Escript: Open Source Environment For Solving Large-Scale Geophysical Joint Inversion Problems in Python

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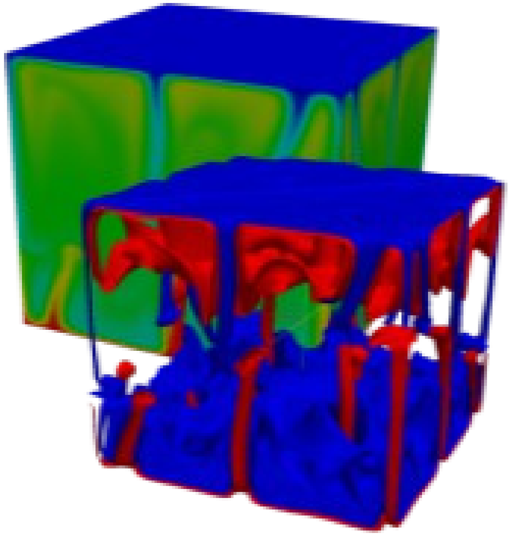
escript

- Environment for mathematical modelling with partial differential equations (PDEs)
  - Multi-physics modelling
  - python interface
  - uses PDE terminology
  - 2D+3D FEM
  - MPI+OpenMP



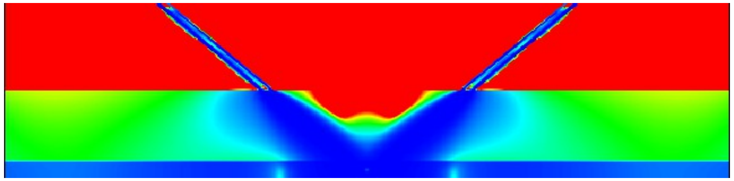
see https://launchpad.net/escript-finley

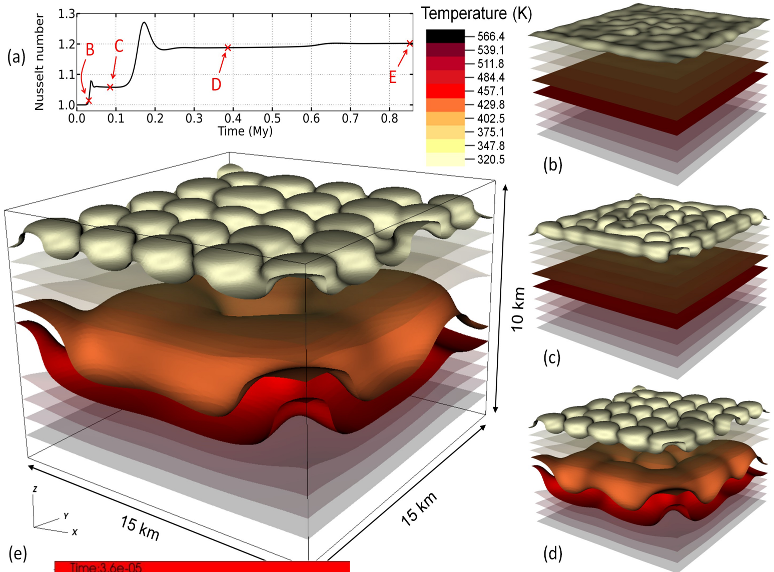
Escript status

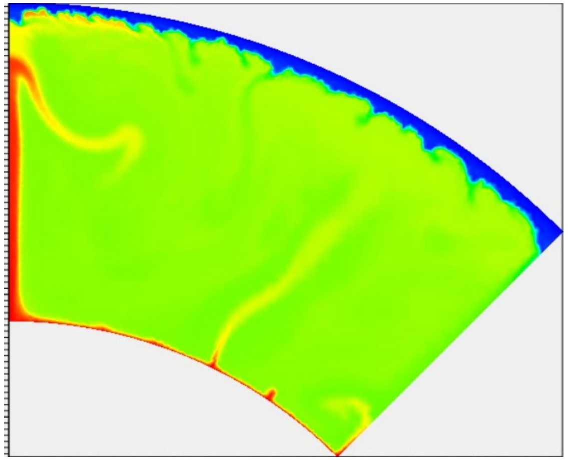
- Since 2003 with about two software engineers at any time
  - AuScope NCRIS, CRIS, NCRIS2
  - AGOS EIF
  - Total Funding $A ~ 2.6 Million (until July'15)
- Open Source under OSF 3.0
- Using best best practice
  - SVN
  - Nightly testing
    - >60000 functional tests
    - On ~10 platforms
  - Source and binary distribution via https://launchpad.net/escript-finley
  - Bug tracking

