Towards Combining Numerical and Symbolic Computing in Python

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Goal: Software toolbox to build and run joint inversions
First Steps: Symbolic generation and manipulation of misfit functions with linking to numerical solution techniques
Case Study: Minimization problems constraint by a partial differential equation (PDE)

Generic Inversion Problem

$$\min_{u,r} \int_\Omega H\left(u, u_{,i}, r, r_{,i}\right) dx$$

u solution for parameter *r*:

$$-X_{i,i} + Y = 0$$
$$X, Y = f\left(u, u_{,i}, r\right)$$

Variation and Linearization

for $\int_\Omega \overline{H}\,(U) dx$

with $U = (r, u, \lambda)$

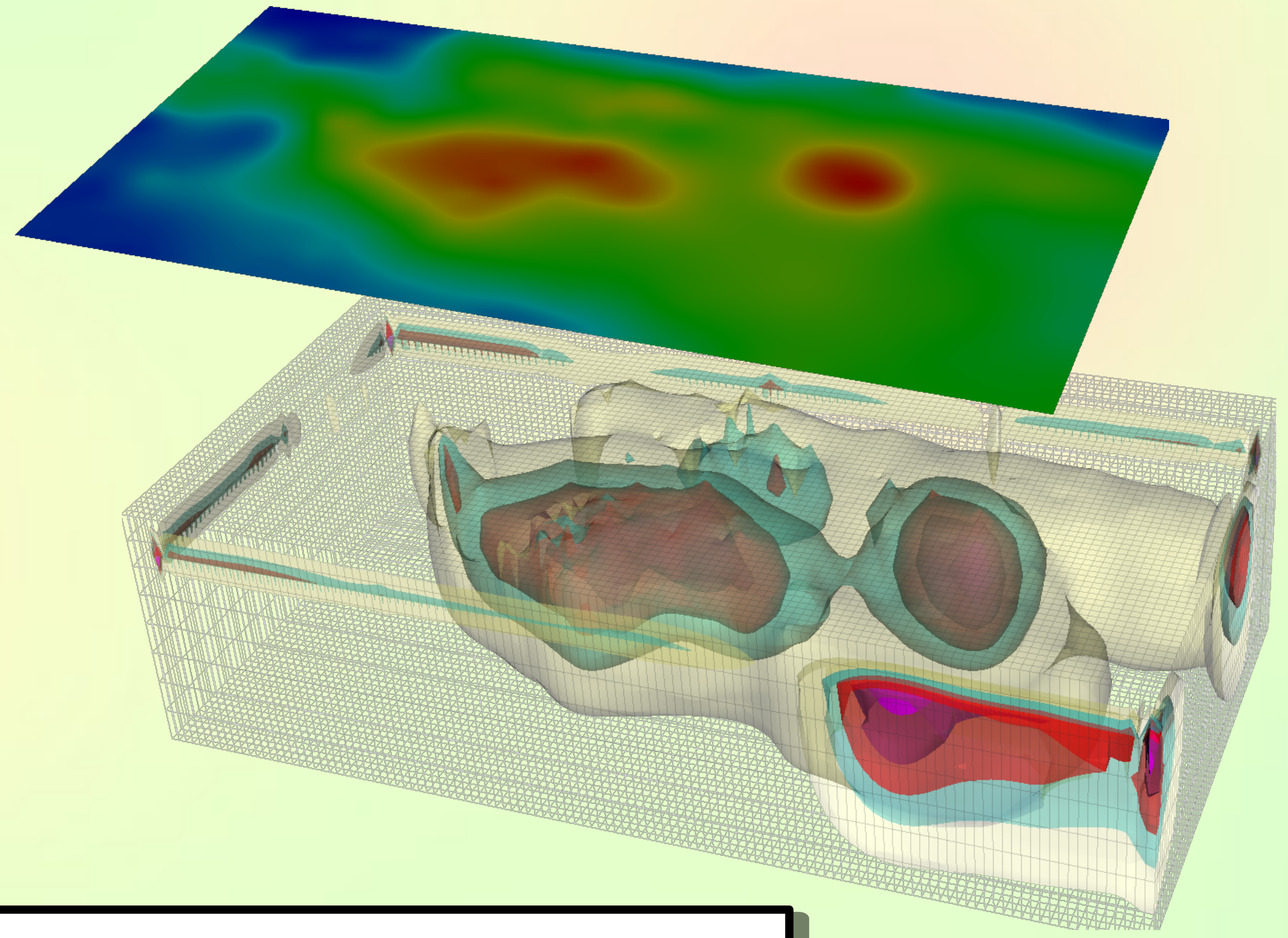
$$\overline{H} = H + \lambda_{,i} X_i + \lambda Y$$

