



# The Programming Language Python In Earth System Simulations

L Gross, I Azeezullah, P Mora, E Saez,  
J Smillie, C Wang, and Paul Cochrane

Earth Systems Science Computational Centre, and  
Australian Computational Earth Systems Simulator,  
The University of Queensland, Brisbane, Australia

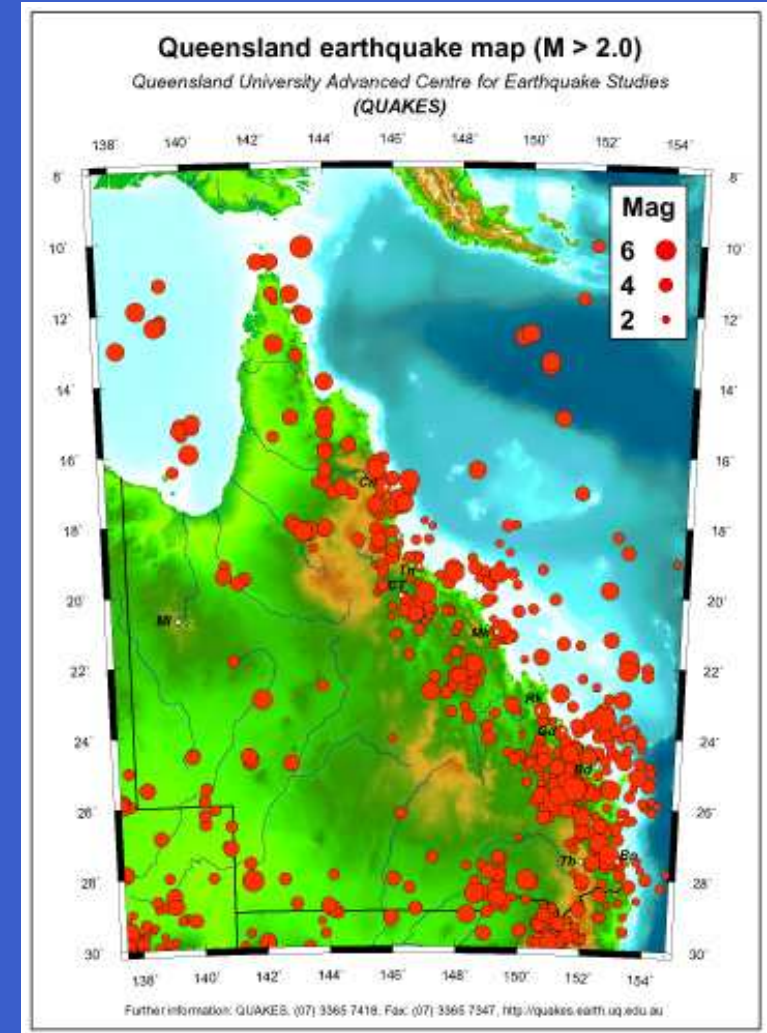


# Fault simulation

- Hazard assessment
  - determine areas of high risk
- Earthquake prediction
  - try to determine “when”
- Typical Fault Model
  - Wave propagation:

$$0 = \rho \frac{\partial u_i^2}{\partial t^2} - \sum_j \frac{\partial \sigma_{ij}}{\partial x_j}$$
$$\sigma_{ij} = \lambda \sum_k \frac{\partial u_k}{\partial x_k} \delta_{ij} + \mu \left( \frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i} \right)$$

- on faults:  $n_j \sigma_{ij} = f_n n_i + f_\tau \tau_i$ ; restoring force:  $f_n = \max(E_n[u]_j n_j, 0)$
- tangential stress:  $f_\tau = \max(E_\tau[u]_i \tau_i, \mu f_n)$

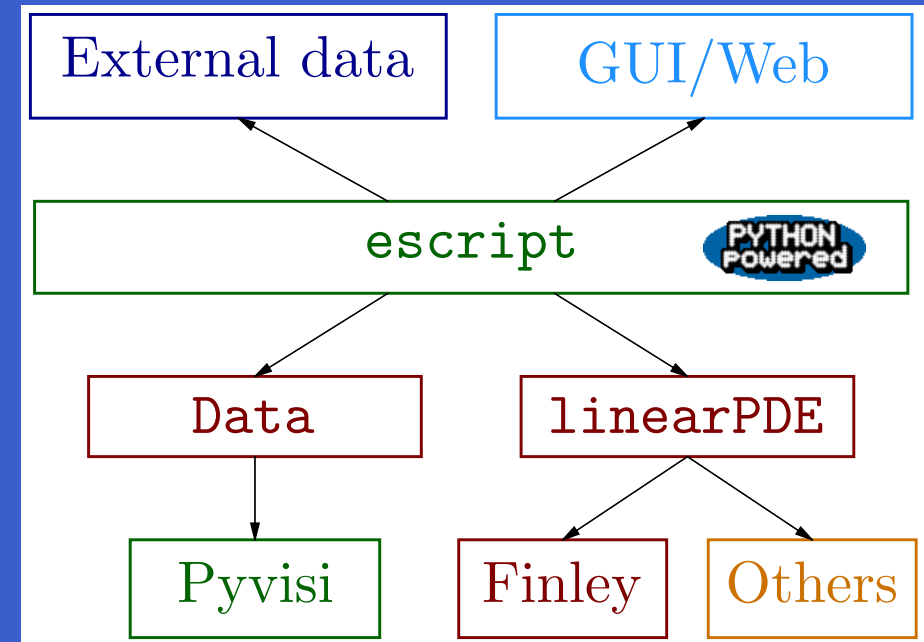


# Simulation Approach

- Simulations scripted with `escript`
  - High-level Python-based modular simulation scripting language
  - Independent of underlying PDE solving software
  - Our simulations use Finley:
    - flexible, high-performance PDE solver for `escript`
- Spatial discretisation
  - Within PDE solving software
    - use the finite element method
- Time discretisation
  - Handled at the `escript` level
    - linear PDE is solved at each step

