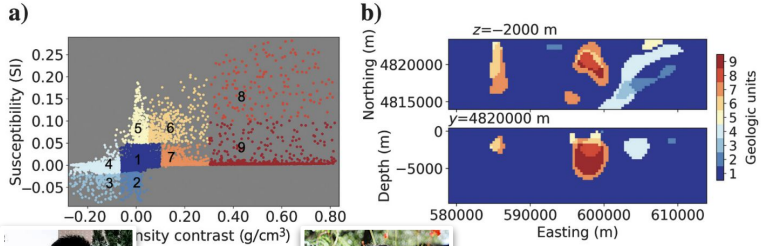
(Kang & Knight, 2022)

combining methods: joint inversions

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

Probabilistic geologic differentiation: cross gradient, Lp norms, physical properties (Wei & Sun, 2021)



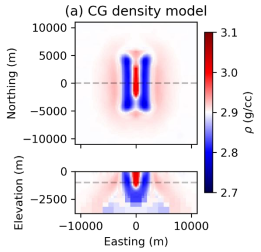


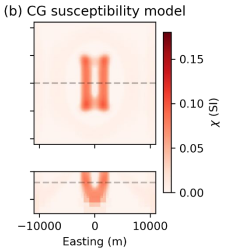
J. Sun

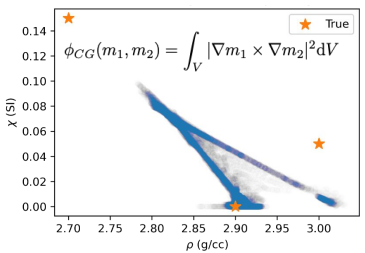
X. Wei

Joint inversions for carbon mineralization

Cross Gradient

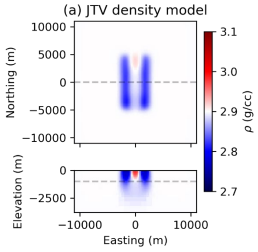


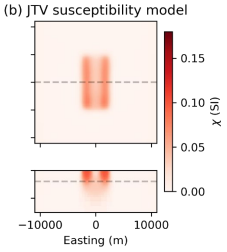


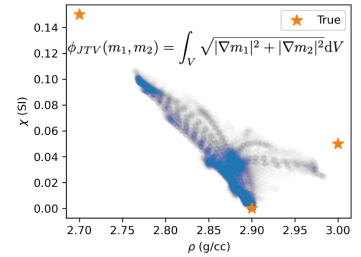


J. Capriotti

Joint total variation

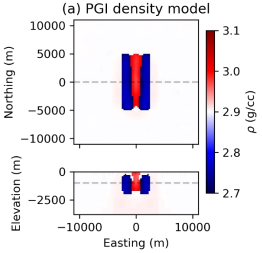


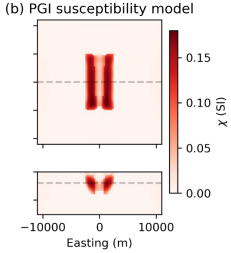


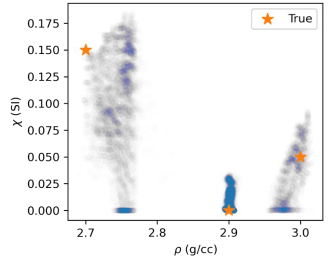


Petrophysically and Geologically guided Inversion (PGI)