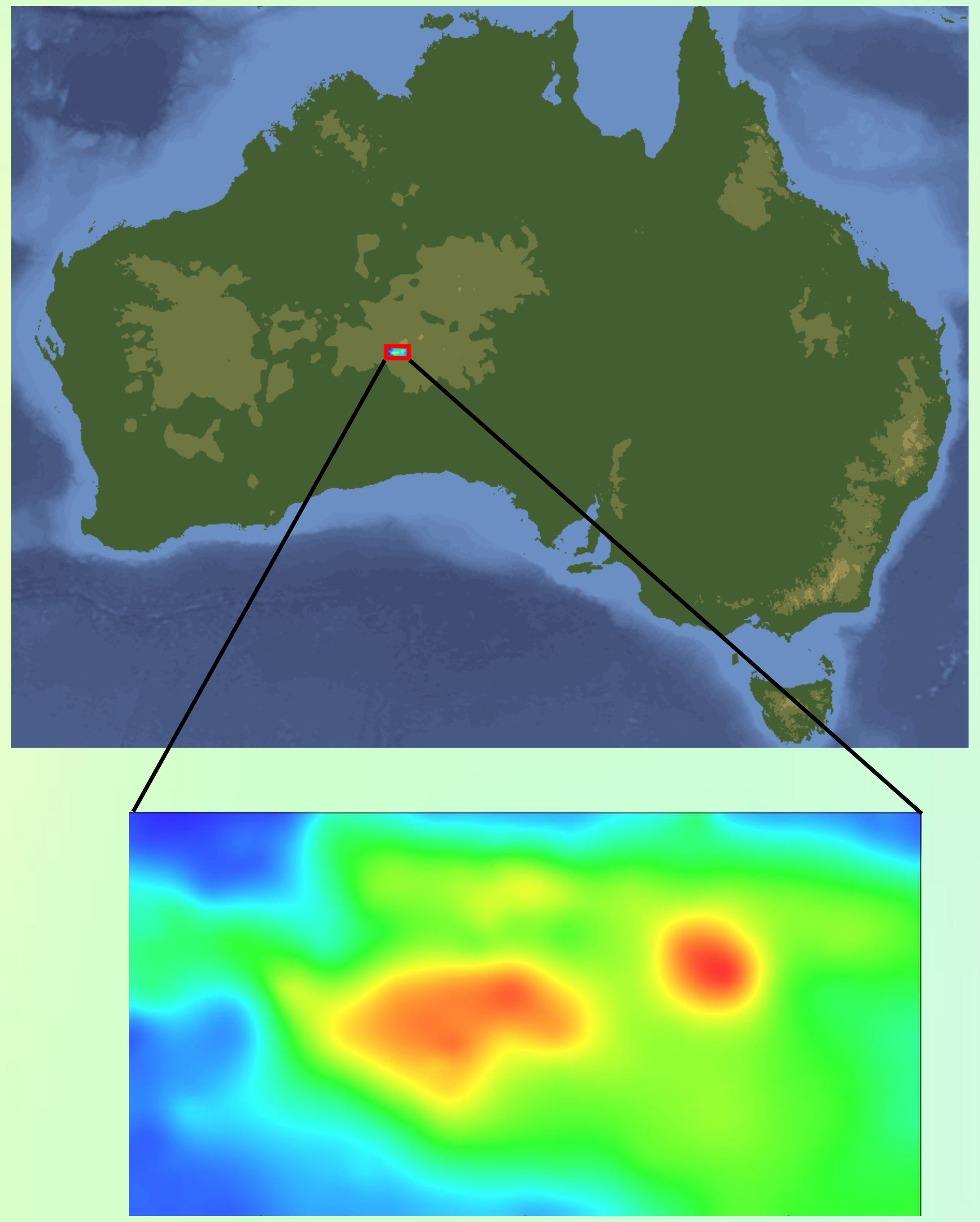
System of linear PDEs for *U*

$$-\left(\frac{\partial^2 \overline{H}}{\partial u_{i,j} \partial u_{k,l}} u_{k,l} + \frac{\partial \overline{H}}{\partial u_{i,j}}\right)_{,j} + \frac{\partial \overline{H}}{\partial u_i \partial u_k} u_k + \frac{\partial \overline{H}}{\partial u_i} = 0$$

Gravity Inversion:

$$\min_{\substack{u,r \\ u_{,ii}=4\pi r}} \int_\Omega h \cdot \left(u_{,2} - g\right)^2 + \|r_{,i}\|^a dx$$





```
dom=Brick(...) # generate FEM mesh
r,u=symbols("r,u")
g=Scalar(..., dom)  # gravity data
v=VariationalProblem(dom, u, r)
v.setValues(X=grad(u), \
    Y=2*pi*r, \
    H=h*(grad(u)[2]-g)**2 \
      +length(grad(r))**a)
r, u = v.getSolution()
```

- Symbolic generation of linear PDE for escript (with sympy)
- Substitute symbols → numerical representation

Numerical solution of linear PDEs using escript

- Finite Element Method
- Performs evaluation of PDE coefficients
- C/C++
- Python interface
- https://launchpad.net/escript-finley

returns numerical representation of solution *u* and parameter *r*

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