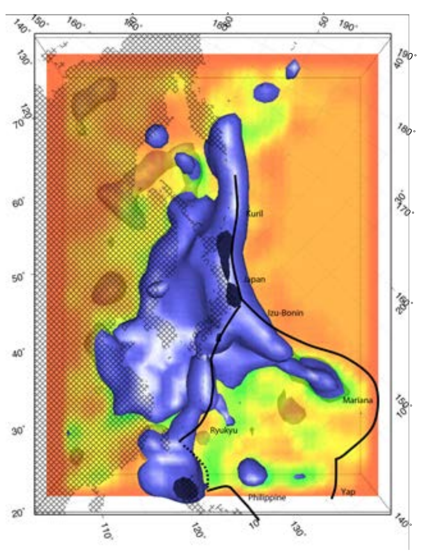
THE UNIVERSITY OF MELBOURNE

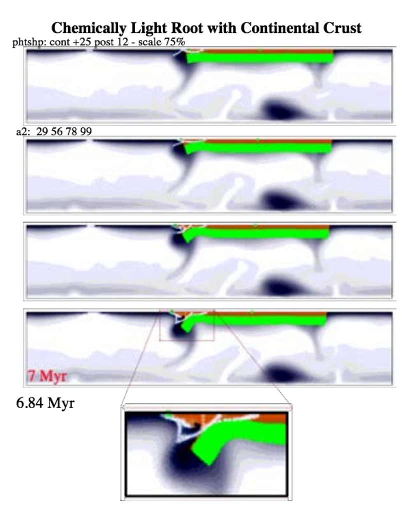
Geodynamic models 20 years — past and future

Louis Moresi, School of Earth Sciences, University of Melbourne

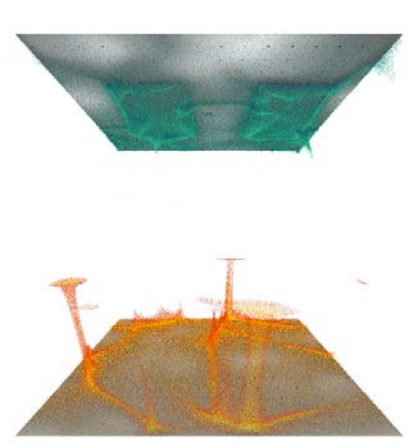
1994



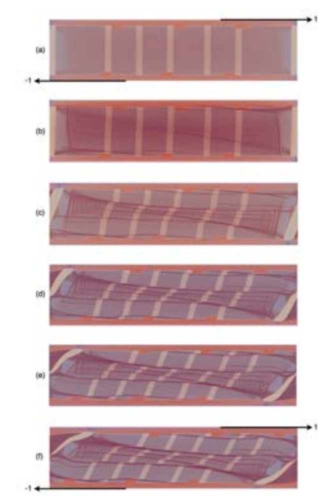
1999



2004



2009



2014

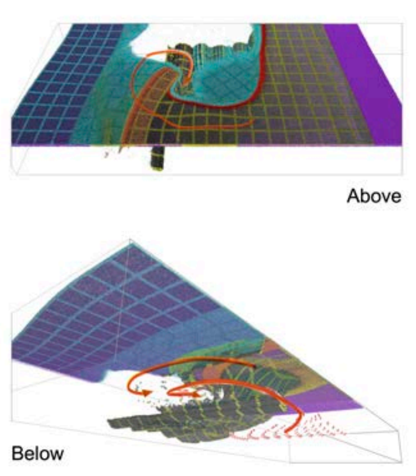
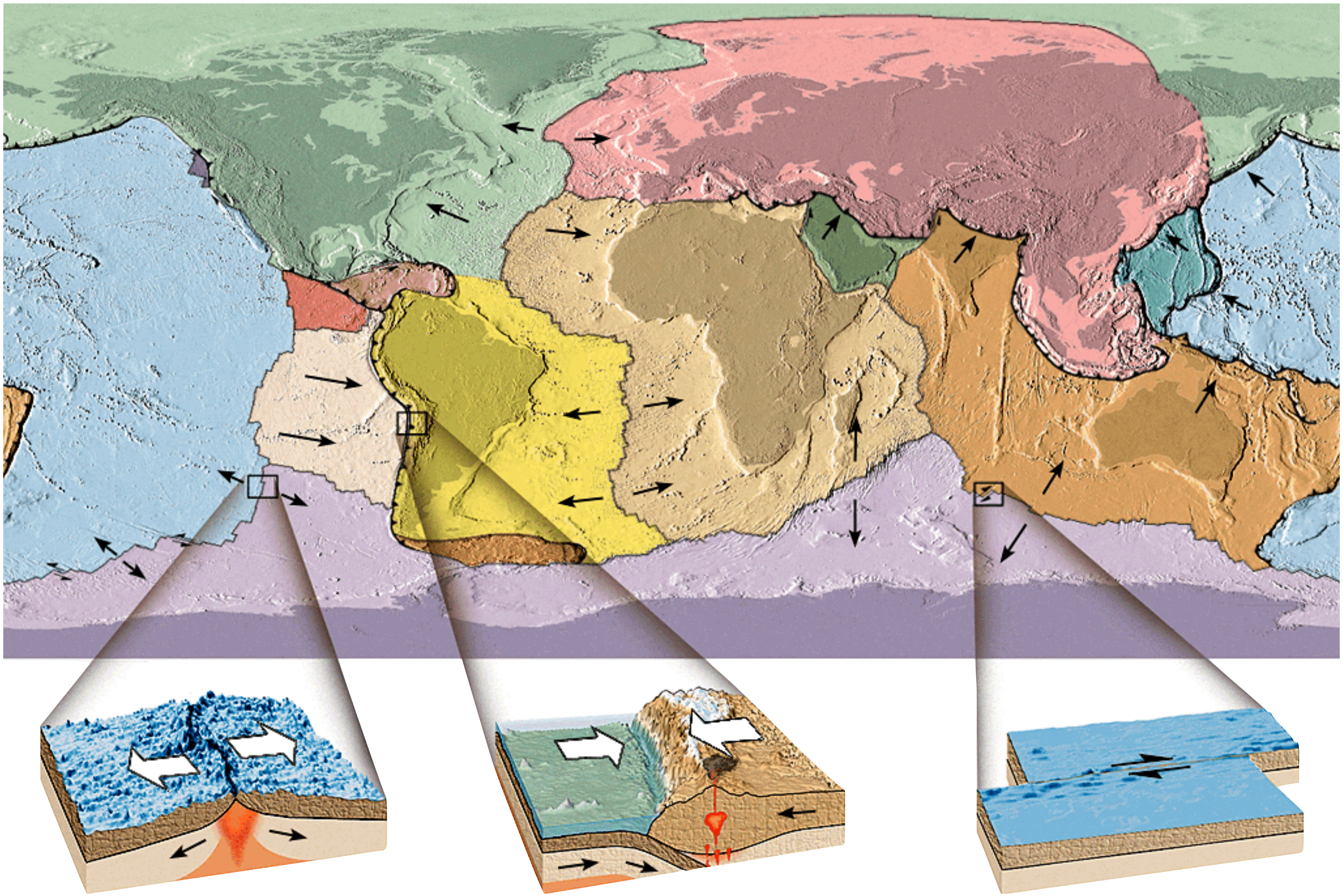
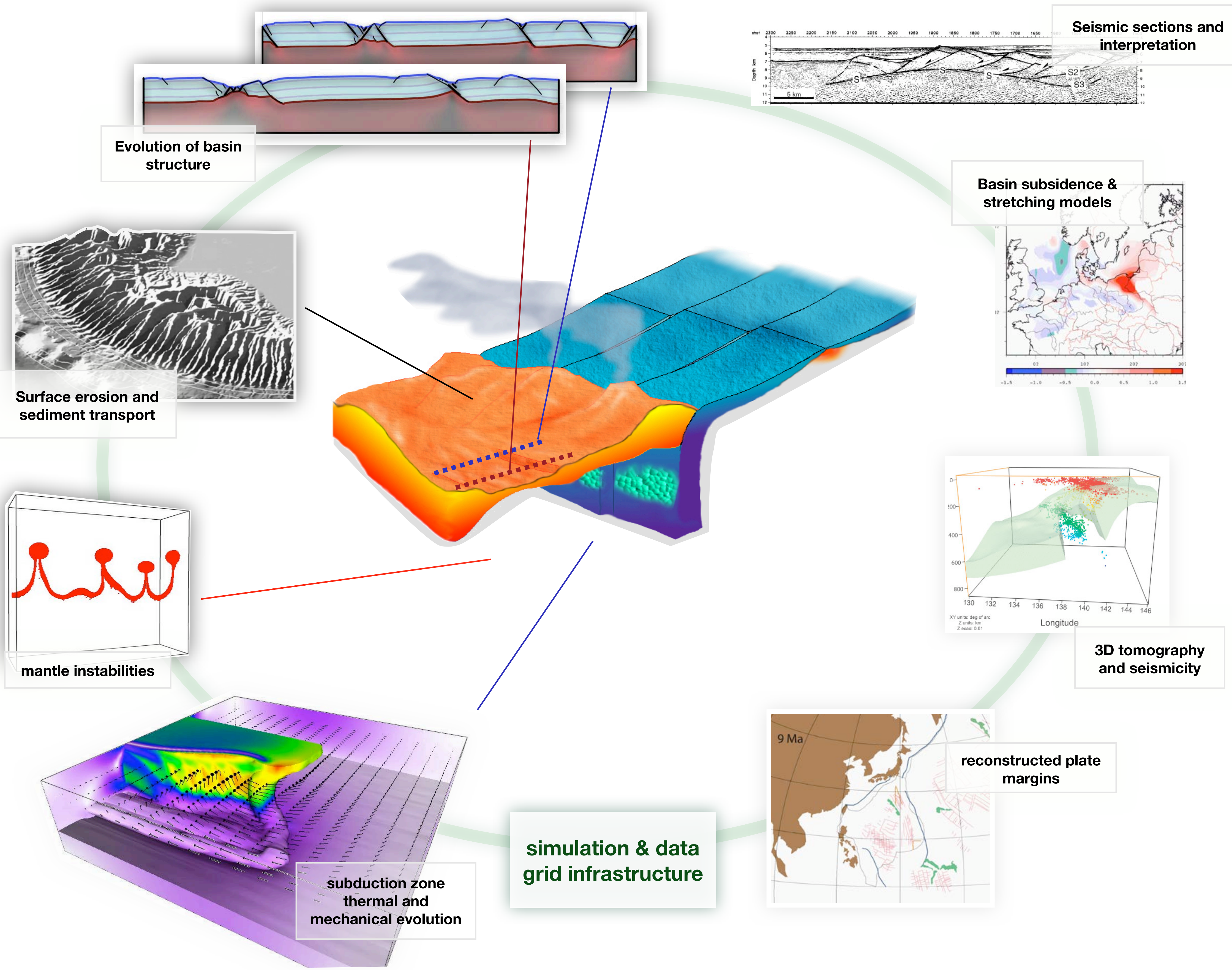