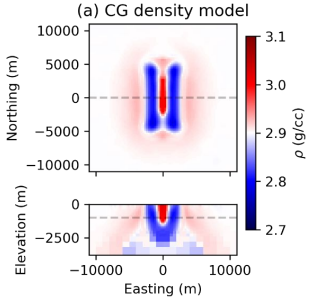
T. Astic

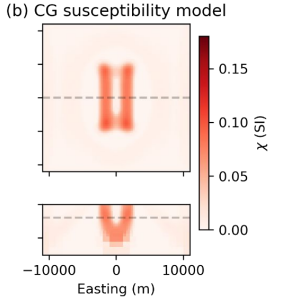


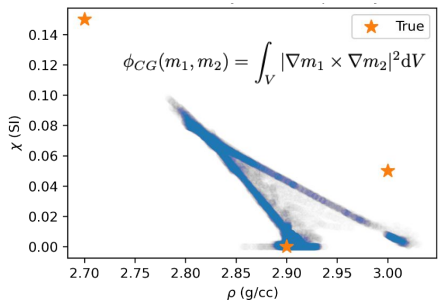




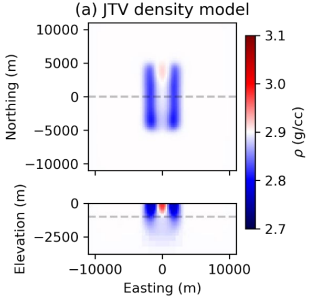
Cross Gradient

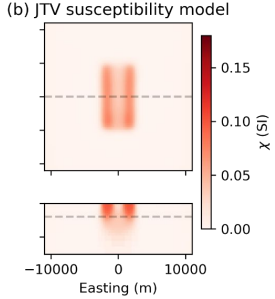


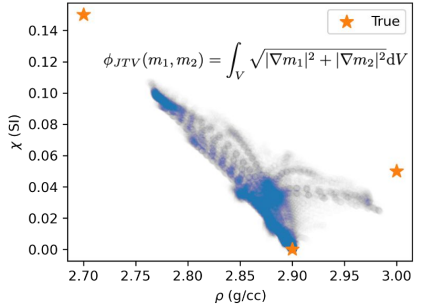




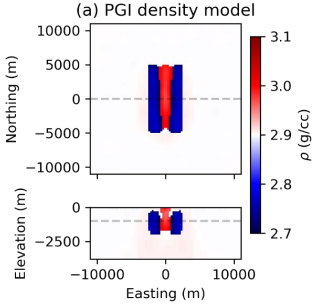
Joint total variation

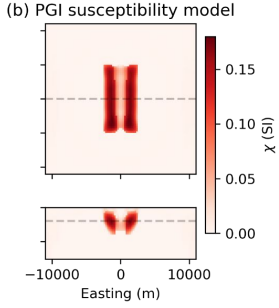


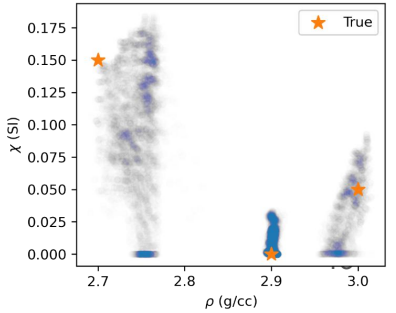




Petrophysically and Geologically guided Inversion (PGI)





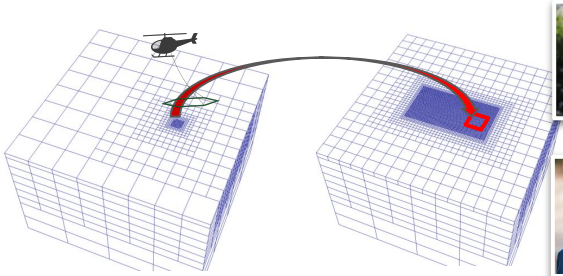


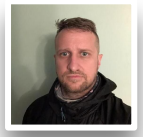
parallelization: an industry-academic collaboration

parallelization motivated initially by large scale 3D DCIP

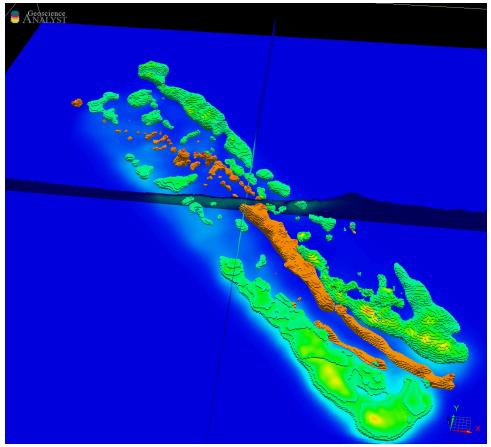
use of dask for parallelization (on any architecture)

