

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

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accelerating research: important problems

opportunities for geophysics



critical minerals



geologic storage of CO₂



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

Choose an open source license

An open source license protects contributors and users. Businesses and savvy developers won't touch a project without this protection.



Which of the following best describes your situation?



I need to work in a community.

Use the [license preferred by the community](#) you're contributing to or depending on. Your project will fit right in.

If you have a dependency that doesn't have a license, ask its maintainers to [add a license](#).



I want it simple and permissive.

The [MIT License](#) is short and to the point. It lets people do almost anything they want with your project, like making and distributing closed source versions.

[Babel](#), [.NET](#), and [Rails](#) use the MIT License.



I care about sharing improvements.

The [GNU GPLv3](#) also lets people do almost anything they want with your project, except distributing closed source versions.

[Ansible](#), [Bash](#), and [GIMP](#) use the GNU GPLv3.



What if none of these work for me?



My project isn't software.

[There are licenses for that.](#)

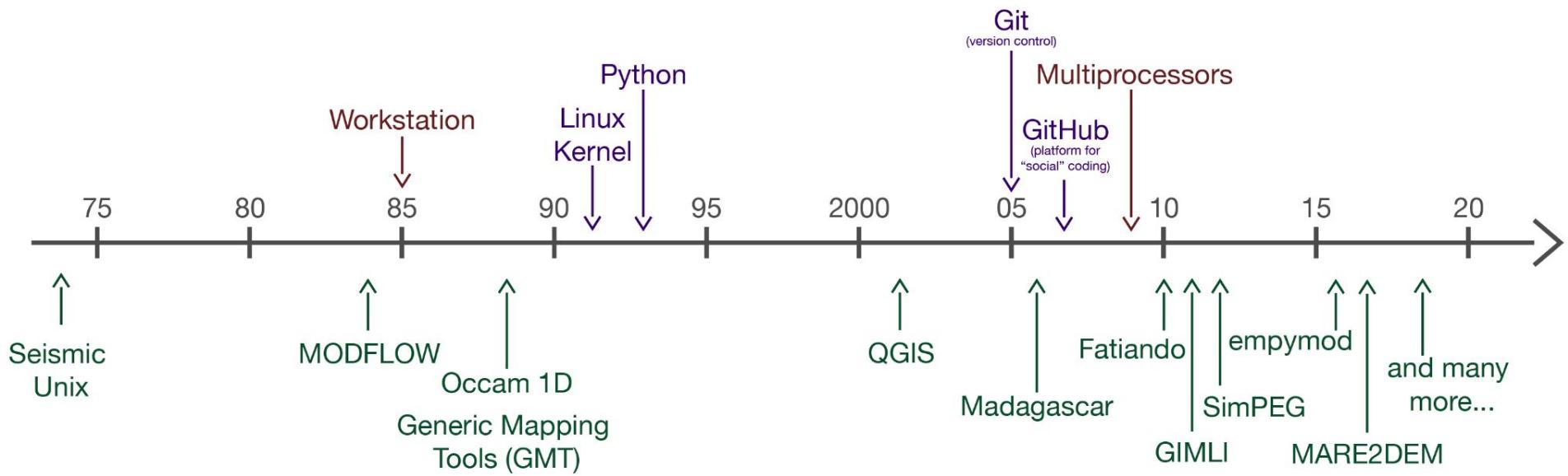
I want more choices.

[More licenses are available.](#)

I don't want to choose a license.

[Here's what happens if you don't.](#)

open source in applied geophysics: a loose timeline



today...

open source tools for

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



PyGMT



And many more!

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



what SimPEG solves...

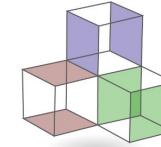
inversion as optimization

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

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

requires:

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



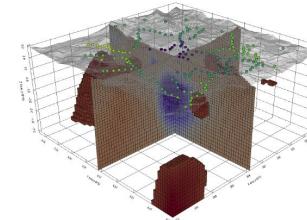
Simulation and Parameter Estimation in Geophysics

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

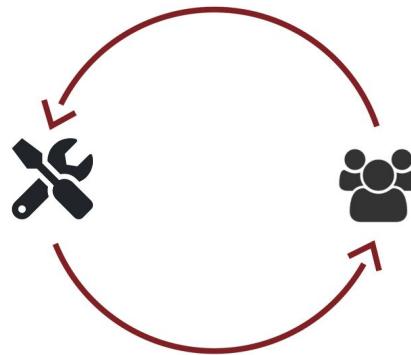
Geophysical Methods

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



advantages of open-source...