Plate tectonics — a multi-scale problem

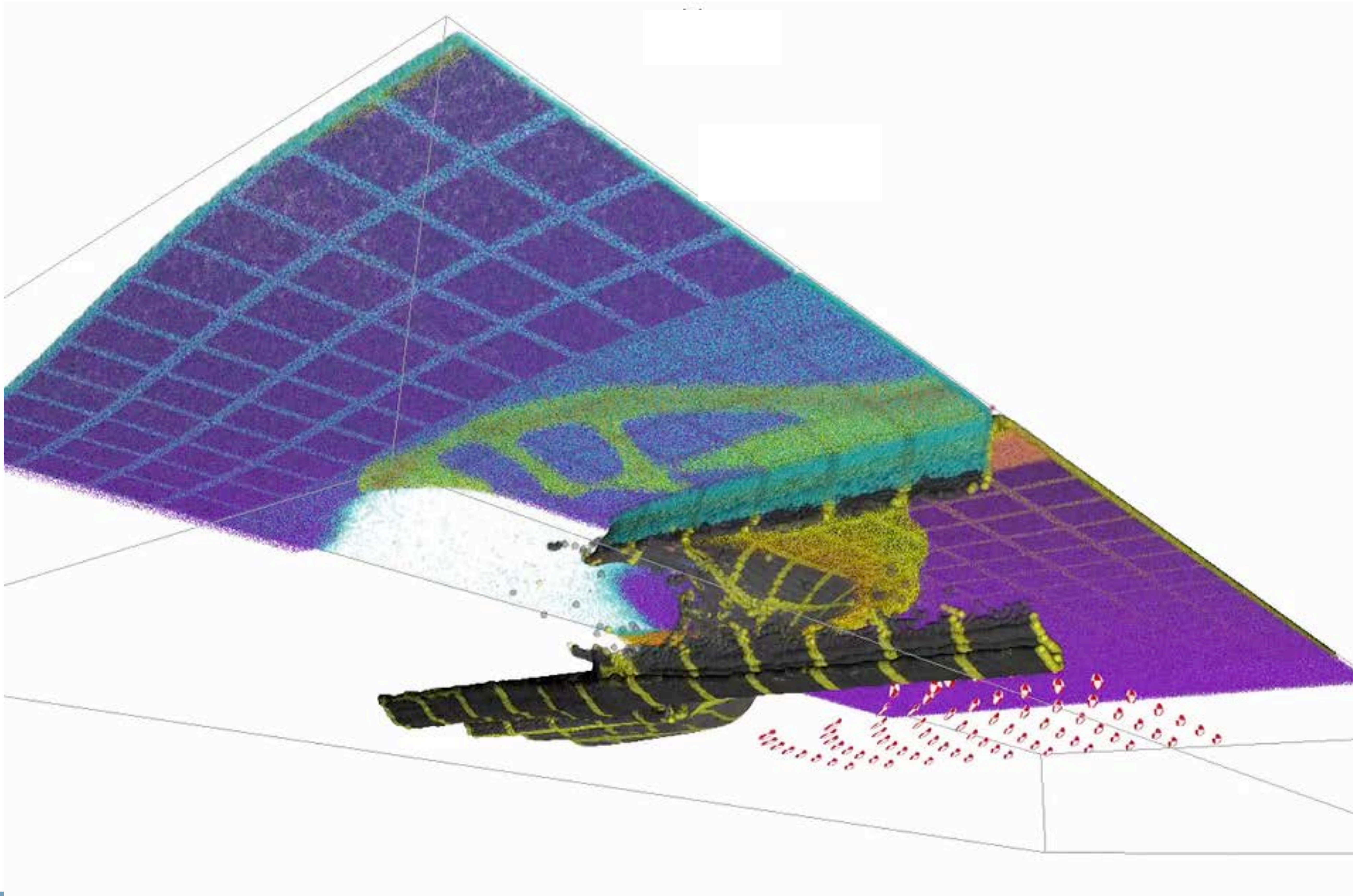


Integrated Earth modelling



Underworld — plate scale models with material history

- Underworld — finite element models with tracking of small-scale physics



Family Tree

Convect b.1988 d 1993
C; FE/FV; 2D Cartesian / Axi

Convect 2 b.1992 d 1992
C; FE; 2D, 3D Cartesian / Axi

Citcom b.1992-1994
C; FE; 2D, 3D Cartesian / Axi, MG

Citcom (parallel) b.1995
C; FE; 2D, 3D Cartesian, **Faults**, MG

Ellipsis b.1997
C; FE; 2D, Cartesian, MG, **PIC, VE/P**

CitcomS b.1998
C; FE; 3D **Spherical**, **parallel**, MG

Ellipsis3D b.2000-2002
C; FE; 2D, Cartesian, MG, **PIC, VE/P**

CitcomCU b. 2002
C; FE; 2D, 3D, MG, VE

StGermain / Snark b.2002
C; FE; 3D, Cart, MG, **PIC, parallel**

Underworld 1.x b. 2006
C; FE; 3D, ALE, MG, **PIC, parallel**

Aspect b.2012
C; FE; 3D/S, **AMR parallel**

Fluidity
C; FE; 3D/S, **AMR parallel**

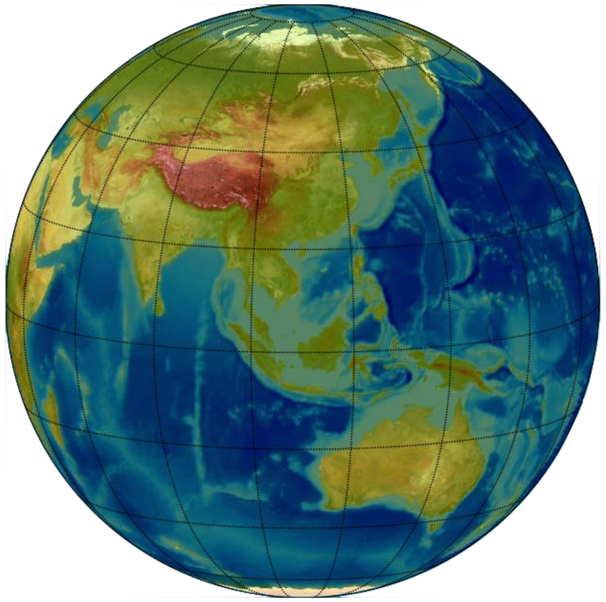
Underworld 2.x b. 2014
C/py; FE; 3D/S, ALE, MG/para, PIC/RBF

Gale 1.x b.2008 d.2012
C; FE; 3D, ALE, MG, **PIC, parallel**

The dotted lines indicate a flow of experience but not lines of code.

This diagram is not intended to be comprehensive !

Why so successful ? — Robust solvers, extensible code



- ★ Stokes flow — viscous, infinite prandtl number, no history
- ★ Simple geometry / boundary conditions (cubes / cylinders / spheres etc)
- ★ Bi/Trilinear velocity / constant pressure elements
- ★ Penalty + direct solver
- ★ Full Multigrid + Uzawa + iterative solver
- ★ Mesh can be constructed by subdividing a "unit cell"
- ★ Boundary conditions can be anticipated; not completely general
- ★ Rheology is most complicated part
    - ★ Non-linear
    - ★ Very strong dependence on temperature / pressure > $10^{6\text{-}10}$ in boundary layers
    - ★ Yield stress

Why so successful ? — Plug and play !