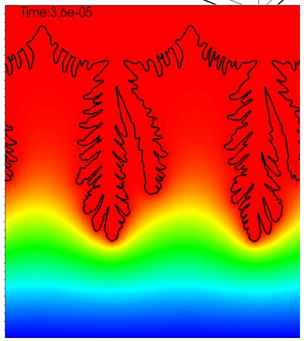
escript applications

- Geophysical inversion
- Mantel Convection
- Pores Media Flow
- Earthquakes
- Reactive Transport
- Volcanoes
- Tsunamis









escript.LinearPDE

Interface to a general linear PDE in variational form:

$$\text{find } u_k : \Omega \rightarrow \mathbb{R},\ u_k = r_k \text{ where } q_k > 0$$

$$\text{for all } v_i : \Omega \rightarrow \mathbb{R},\ v_i = 0 \text{ where } q_i > 0$$

$$\int_\Omega A_{ijkl} v_{i,j} u_{k,l} + B_{ijk} v_{i,j} u_k + C_{ikl} v_i u_{k,l} + D_{ik} v_i u_k \, dx$$

$$= \int_\Omega X_{ij} v_{i,j} + Y_i v_i \, dx$$

with PDE coefficients A_{ijkl}, B_{ijk}, C_{ikl}, D_{ik}, X_{ij}, Y_i, q_k, r_k

Example

Gravitational field anomaly g_i due to density variation ρ

$$-u_{,ii}=4\pi\cdot\rho \qquad -\Delta u=4\pi\cdot\rho$$

$$g_i=-u_{,i} \qquad \boldsymbol{g}=-\nabla u$$

Example (cont.)

Variational Formulation of the PDE:

$$\text{for all } v:\Omega \rightarrow \mathbb{R}$$
$$\int_{\Omega} \underbrace{\delta_{jl}}_{A_{jl}} v_{,j} u_{,l} \, dx = \int_{\Omega} \underbrace{4\pi \cdot \rho}_{Y} \cdot v \, dx$$

$$\text{for all } v:\Omega \rightarrow \mathbb{R}$$
$$\int_{\Omega} \nabla^t v \nabla u \, dx = \int_{\Omega} 4\pi \cdot \rho \cdot v \, dx$$

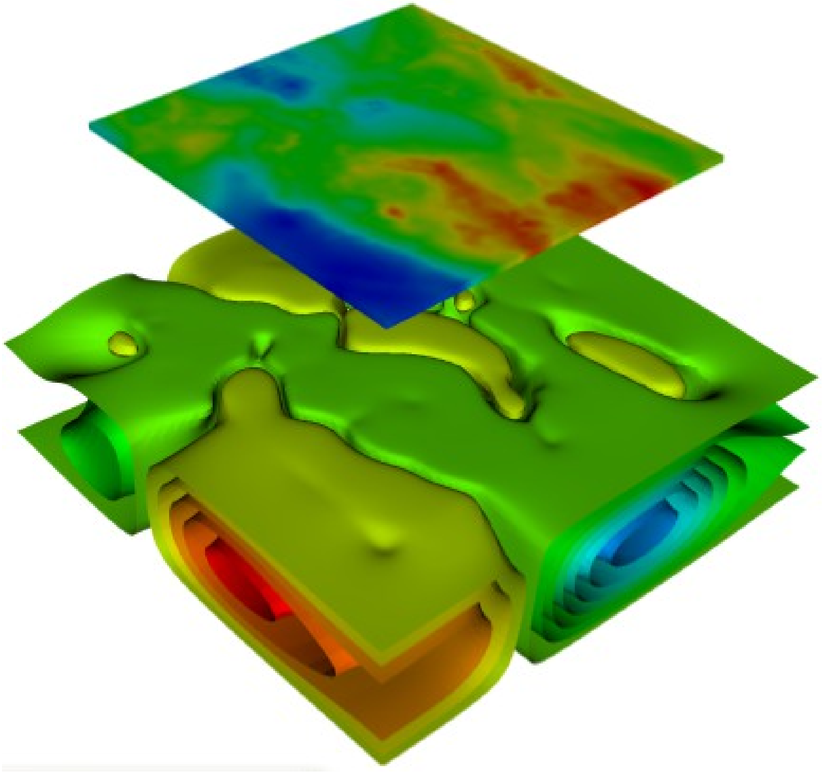
Implementation in python

```
from esys.escript import *
import esys.escript.unitSI as U
rho=200*U.kg/U.m**3
# 100x100x10km with 200m resolution
domain=Brick(500,500,50,100*U.km,100*U.km,10*U.
# solve the PDE:
myPDE=LinearPDE(domain)
z=domain.getX()[2] # get z coordinates
mypde.setValue(A=kronecker(3), Y=4*pi*rho, \
               q=whereZero(z-sup(z)) # fix potential @ top
u=myPDE.getSolution()
g=-grad(u)
# calculate misfit to vertical gravity data
d=getMyGravityData(...)
D=0.5*integrate((g[2]-d)**2)
```

