Durham University

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InLab

Espresso

Earth Science Problems for the Evaluation of Strategies, Solvers and Optimizers

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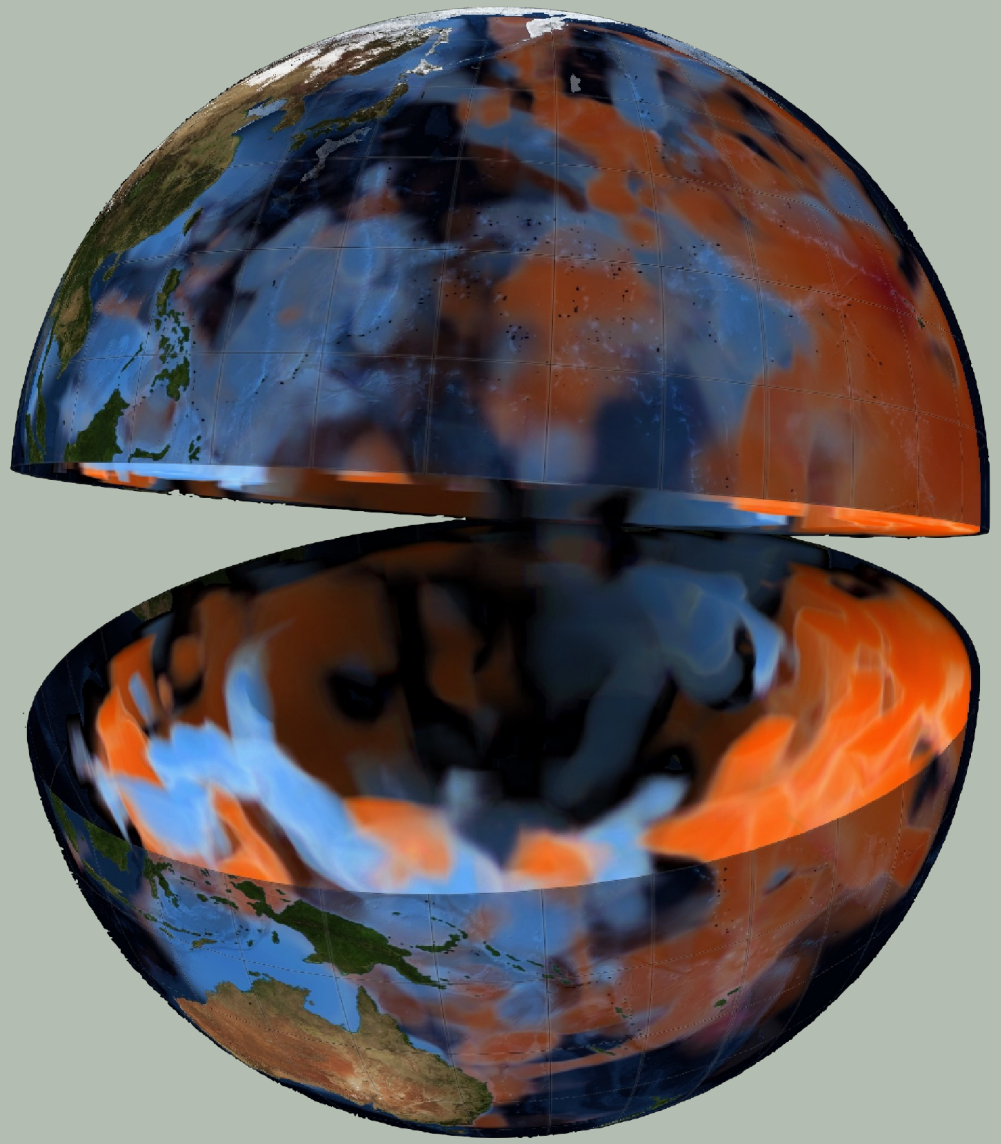


Geoscience relies on inference techniques

- Parameter estimation
- Imaging & inversion algorithms
- Bayesian methods
- Machine learning