Citcom.core.code †

Ground-up redesigned code:

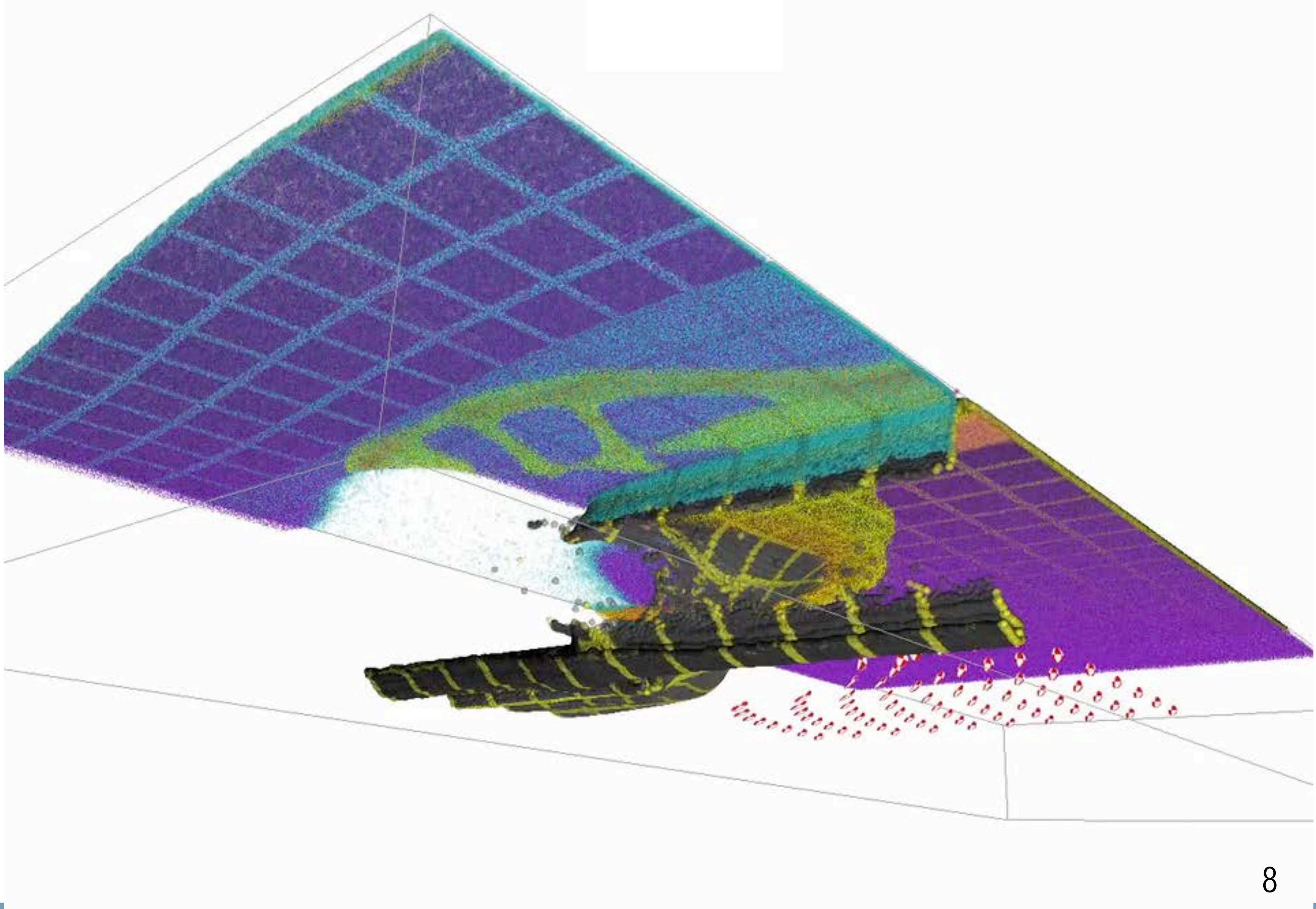
Citcom.c

```
while ( E.control.keep_going   &&  (Emergency_stop == 0) )   {

    time = CPU_time();
    general_stokes_solver(&E);

    E.monitor.cpu_time_on_vp_it += CPU_time()-time;

    process_new_velocity(&E,E.monitor.solution_cycles);
    (E.special_process_new_velocity)(&E,E.monitor.solution_cycles);

    (E.next_buoyancy_field)(&E);

    process_new_buoyancy_field(&E,E.monitor.solution_cycles);
    (E.special_process_new_buoyancy)(&E,E.monitor.solution_cycles);

    (E.problem_update_node_positions)(&E,E.monitor.solution_cycles);  /* caution ! */
    (E.problem_update_bcs)(&E,E.monitor.solution_cycles);

    E.monitor.cpu_time_elapsed = CPU_time();
    fprintf(E.fp,"Cpu time elapsed after %d cycles  = %g seconds\n\n\n",
        E.monitor.solution_cycles, E.monitor.cpu_time_elapsed); fflush(E.fp);
    E.monitor.solution_cycles++;
    if(E.monitor.solution_cycles>E.control.print_convergence)
    E.control.print_convergence=0;

}
```

† Simple strategy for building multiple problem types / extensions to code at compile time (

Underworld — plate scale models with material history

- Underworld — finite element models with tracking of small-scale physics
- Highly parallel code for modern petascale machines
- Open source / based on open libraries (StGermain and PETSc)
- Checkpointed and so forth
- Adopted child of CITCOM



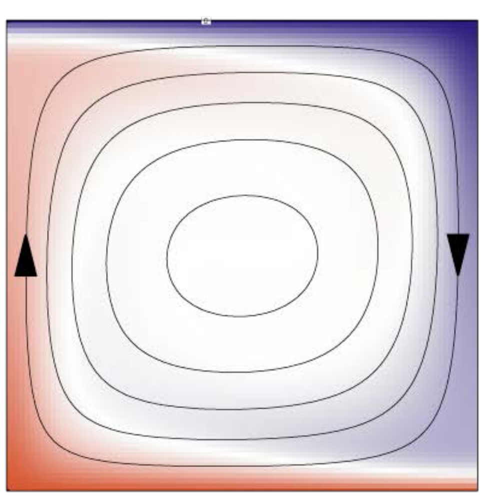
Moresi, Betts, Miller, Cayley,
Dynamics of continental accretion.
Nature, 2014, doi: 10.1038/nature13033

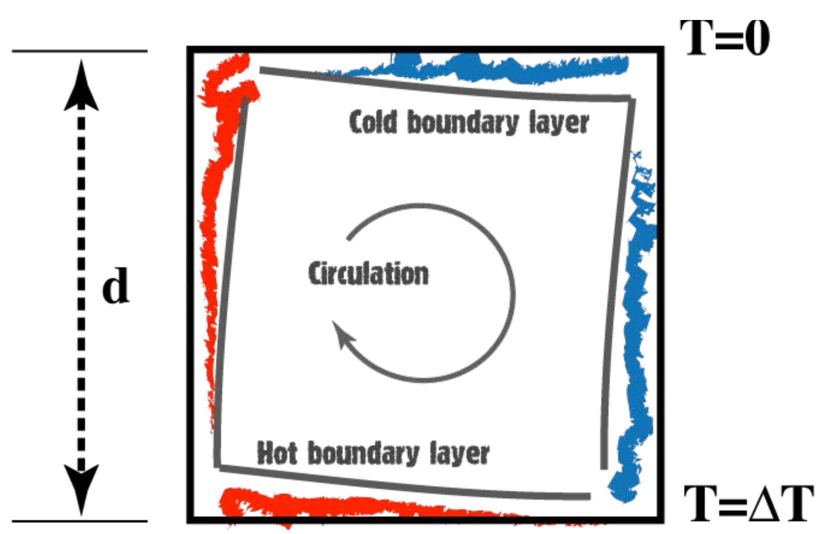
Challenges: High strain accumulation during fluid-like deformation

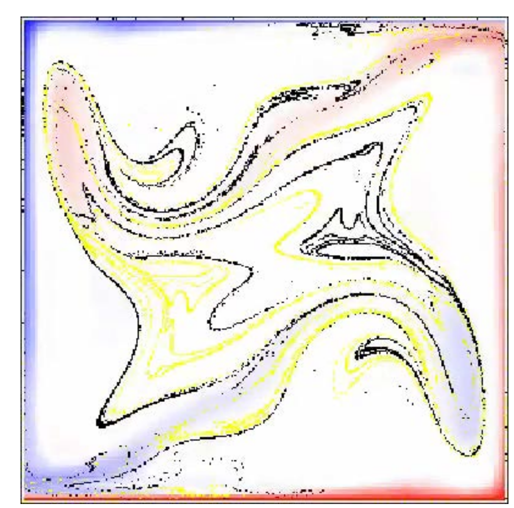
This is a Rayleigh-Bénard convection model which evolves to a straightforward balance between thermal diffusion and thermal advection in narrow boundary layers.

At modest Rayleigh number, the structure which develops is steady despite strongly developed convective flow.