# escript objects

- `escript.Data`
  - Represents data with spatial distribution
    - stored on sample points
    - tensors up to order 4
- Data manipulation
  - eg: `+`, `-`, `*`, `/`, `cos`, `sin`, `exp`, `sqrt`, ...
  - without spatial dependency
  - data parallel: OpenMP and MPI
- `escript.linearPDE`
  - Interface to a general linear PDE



# escript example

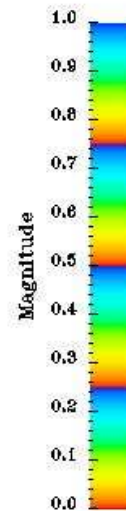
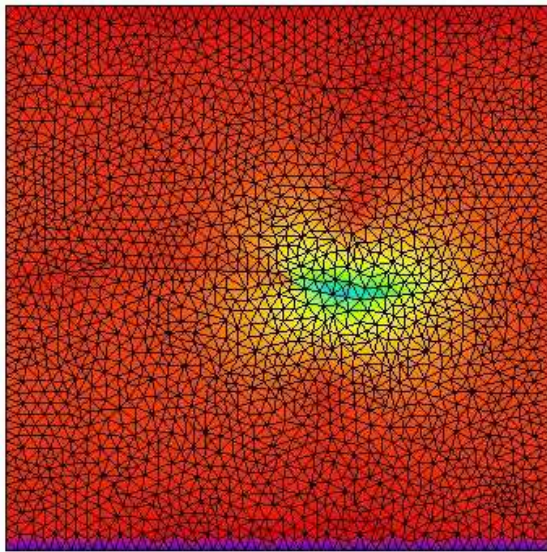
```
from escript import *
myPDE = linearPDE(mydomain)
myPDE.setMatrixType(LUMPED)
while <something true>:
    g = grad(u)
    stress = l*trace(g) + m/2*(g+transpose(g))
    jump = u.interpolate(faultface1) - u.interpolate(faultface0)
    fn = max(En*inner(jump,n), 0)
    ftau = max(Etau*inner(jump,tau), mu*fn)
    myPDE.setCoefficients(X=stress, y_contact=fn*n+ftau*tau)
    # velocity-verlet scheme:
    anew = myPDE.getSolution()
    v += h/2*(a+anew)
    u += h*v + h**2/2*a
    a = anew
```



# Typical simulation results

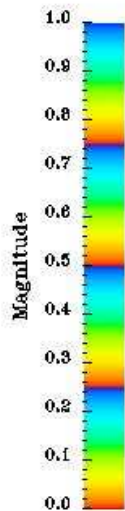
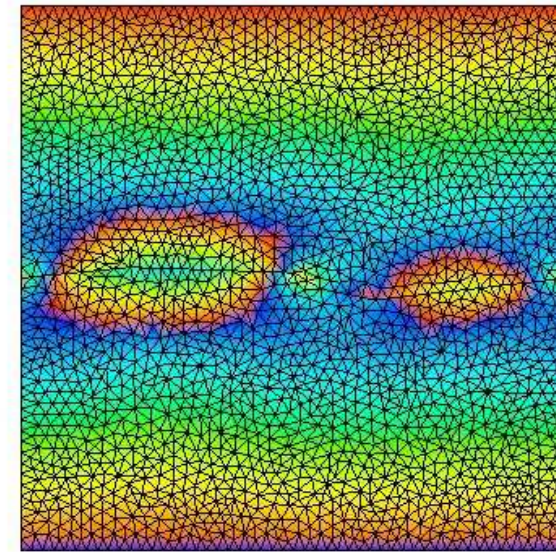
- Courtesy: Estelle Saez, Poster: *A dynamic Finite Element Method for simulating the physics of fault system*. Section: SF09, Thursday morning session.

VELOCITY



Time: 1.000100e-01 [s]

VELOCITY



Time: 2.400000e-01 [s]

- Project to have a consistent interface to many visualisation and rendering backends
- For example:
  - vtk—the visualisation toolkit
  - OpenDX
  - gnuplot
  - povray
  - . . .
- Independent of underlying visualisation software
- Project is in its infancy



# Pyvisi in escript scripts

- Inserting visualisation code into previous example

```

from pyvisi import *
scene = Scene(renderer='vtk')
plot = ContourPlot(scene)
plot.title = "Fault system simulation"
scene.add(plot)
myPDE = linearPDE(mydomain)
while <something true>:
    <set up pde>
    myPDE.setCoefficients(X=stress, y_contact=fn*n+ftau*tau)
    # velocity-verlet scheme:
    anew = myPDE.getSolution()
    plot.setData(anew)
    scene.render()
    u += h*v + h**2/2*a
    v += h/2*(a+anew)
    a = anew

```



# Closing comments

- `escript`
  - High performance, modular scriptable simulation system
  - Rapid development of high-level solution algorithms
    - <http://www.esscc.uq.edu.au/Research/EsriptFinley>
- `Pyvisi`
  - Clean, easy-to-use interface to visualisation packages
  - Project page:
    - <http://pyvisi.sourceforge.net>

# Supporting Institutions

- Australian Commonwealth Government 
- Australian Computational Earth Systems Simulator Major National Research Facility 
- Queensland State Government
  - Smart State Research Facility Fund 
- The University of Queensland 
- SGI 