now adapted for Mag, Grav, and working on AEM, MT

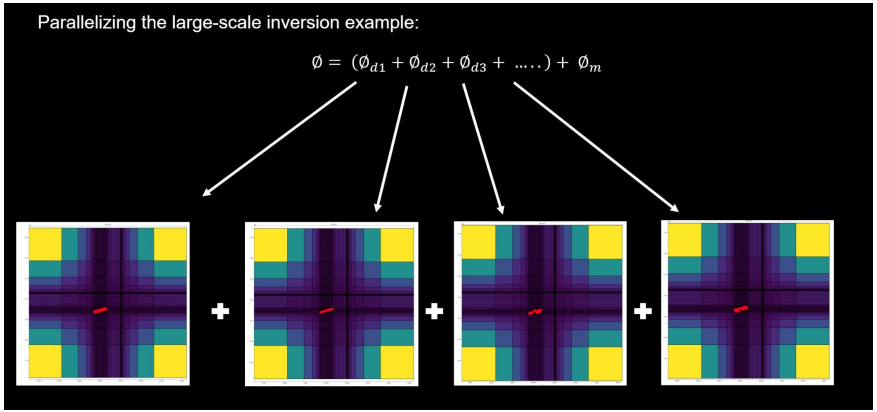




J. Kuttai



17.1 million cells 783 injections

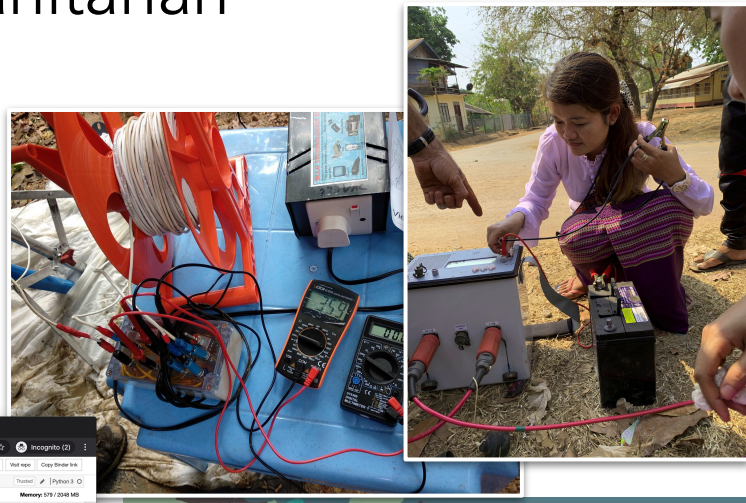


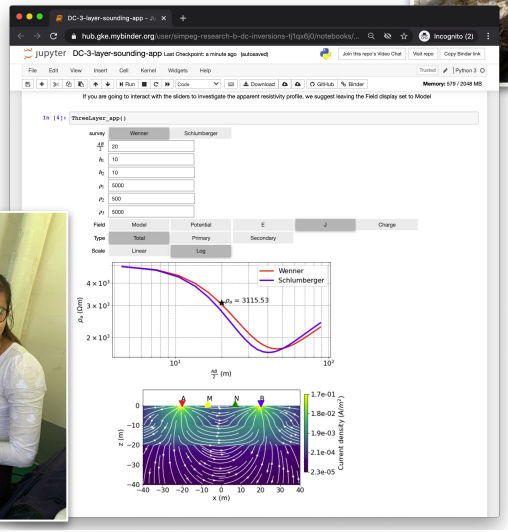
broader impact: educational & humanitarian