accelerates re-use and extension of ideas

enables combination of methods

facilitates collaboration

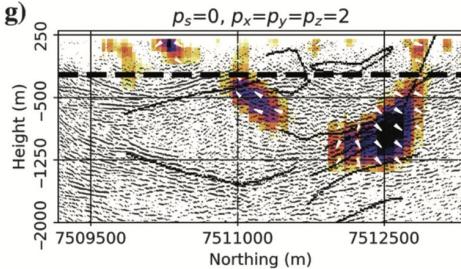
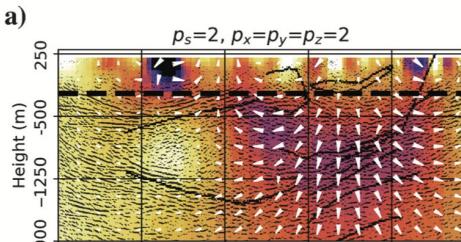
broadens impact

re-use and extension: sparse norms

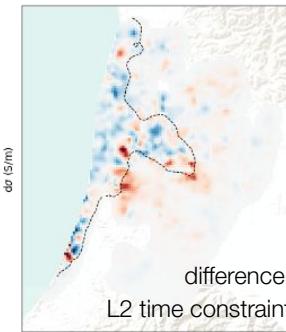
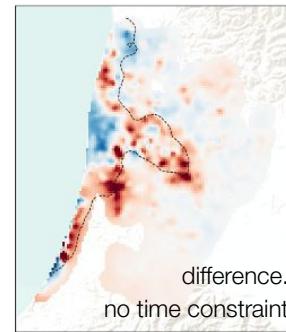
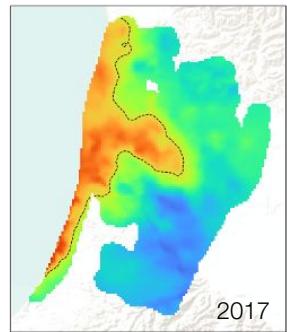
developed in potential fields

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

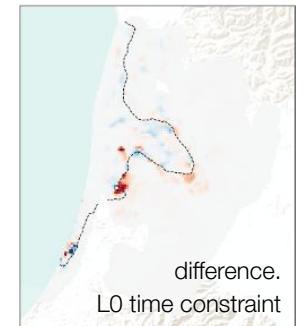
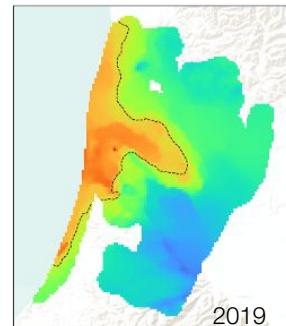
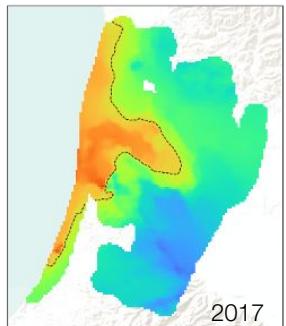
adapted to time-lapse AEM



(Fournier et al.
2019)



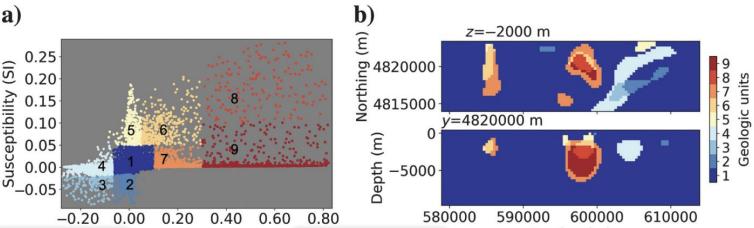
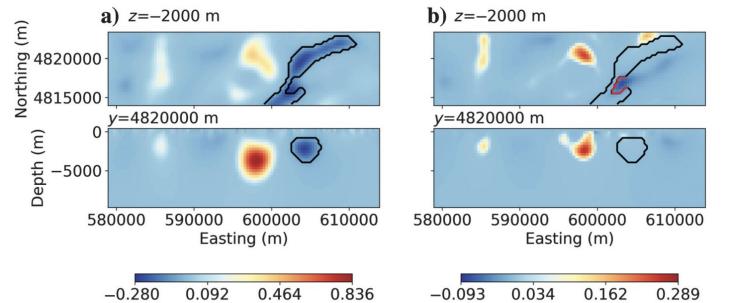
(Kang & Knight,
2022)



combining methods: joint inversions

$\phi_{\text{data}} = \phi_{\text{grav}} + \phi_{\text{mag}}$ # one earth?