This system can be solved very efficiently on a fixed mesh







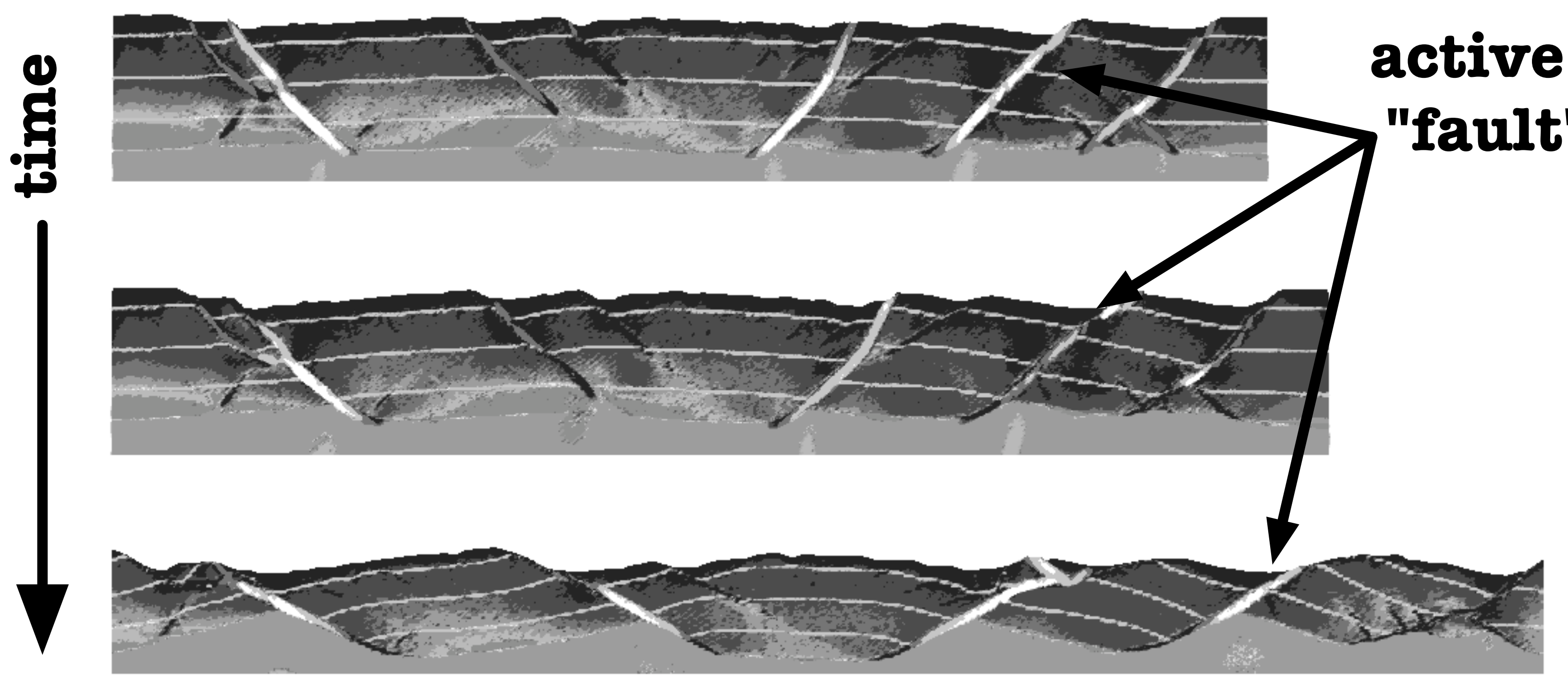
$\mathrm{Ra} = 10^7$

Challenges: Strain-dependence of lithospheric deformation

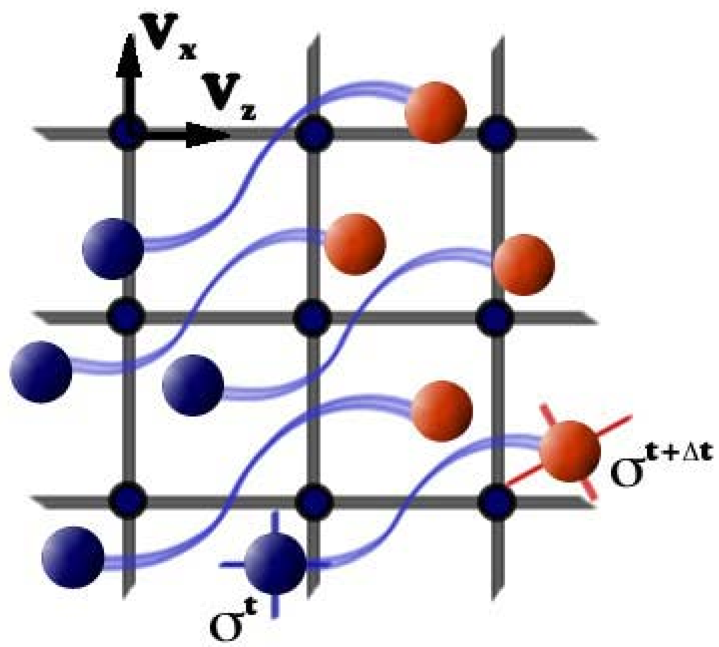
This is a simulation of continental crust being stretched in response to far field stresses imposed by plate motions.

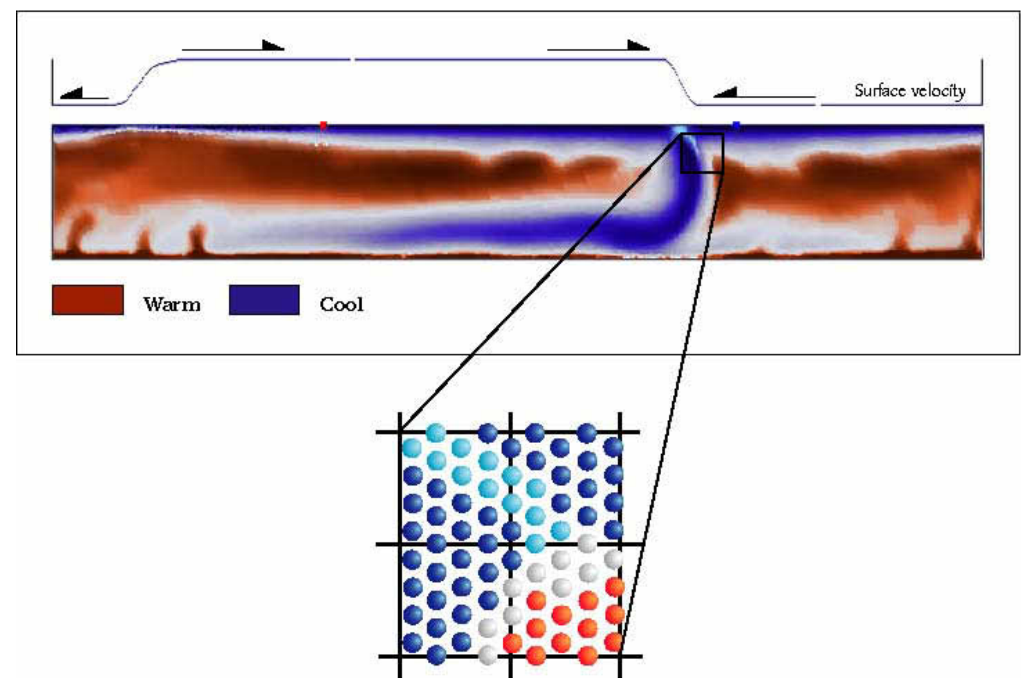
At modest strain, the deformation will often localise onto faults which can be very long-lasting structures; very fine scale in width, but with large lateral dimension and relatively weak.

The history dependence of shear deformation is tractable if we use a Lagrangian reference frame.



In the **material point method** we can keep a mesh which is computationally efficient for diffusion-dominated problems (including Stokes flow) and material points — a.k.a. particles — for tracking history variables.





This is the technique implemented in Underworld (and other similar codes) and leads to a very natural approach to many “difficult” issues in geological thermal / mechanical models (www.underworldproject.org)

Equations

Ugly !!

$$\tau_{ij} = 2\eta D_{ij} = \eta(u_{i,j} + u_{j,i})$$

$$\tau_{ij,j} - p_{,i} = f_i$$

$$u_{i,i} = 0$$

$$f = \mathbf{g}\rho_0\alpha\Delta T$$

Stokes flow, incompressible
Elliptic problem - multigrid

$$T_{,t} + u_k T_{,k} = (\kappa T_{,k})_{,k} + Q$$

Advection / diffusion

Robust solution is possible

The general approach is like this

mg configuration
accuracy ?

"outer" solve for p

$$(G^T \tilde{K}^{-1} G)p = (G^T \tilde{K}^{-1})F$$

"inner" mg solve for v*

$$\tilde{K} v_i^* = f_i^*$$

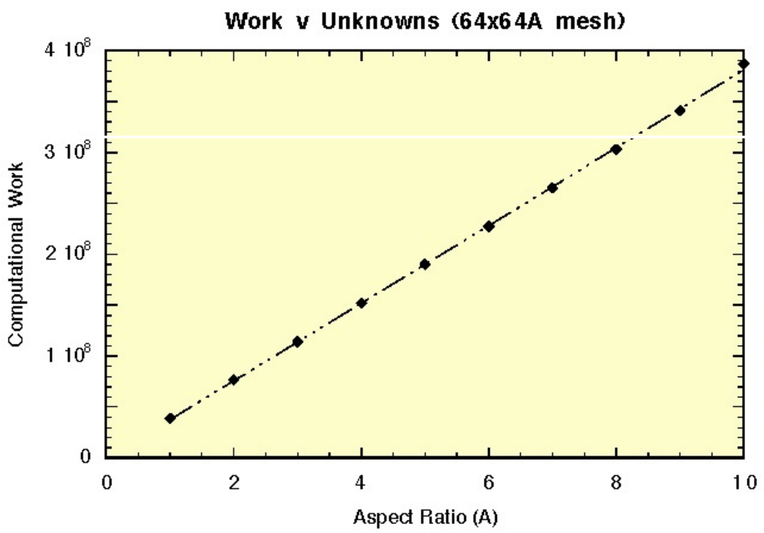
solve for v

$$Kv = F - Gp$$

which ksp / pc ?
accuracy ?
penalty ?