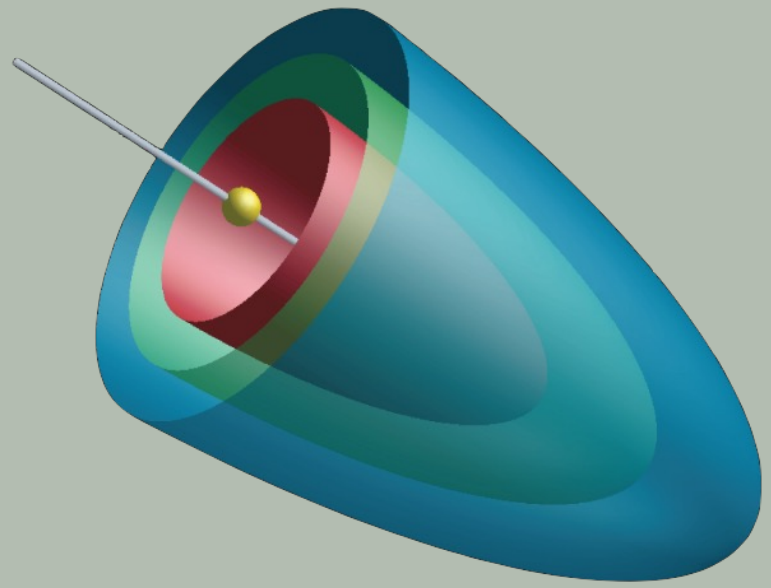
Geoscience drives inference innovation

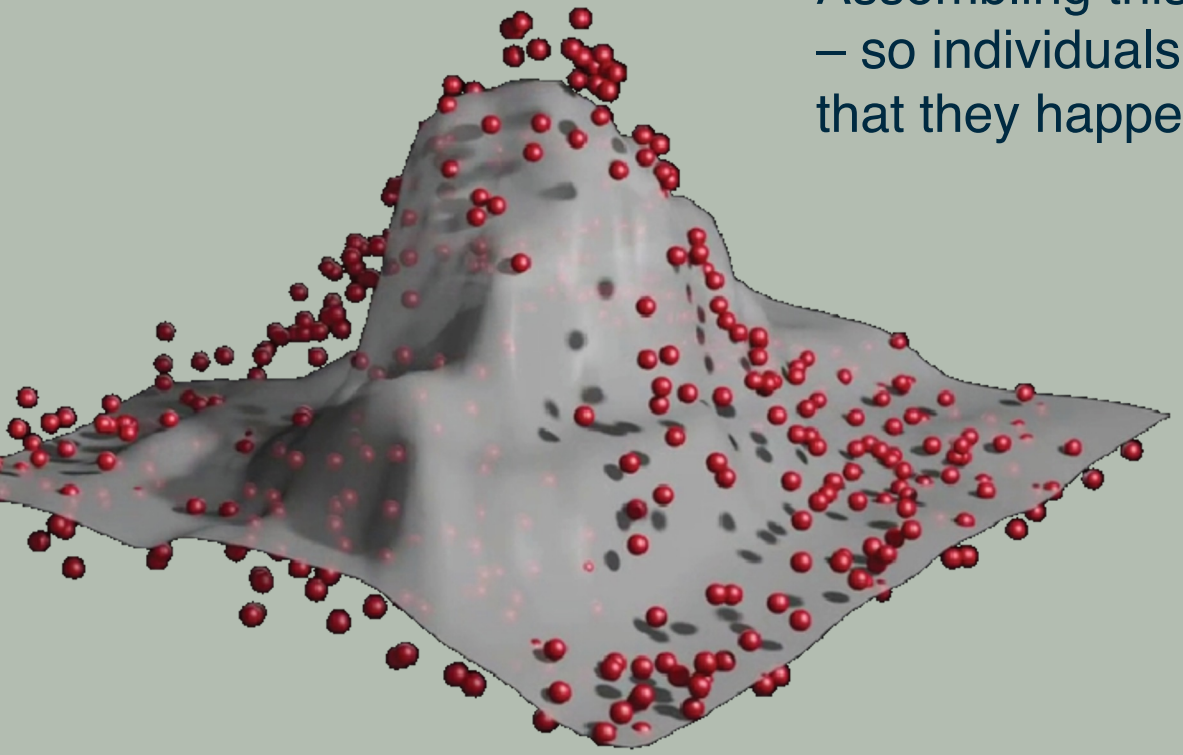
- Data: big, small, uncertain, uneven
- Computational complexity
- Interpretation & propagation of uncertainty
- Practicalities: real-time, autonomous, low-power…