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

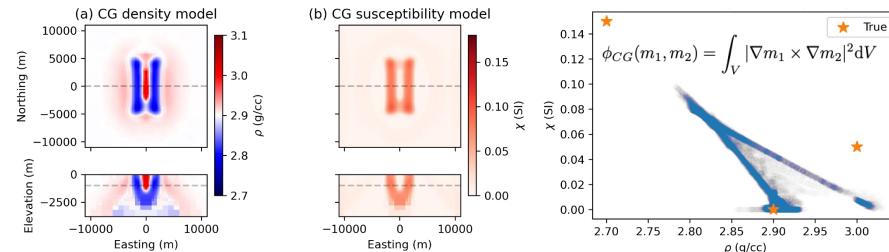


J. Sun

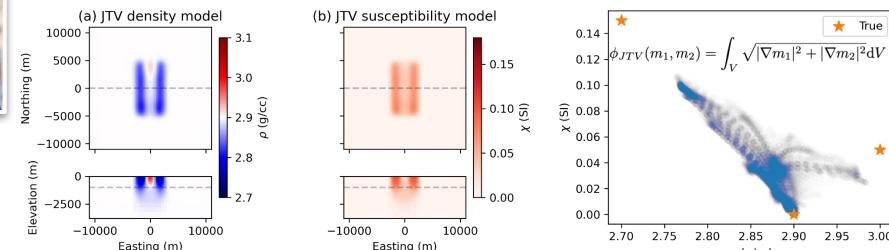
X. Wei

Joint inversions for carbon mineralization

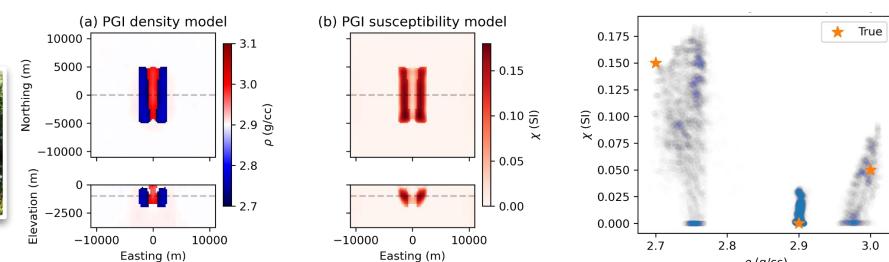
Cross Gradient



Joint total variation

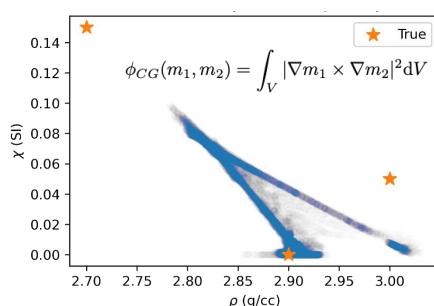
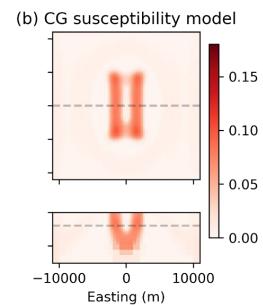
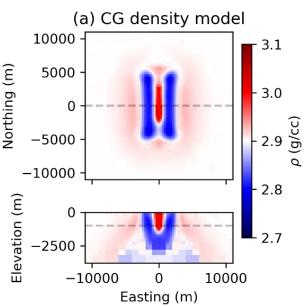


Petrophysically and Geologically guided Inversion (PGI)