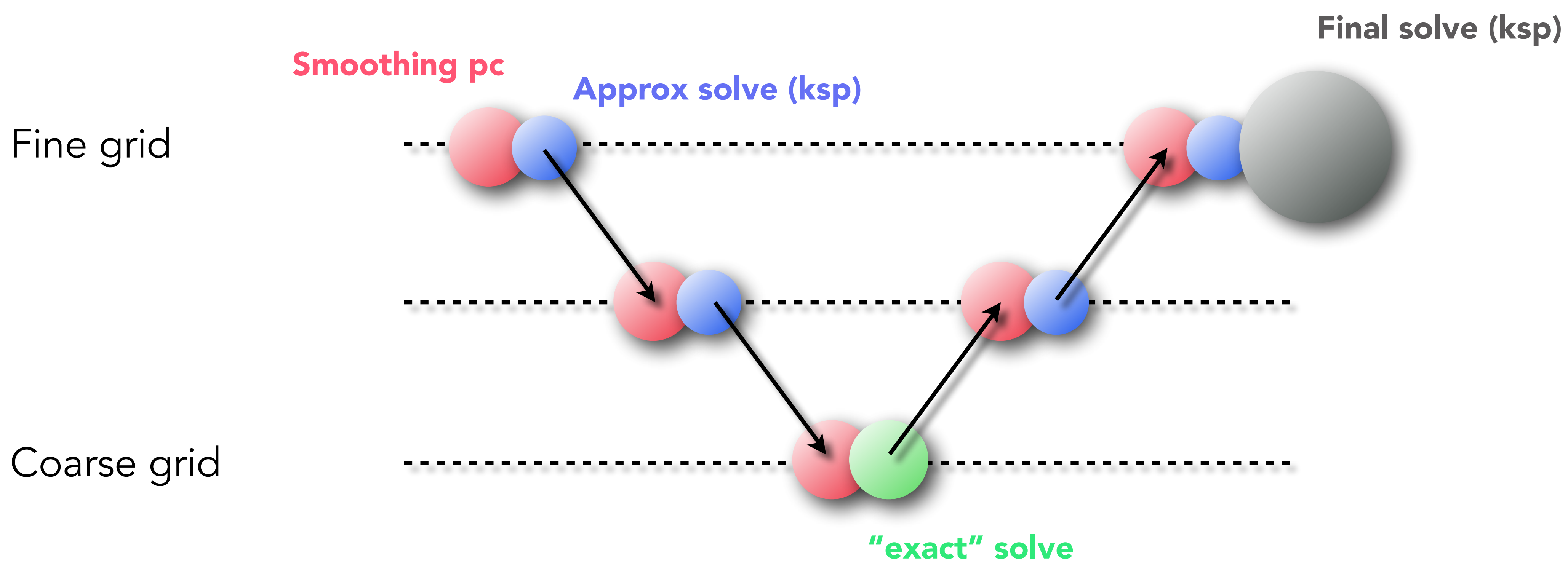
which ksp ?
accuracy ?
penalty ?

Multigrid "Inner solve"



Geometric multigrid

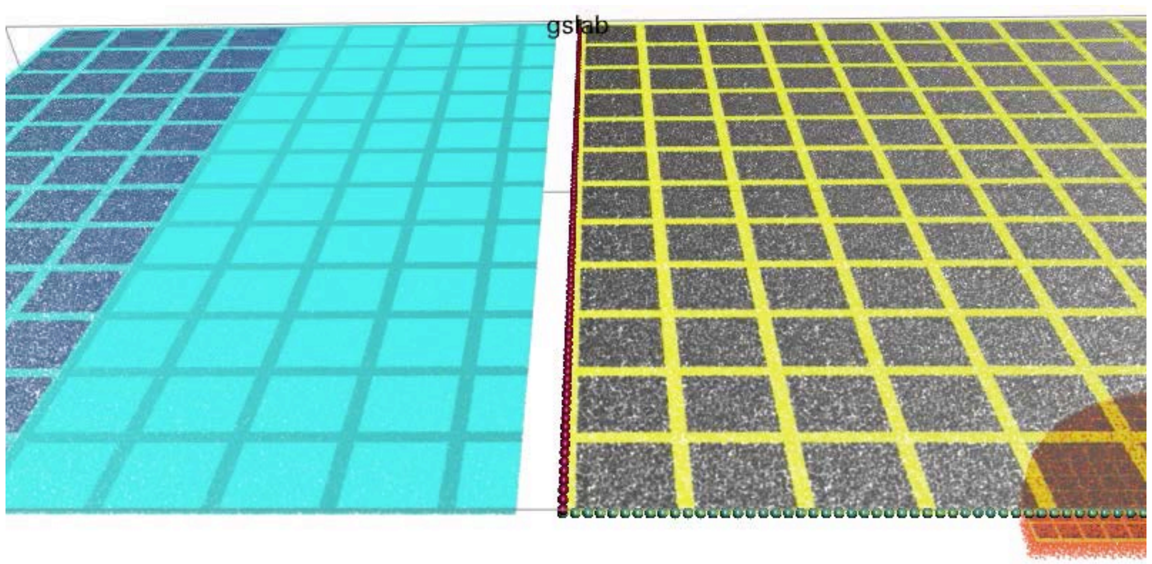
- Multiple, nested grids sharing common nodes
- Solution is obtained by combining solutions on all grids
- Ideal for elliptic problems in which information propagation is not local and is instantaneous



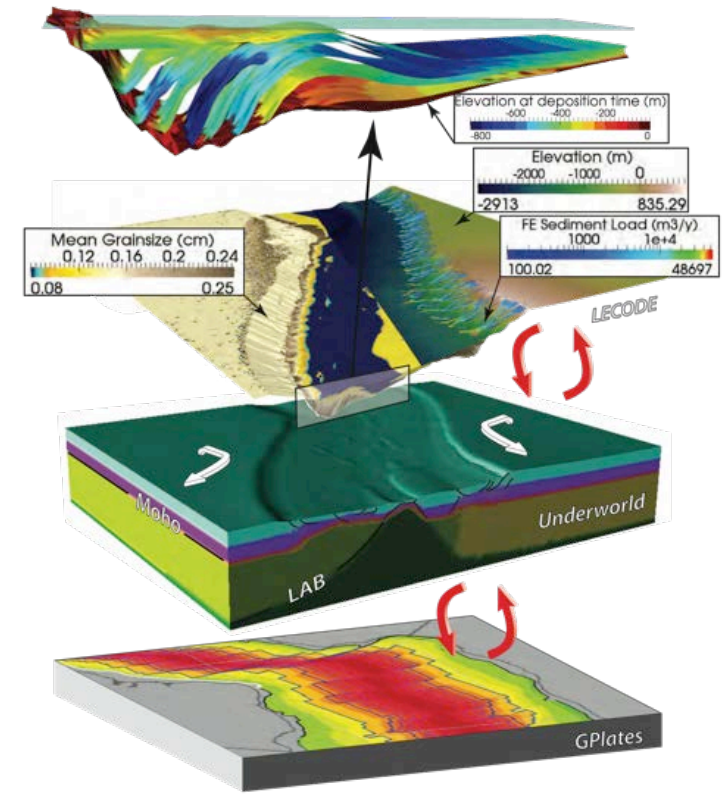
"V cycle" is MG preconditioner on final solver

Integrated workflows

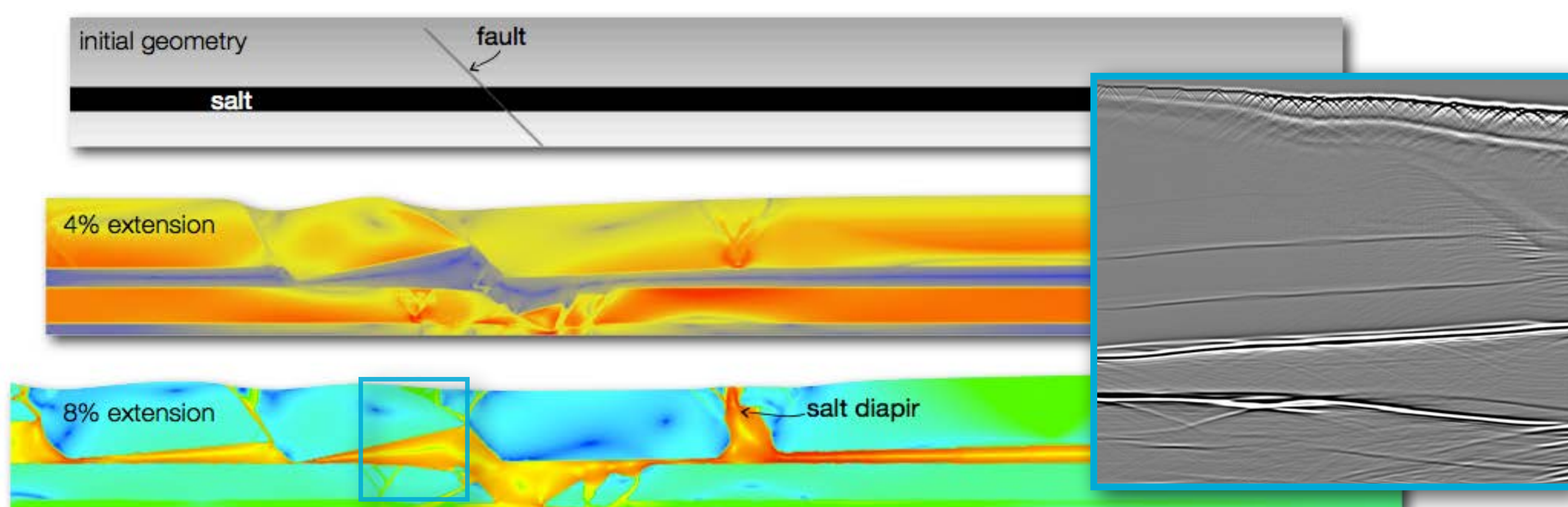
Multiple data types mean multiple modelling techniques