- constant
- tagging
- PDE solution

Inversion

Recover physical properties in the subsurface from measurements near/above surface.



PDE constraint Optimisation

Find $\underset{\rho}{\arg\min}\, J(\rho) := D(u) + \mu \cdot R(\rho)$

data misfit : $D(u) = \frac{1}{2} \int_{\Omega} (u_{,2} - \hat{g})^2 \, dx$

PDE constraint : $u = Q[\rho]$ defined by
for all $v : \int_{\Omega} v_{,l} u_{,l} \, dx = \int_{\Omega} 4\pi \cdot \rho \cdot v \, dx$

regularization: $R(\rho) = \frac{1}{2} \int_{\Omega} \rho_{,l} \rho_{,l} dx$

escript.downunder

find property functions : $\boldsymbol{m} = (\text{density}, \text{susceptibility}, \ldots)$

cost function $J(\boldsymbol{m}) := R(\boldsymbol{m}) + \sum_f D^f(u^f)$

data misfit for forward model f : $D^f(u^f) = \frac{1}{2} \int_\Omega \left(w_i^f \cdot u_{,i}^f - \hat{g}^f \right)^2$

PDE constraints : $u^f = Q^f[\boldsymbol{m}]$

Regularization Term

$$R(\boldsymbol{m}) = \sum_{k} \int_{\Omega} \mu_k S(m_k) + \sum_{i<k} \int_{\Omega} \mu_{ik} C(m_k, m_i)$$

$$\text{smoothing}: S(m) = \frac{1}{2}\left(w_1 \cdot m_{,l} m_{,l} + w_0 \cdot m^2\right)$$

$$\text{cross-gradient}: C(m,n) = \frac{1}{2}\left(\left(m_{,l} m_{,l}\right) \cdot \left(n_{,l} n_{,l}\right) - \left(m_{,l} \cdot n_{,l}\right)^2\right)$$

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Gradient

find $\boldsymbol{m} : \langle \nabla J(\boldsymbol{m}), \boldsymbol{p} \rangle = 0$ for all increments $\boldsymbol{p}$ to $\boldsymbol{m}$

$$\langle \nabla J(\boldsymbol{m}), \boldsymbol{p} \rangle = \int_{\Omega} X_{ij}\, p_{i,j} + Y_i\, p_i \; dx$$

- with suitable functions X_{ij} and Y_i of $\boldsymbol{m}$
- calculate via superposition
- extra adjoint PDE per forward problem

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Quasi-Newton Method

iteration count $\nu=0$; initial guess $\boldsymbol{m}^{(\mathbf{0})}$

$$\boldsymbol{g}^{(\nu)}=\nabla J\left(\boldsymbol{m}^{(\nu)}\right)$$

find $\boldsymbol{p}^{(\nu)}$ with: for all $\boldsymbol{q}:\left\langle \mathrm{H}^{(\nu)}\boldsymbol{p}^{(\nu)},\boldsymbol{q}\right\rangle=\left\langle \boldsymbol{g}^{(\nu)},\boldsymbol{q}\right\rangle$