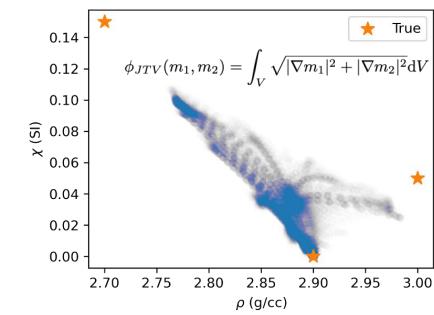
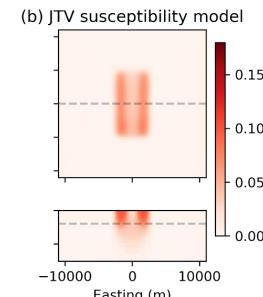
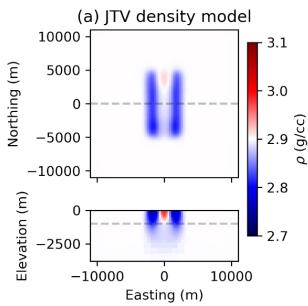


T. Astic

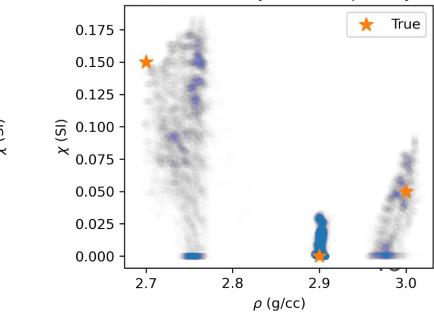
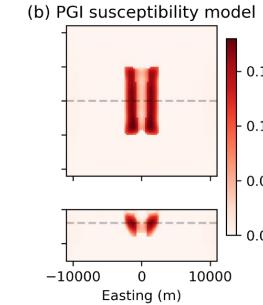
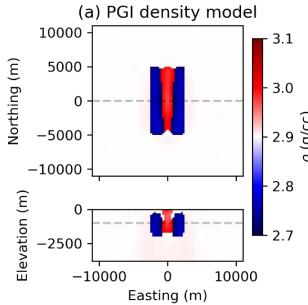
Cross Gradient



Joint total variation



Petrophysically and Geologically guided Inversion (PGI)



parallelization: an industry-academic collaboration

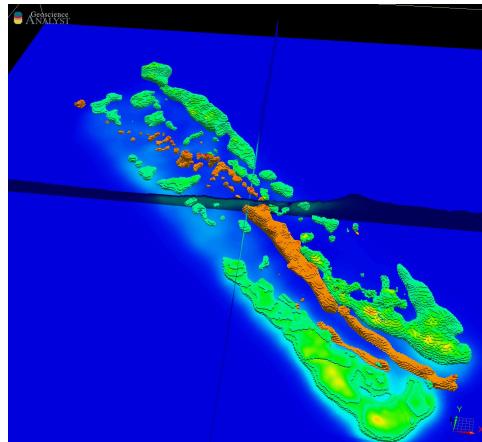
parallelization motivated initially by large scale 3D DCIP

use of dask for parallelization (on any architecture)

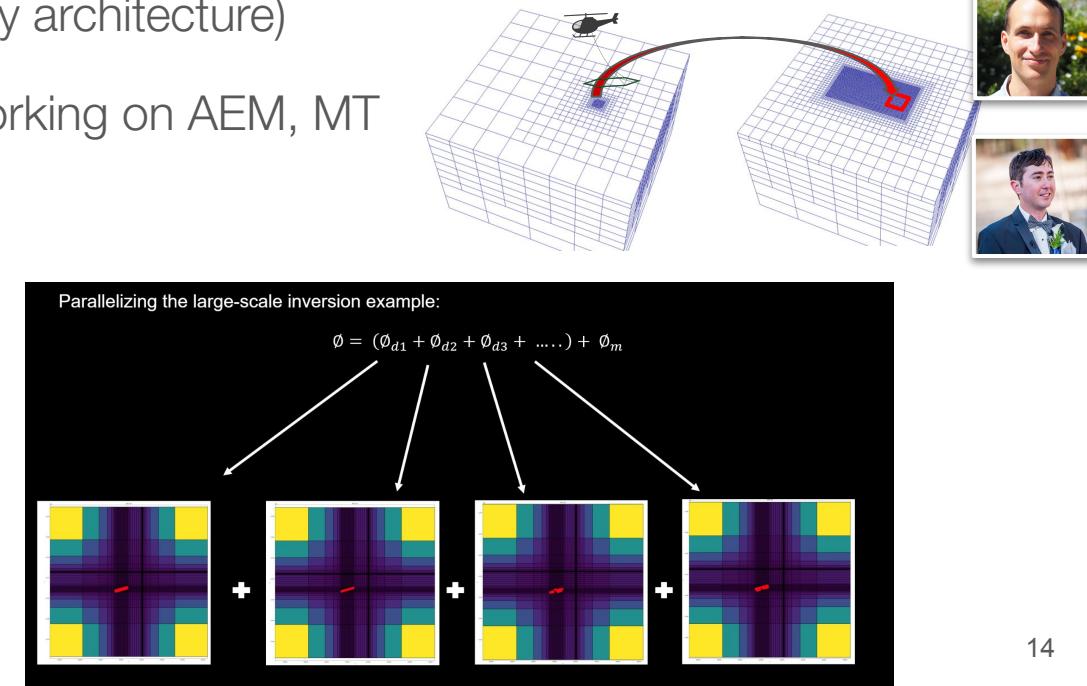
now adapted for Mag, Grav, and working on AEM, MT