Betts et al - Underworld + conceptual models



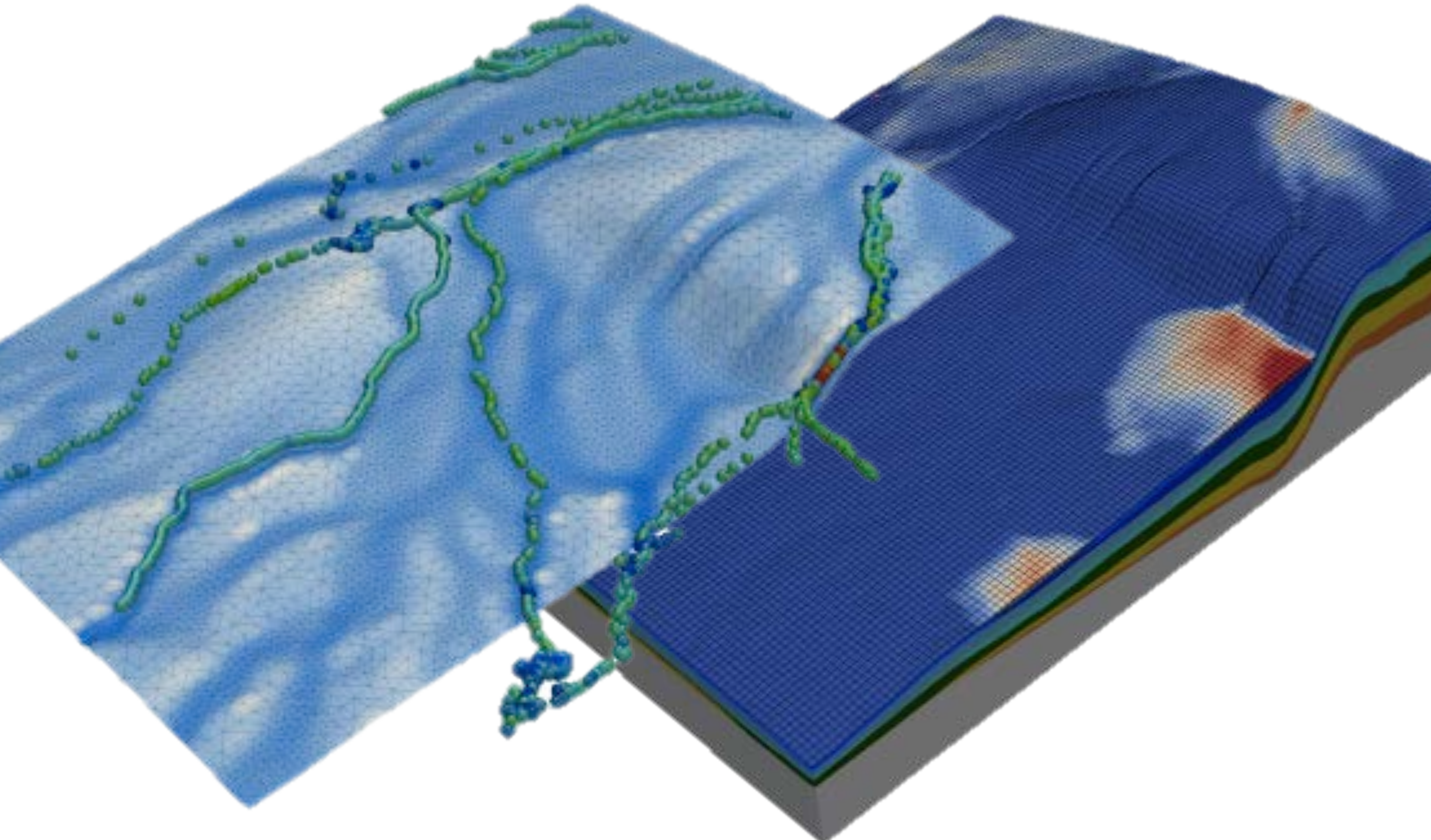
Australia et al — Underworld & gPlates & LeCode



Mondy et al — Underworld & Madagascar

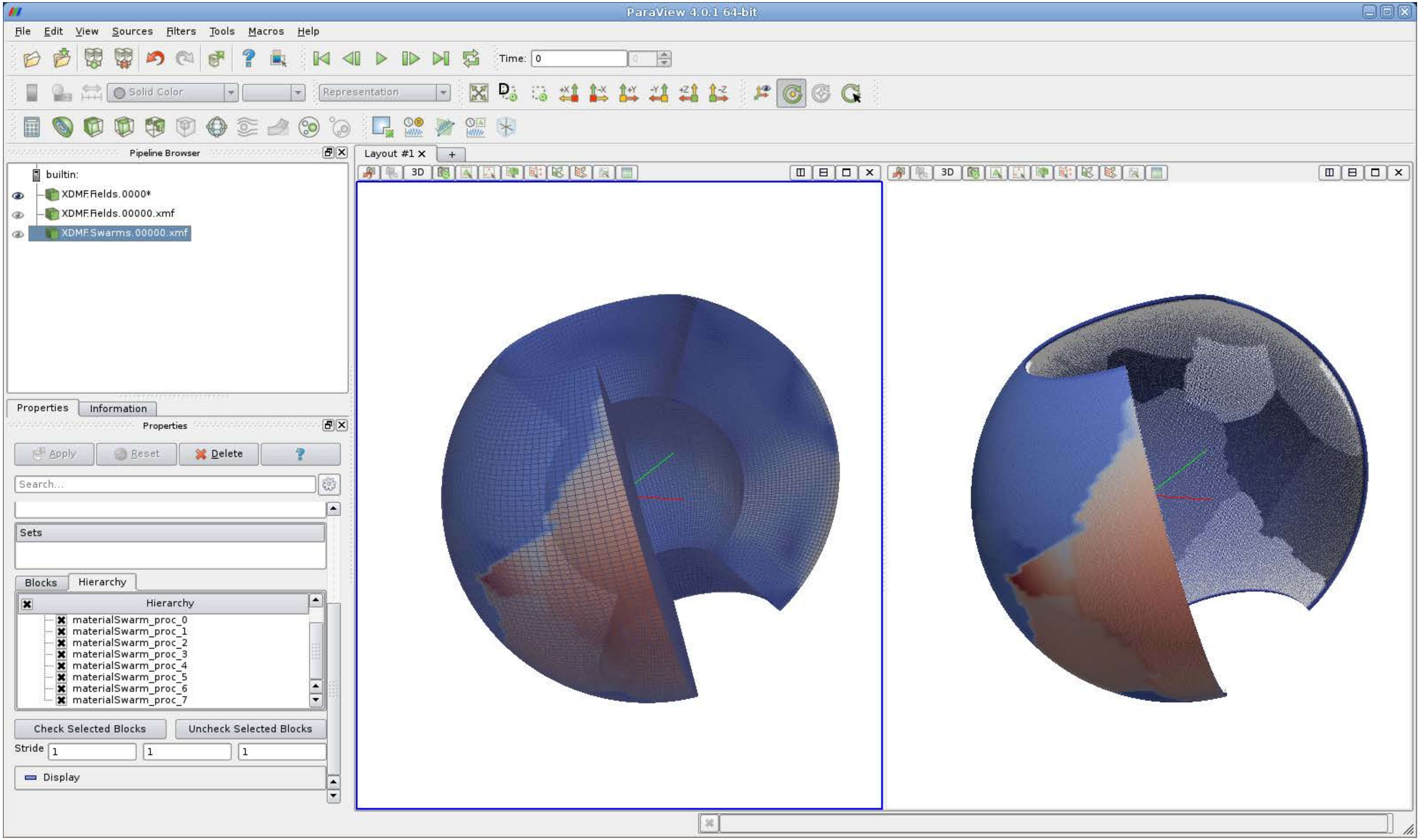
Coupling with LeCode & Badlands

details: guillaume.Duclaux@csiro.au



Underworld and gPlates

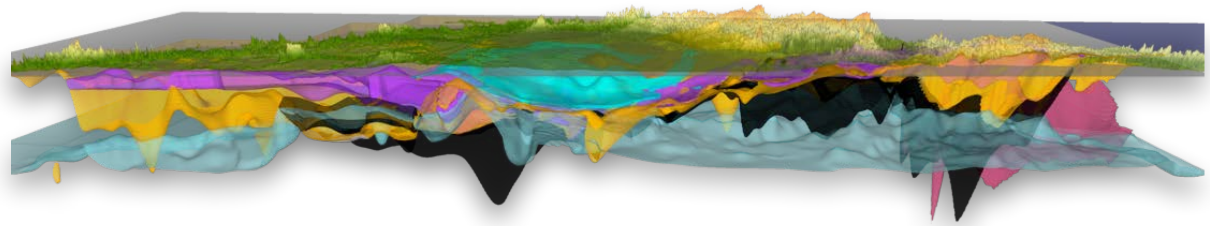
john.mansour@monash.edu, mirko.velic@unimelb.edu.au