$\mathrm{H}^{(\nu)}\approx$ Hessian Operator at $\boldsymbol{m}^{(\nu)}$

$m^{(\nu+1)}=m^{(\nu)}+\alpha\cdot p^{(\nu)}$ with

$\min_{\alpha} J\left(m^{(\nu)}+\alpha\cdot p^{(\nu)}\right)$ via line search

$$\nu\leftarrow\nu+1$$

Hessian Operator

- Ignore forward models
- If no cross gradient term

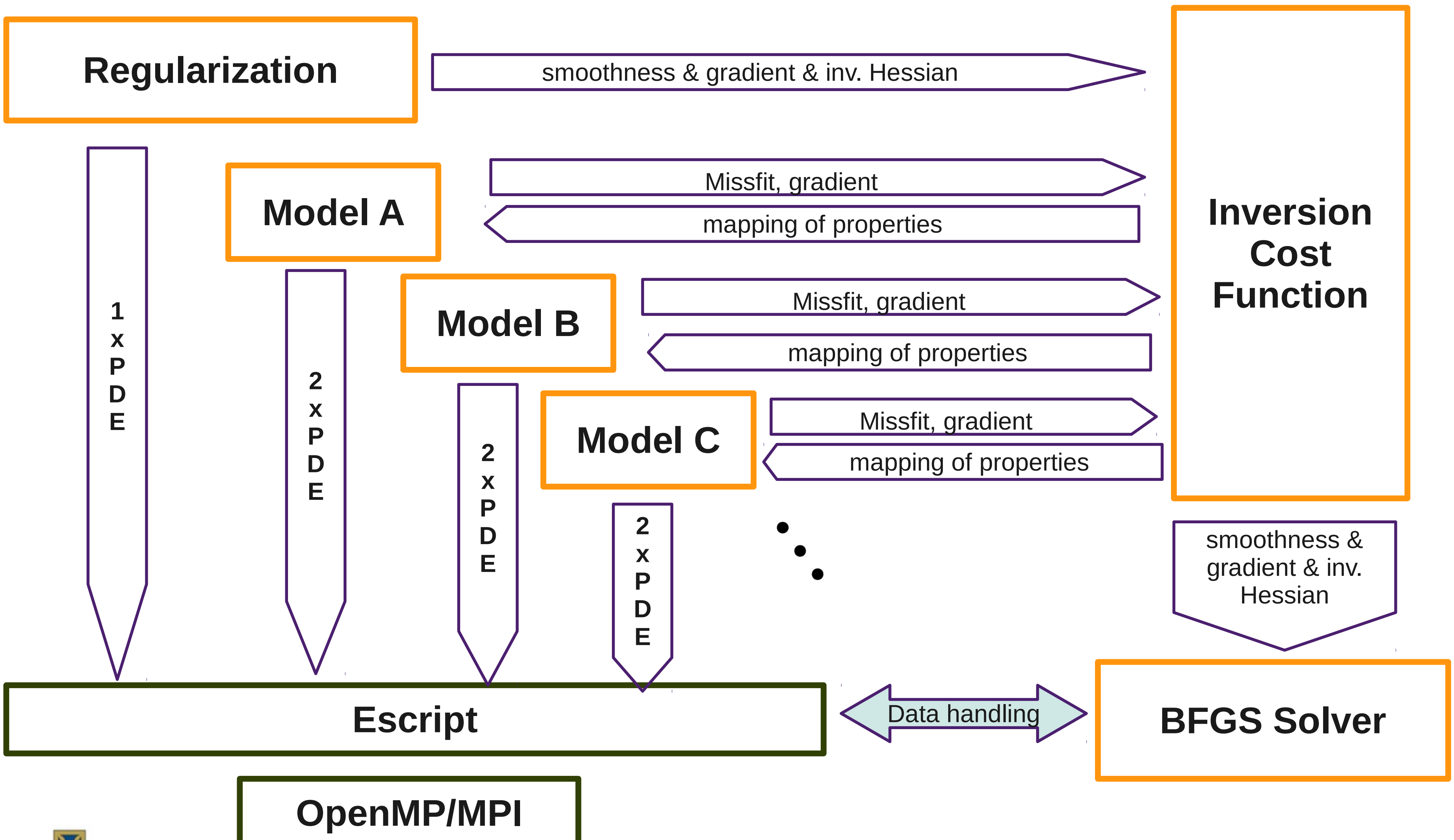
$$\left\langle \mathrm{H}^{(\nu)} \boldsymbol{p}^{(\nu)}, \boldsymbol{q} \right\rangle = \left\langle \boldsymbol{g}^{(\nu)}, \boldsymbol{q} \right\rangle$$