J. Kuttai



17.1 million cells 783 injections

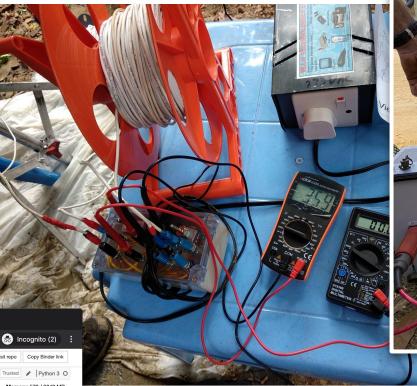
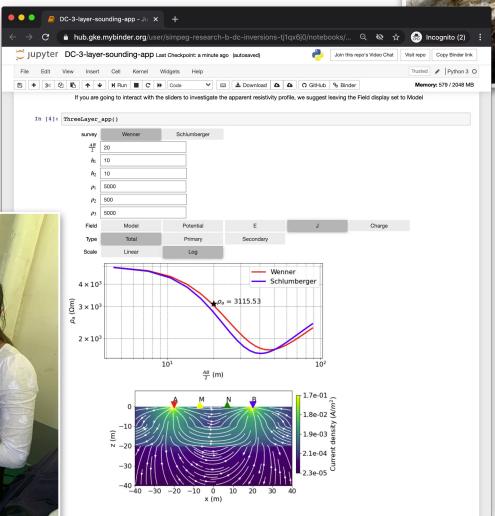
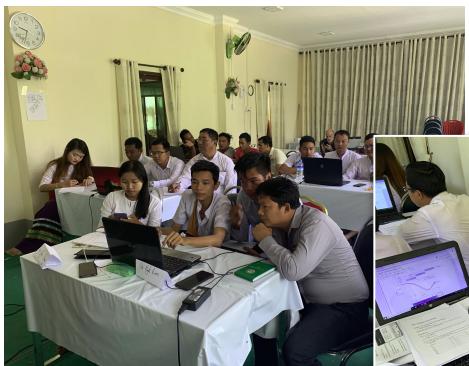


broader impact: educational & humanitarian

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:

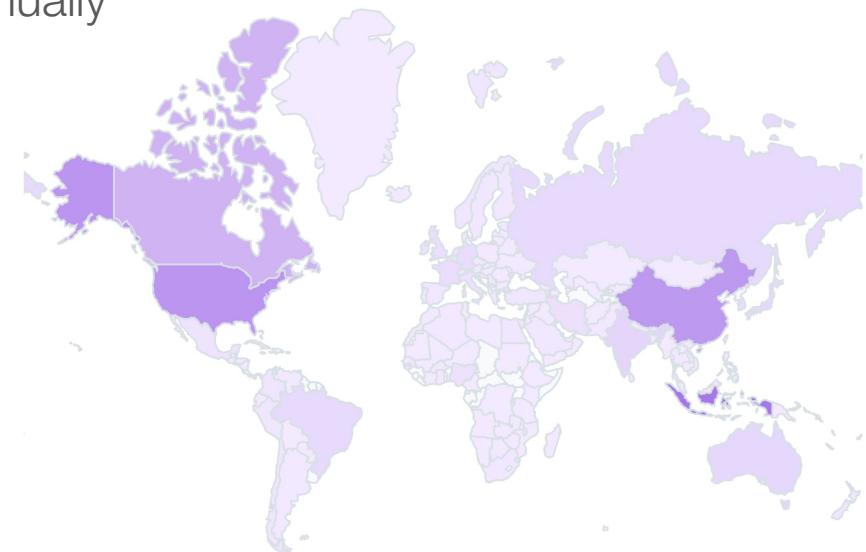
15000+ visitors to the simpeg website annually