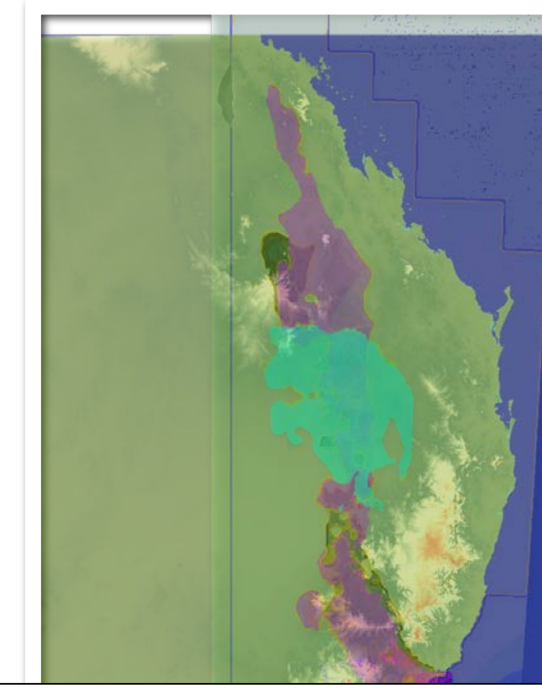


Coupling with GoCAD & GeoModeller

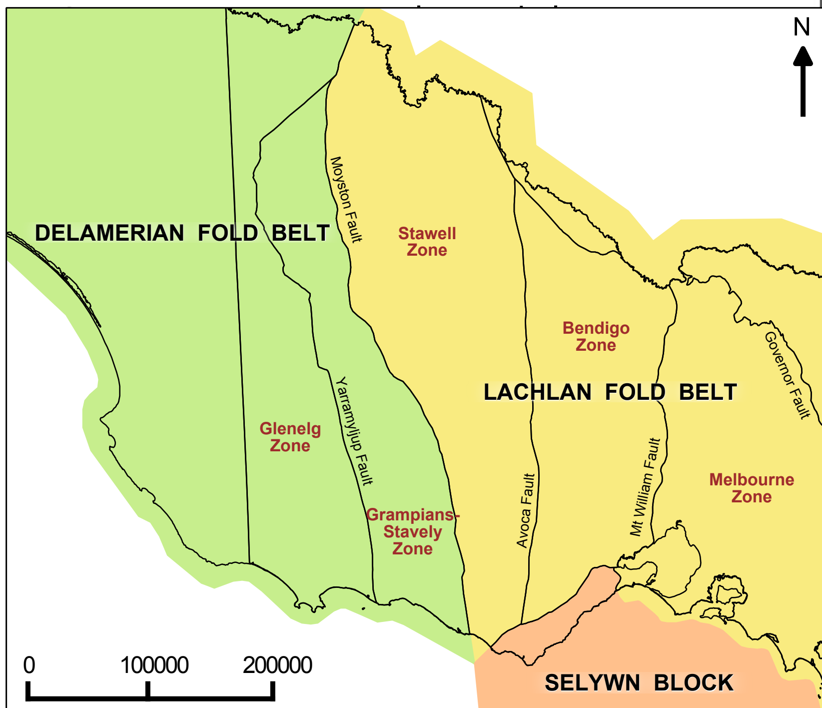
Heat flow models at the 1000km scale

- Incorporating 3D structure — ingest 3D structural models from geophysical interpretation



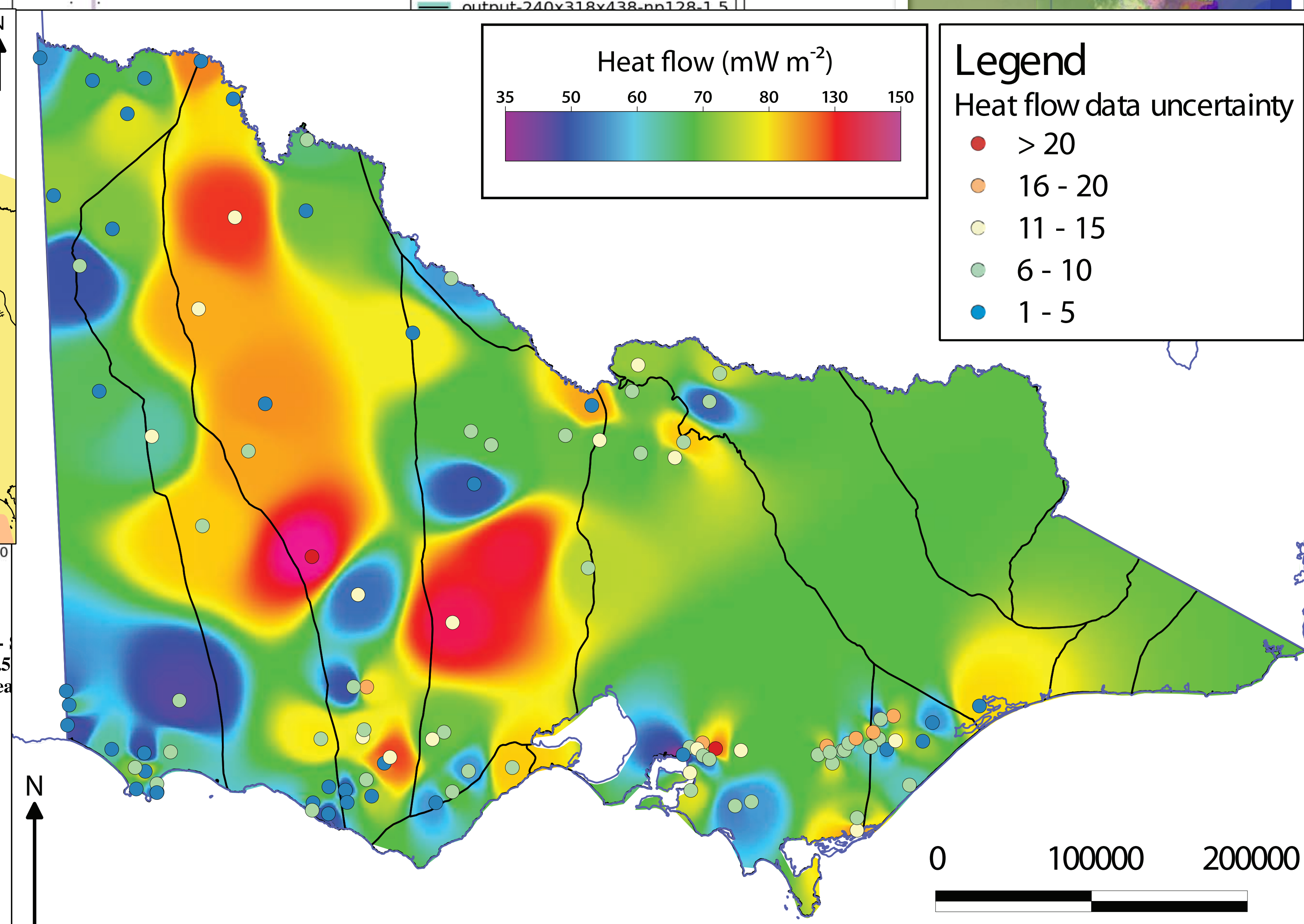


Drillcore profile difference - temperature



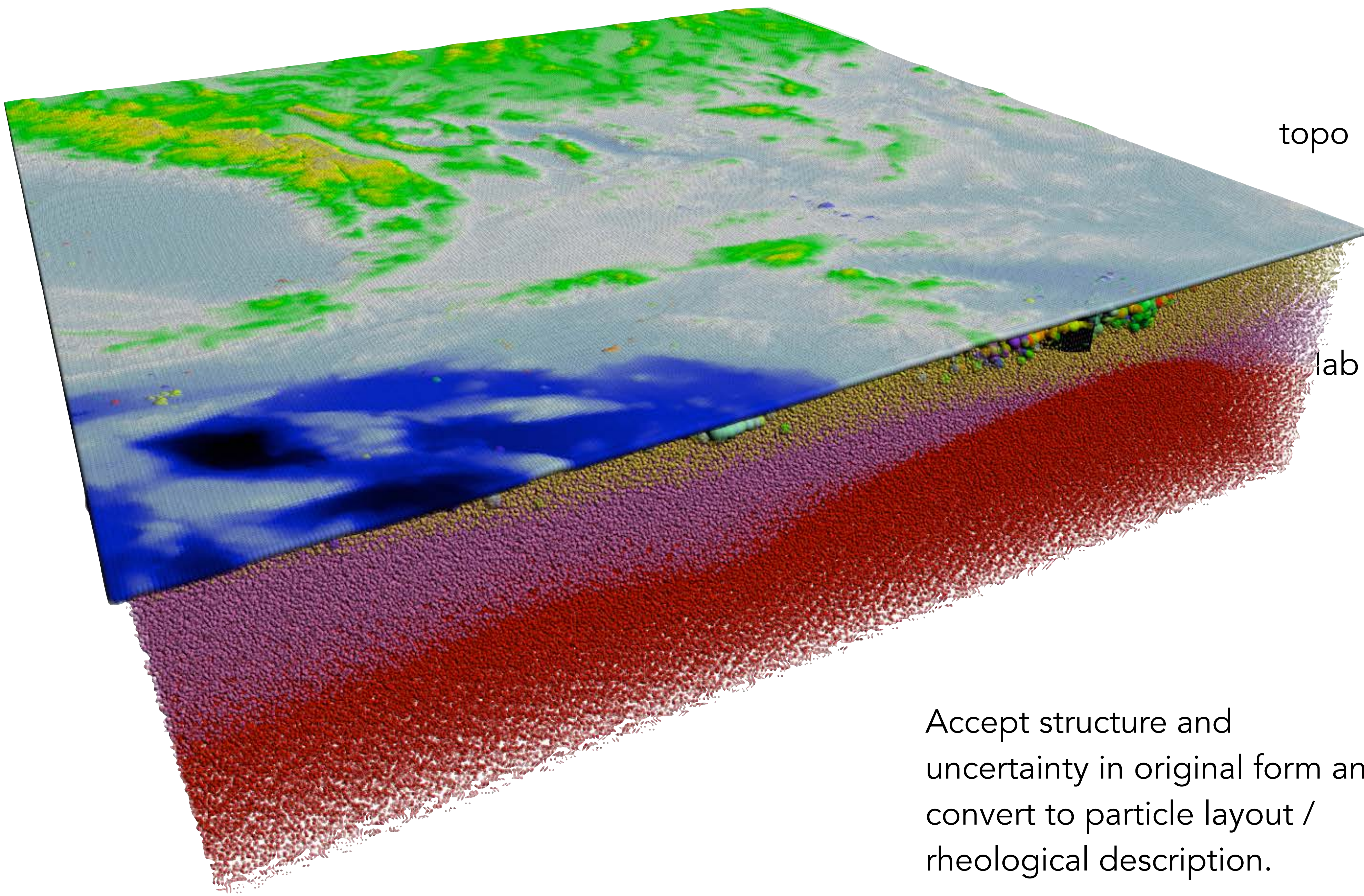
assessments for geothermal exploration

Figure 3 -
K_{Crit} at 1.5
of fit for ea



- *Towards a risk analysis for management of basins with competing uses (groundwater, geothermal, CO_2 storage, petroleum extraction)*