$$\downarrow$$

$$\int_{\Omega} w_{1\mathrm{k}}\, p_{k,l}\, q_{k,l} + w_{0\mathrm{k}} \cdot p_k q_k \; dx = \int_{\Omega} X_{ij}\, q_{i,j} + Y_i q_i \; dx$$

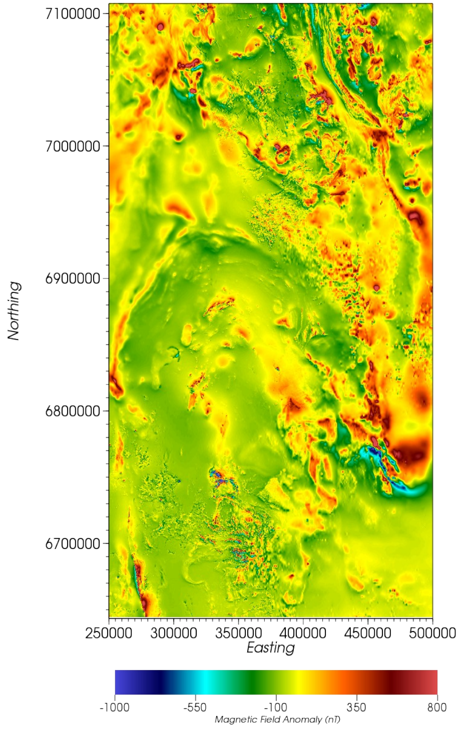
→ PDE solved by escript

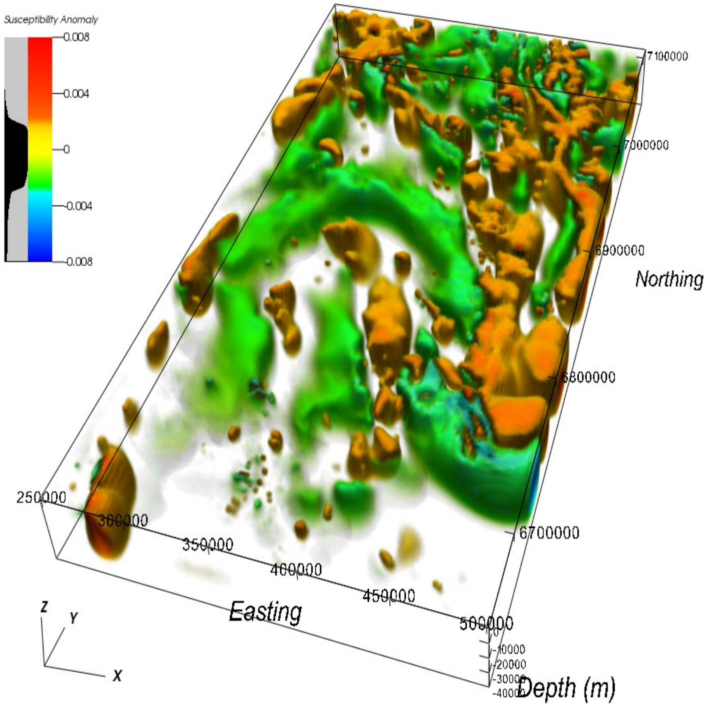
Inversion Framework in Python



Example: Clarence-Moreton Basin

- Magnetic data from vgl.auscope.org.au, resolution <100m
- 500Million cells on 8000 cores in < 1.5 hours





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Summary

- Inversion as PDE constraint optimization
  - "First optimize then discretize"
  - Adaptive meshing
  - Computational scalability
- Escript based inversion framework
- Visit https://launchpad.net/escript-finley