GWB project: groundwater in Myanmar

notebook “apps” for fundamentals, inverting data

“living” resources can be adapted to needs

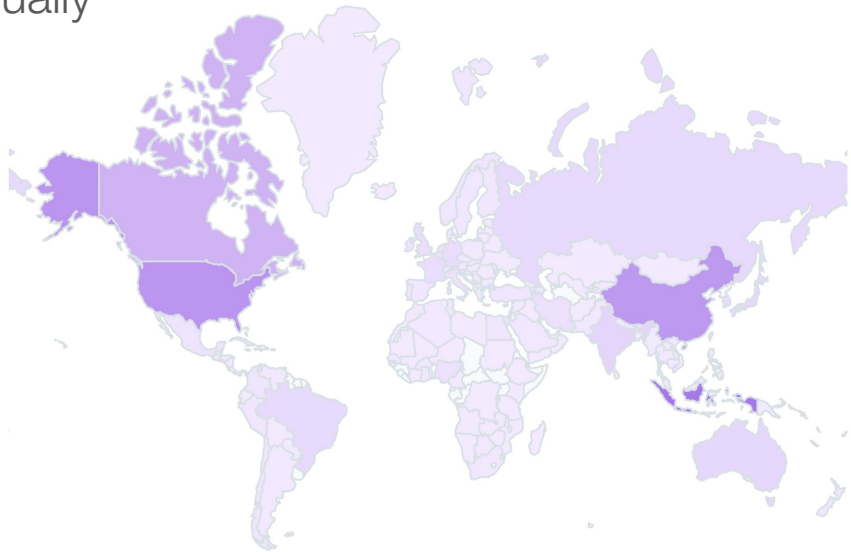




hypothesis: open-source software & open-science practices can accelerate research

some additional evidence:

- 15000+ visitors to the simpeg website annually
- 1000+ downloads per month (from pypi)
- 250+ citations to the SimPEG papers
- 39+ contributors to the codebase
- 20+ institutions using SimPEG



locations of visitors to the simpeg.xyz in the last year

challenges & opportunities

mechanisms for academic credit

- role of professional societies
- doi's for software

zenodo

new funding models

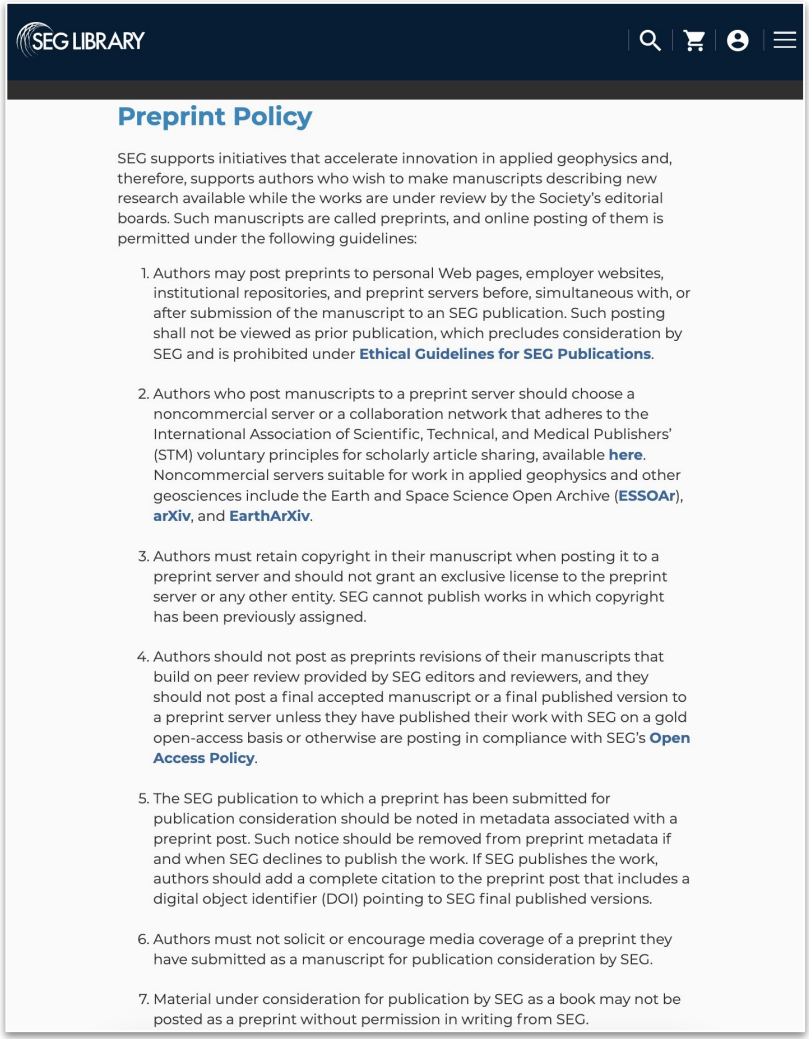
- industry support: contributions & research funding
- also related to academic credit, tracking impact

pyOpenSci

Peer review of Python software to support open science

beyond software: open science

- not all research code needs to be an “open source project”
- sharing (even messy!) code facilitates reproducibility, extensibility
- “green open access”: preprints support open science