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

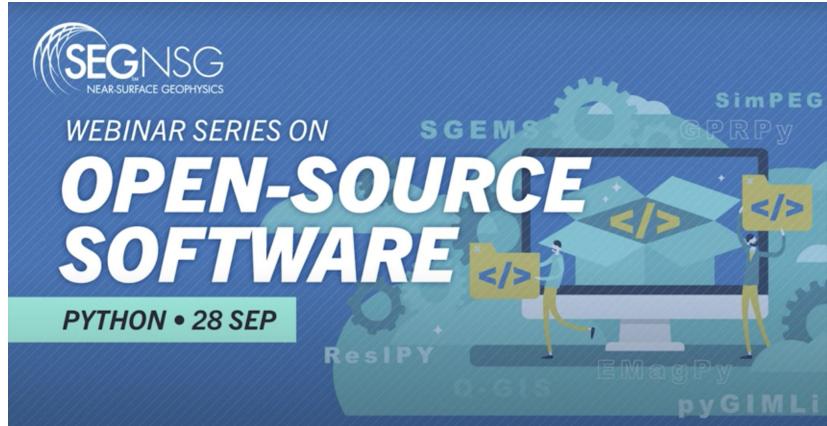
mechanisms for academic credit

- role of professional societies
- doi's for software



new funding models

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



Peer review of Python software to support open science



Python Package Peer Review



Community Partnerships



Simplifying Packaging



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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Preprint Policy

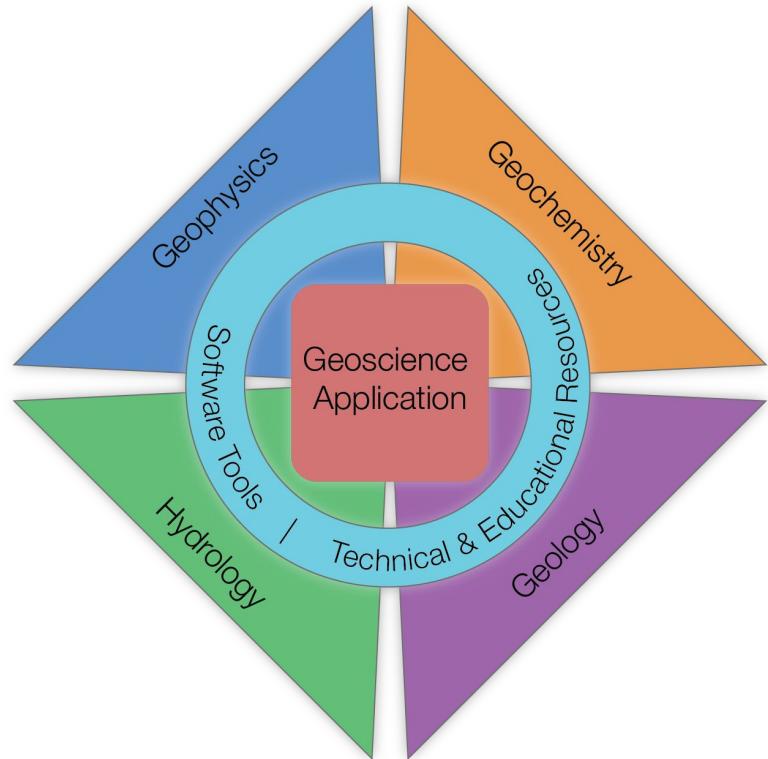
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geophysics and multidisciplinary problems