Valentine & Sambridge, *in press*. Emerging Directions in Geophysical Inversion

Developing & testing new inference strategies requires **exemplar inference problems:**

- Problem definition
- Dataset (QC'd, preprocessed, etc)
- Simulation package (+ appropriate configuration choices, input files, etc)





The challenge:
Assembling this is hard & requires domain knowledge – so individuals tend to rely on a handful of problems that they happen to understand!

The consequences:

- Progress becomes siloed within domains
- Limited range of problem characteristics
- Difficult to compare/benchmark methods

The solution: Espresso!

Earth Science Problems for the Evaluation of Strategies, Solvers and Optimizers

A community-sourced collection of geoscience inversion and inference scenarios

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Small	Examples are chosen to be modest in scale
Quick	Problems are defined and set up by domain-expert contributors
Stimulating	Find opportunities from across the spectrum of geoscience
Not to everyone's taste	We prioritize standardization at the expense of flexibility
A starting point	Identify new directions worth pursuing further
Enjoyed with friends	Build community of inference **users** and inference **developers**
Helps you learn	A resource for use in education

python™

```
from espresso import <NAME> as problem
p = problem()
```

Required:

- Dataset, **d** (QC'd, preprocessed…)
- Model parameterization, **m**
- Forward simulation code, **f(m)**
- Suggested initial/background model, $\mathbf{m_0}$
- Example solution vector, $\mathbf{m_s}$
- Documentation & metadata

```
p.data
p.model_size
p.forward(model)
p.starting_model
p.good_model
```

Optional:

- Data covariance matrix, $\mathbf{C_d}$

- Routine to compute Jacobian, $\partial\mathbf{f}/\partial\mathbf{m}$
- Misfit and/or Likelihood functions

- Prior distribution on model parameters
- Tools to visualize models and/or data

```
p.covariance_matrix
p.inverse_covariance_matrix
p.jacobian(model)
p.misfit(d1, d2)
p.log_likelihood(d1, d2)
p.log_prior(model)
p.plot_model(model)
p.plot_data(d1[, d2])
```

Select a different problem here - everything else stays the same!

```
from espresso import <EspressoProblem> as problem

p = problem(example_number = 1)

niterations = 100
eps = 0.01

model = p.starting_model
for i in range(niterations):
    predictions, G = p.forward(model, with_jacobian = True)
    residuals = p.data - predictions
    model -= eps * G.T.dot(residuals)
p.plot_model(model)
```

Capacity for multiple examples within a single problem - showcase different datasets, parameterizations, etc.

Infrastructure:
The Espresso Machine

github.com/inlab-geo/espresso

CI/CD workflow checks
& builds automagically

```
pip install geo-espresso
```

```
from espresso import Problem1 as problem
```

```
contrib/
  Problem 1/
    Data/
      example1.dat
      example2.dat
    __init__.py
    my_code.py
    my_library.py
    README.md
    LICENCE
  Problem 2/
  ...
```

Handle system-dependent file paths
(ToDo: lazy file downloads)

Integrate into documentation:
https://geo-espresso.readthedocs.io

Espresso: Earth Science Problems for the Evaluation of Strategies, Solvers and Optimizers

Currently 8 exemplars:

- 1D regression
- 2D X-ray imaging
- Geophysics
  - Gravity modelling
  - Magnetotellurics
  - Receiver functions
  - Travel-time seismology
- Hydrology
  - Aquifer slug test
  - Aquifer pumping test

More coming soon!

With thanks to early contributors: Hannes Hollmann, Nick Rawlinson, Hoël Seillé & Chris Turnadge

How you can help:

- Try it out
- Give us feedback on the concept/design
  - Missing functionality?
- Contribute an example or two
  - Get in touch if you need support!
- Tell your friends!

Install: `pip install geo-espresso`
Info: `geo-espresso.readthedocs.io`
GitHub: `inlab-geo/espresso`

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