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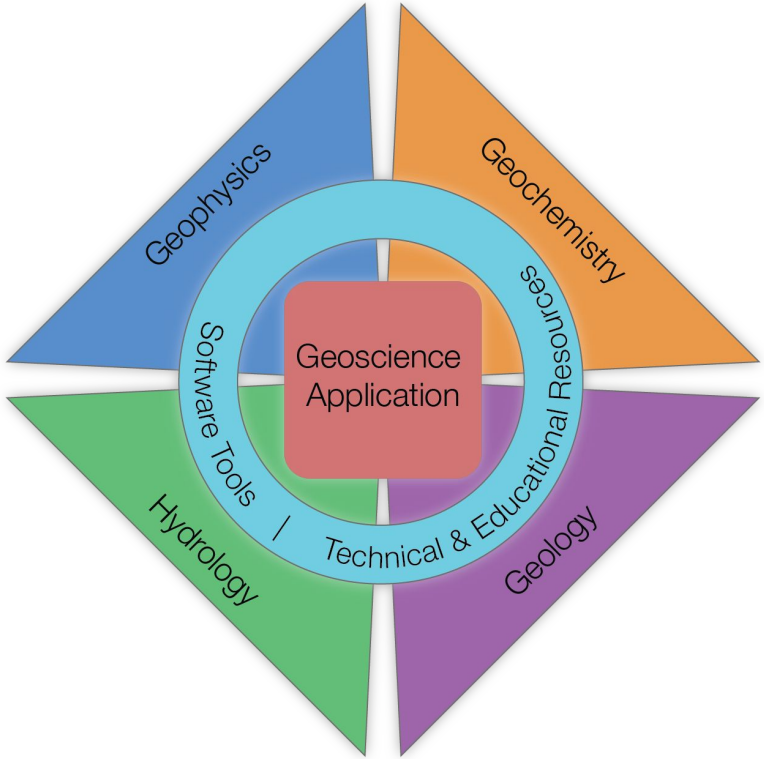
geophysics and multidisciplinary problems




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



opportunities with open science




accelerates re-use and extension of ideas

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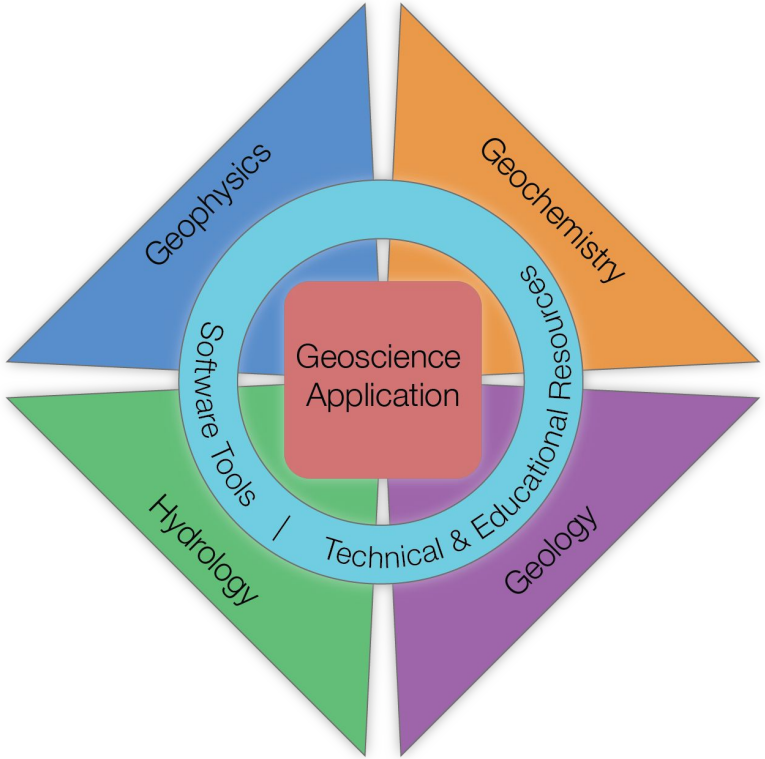

thank you & questions

email: lheagy@eoas.ubc.ca

slides: bit.ly/heagy-2023-image