- 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

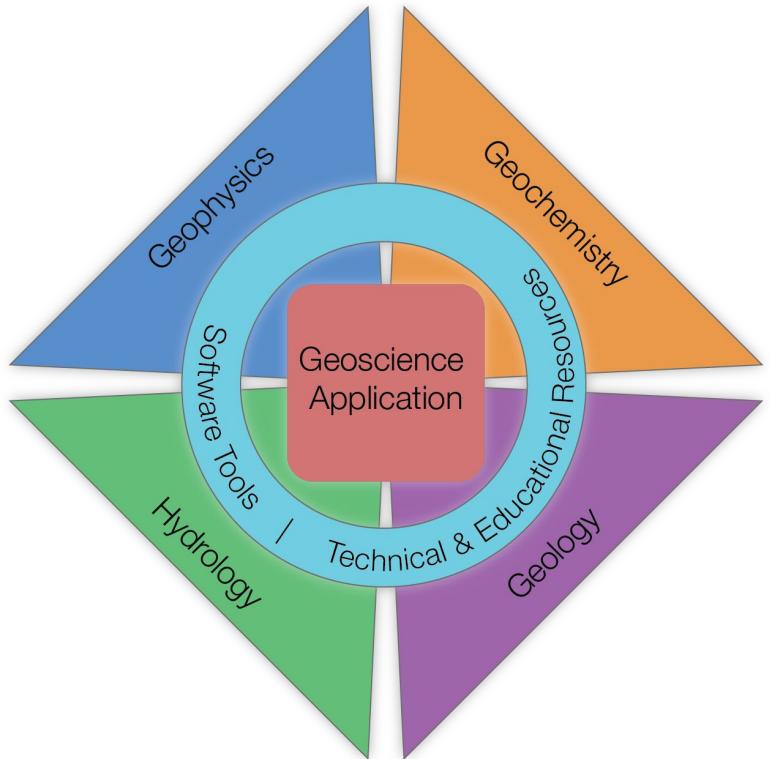


accelerates re-use and extension of ideas

enables combination of methods

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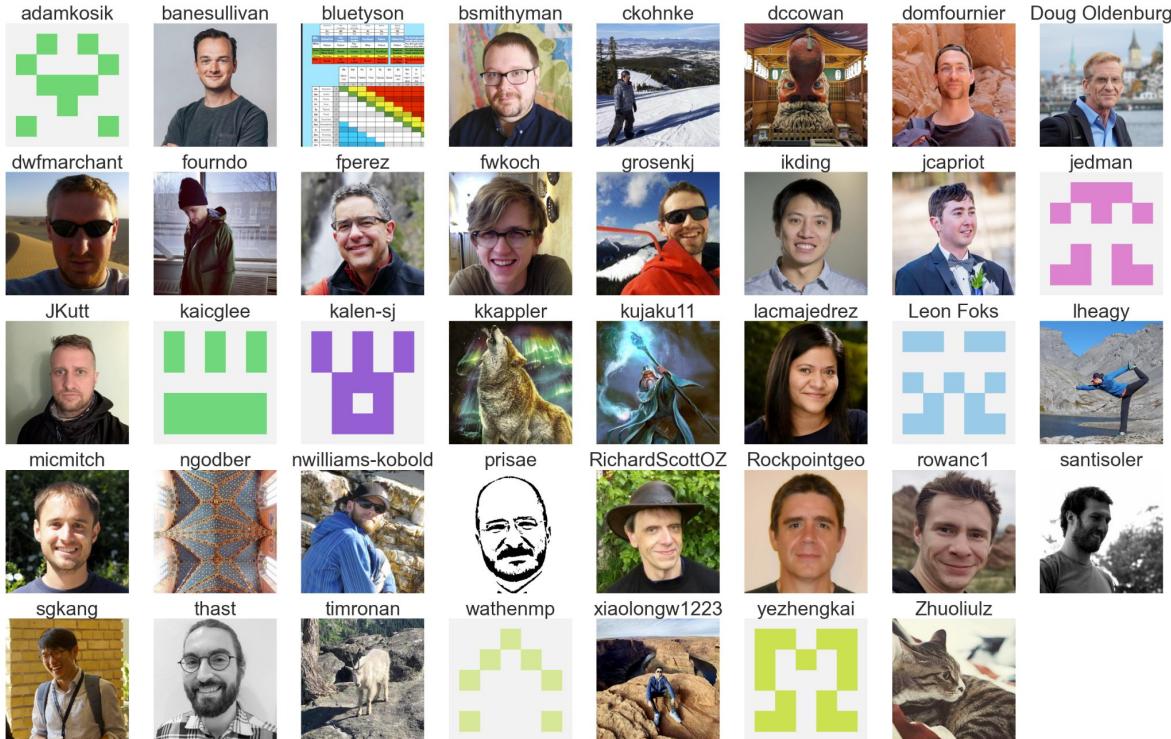
broadens impact



thank you & questions

email: lheagy@eoas.ubc.ca

slides: bit.ly/heagy-2023-image



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