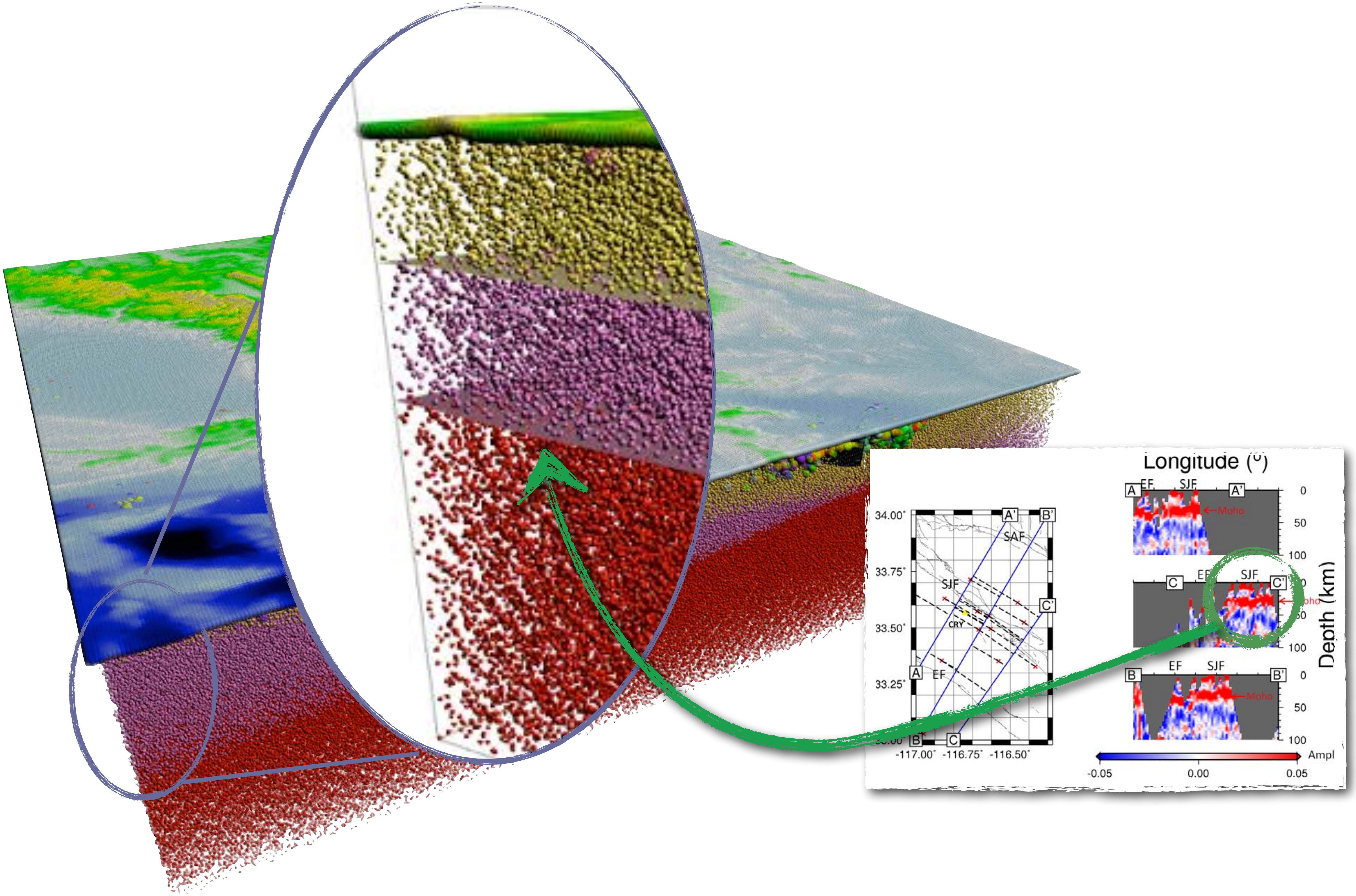
Automated workflows — prerequisite for inversion



Accept structure and uncertainty in original form and convert to particle layout / rheological description.

Keep both representations for analysis purposes.

Automated model building — prerequisite for inversion



Geographical / spherical meshes needed !

Models in a structural inversion workflow

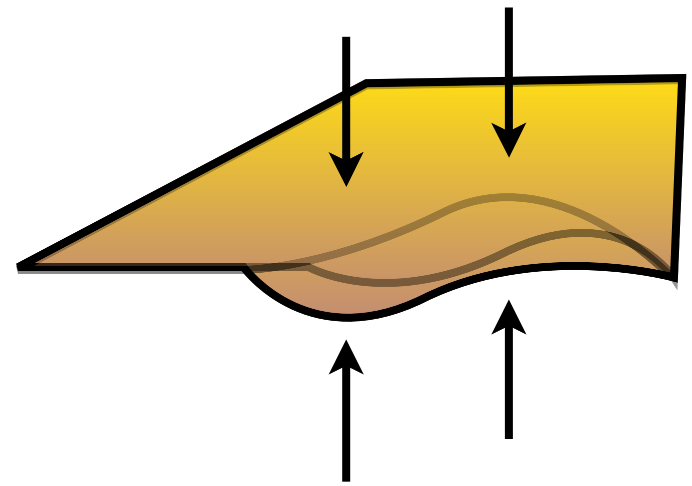
Geothermal models: we import structures / properties from geophysically constrained 3^{rd} party interpretations (gravity, magnetics, seismic sections)

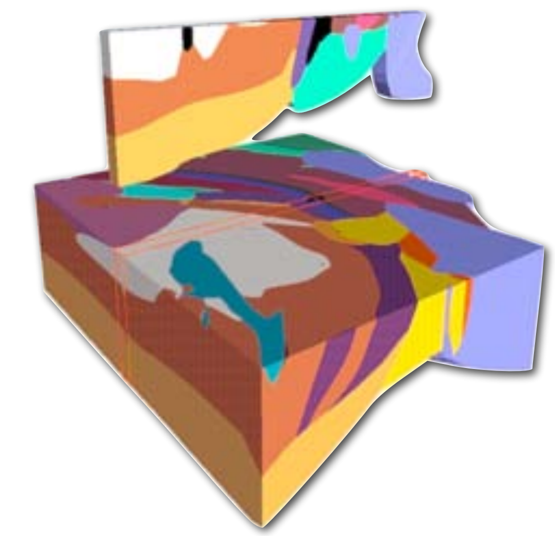
Any observed structure we use to construct a model has uncertainty; so do material properties inferred for structures; so does the possibility of unknown structure.

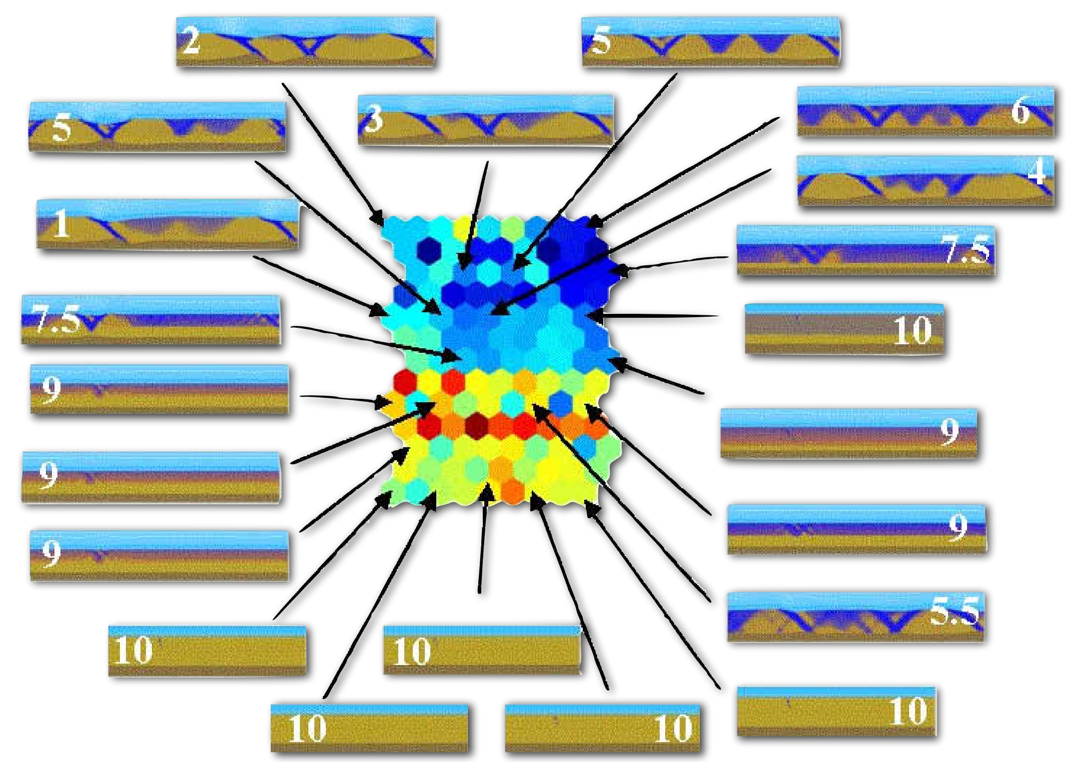
Various approaches to exploring this uncertainty including running multiple realisations and "interactive inversion"

Requires us to be able to build u/w models quickly given {starting condition + uncertainty} in their native format (e.g. fault + uncertainty in dip / strike; moho depth + observational error)

Would rather solver related problems together and not have a black box code + black box inversion engine.



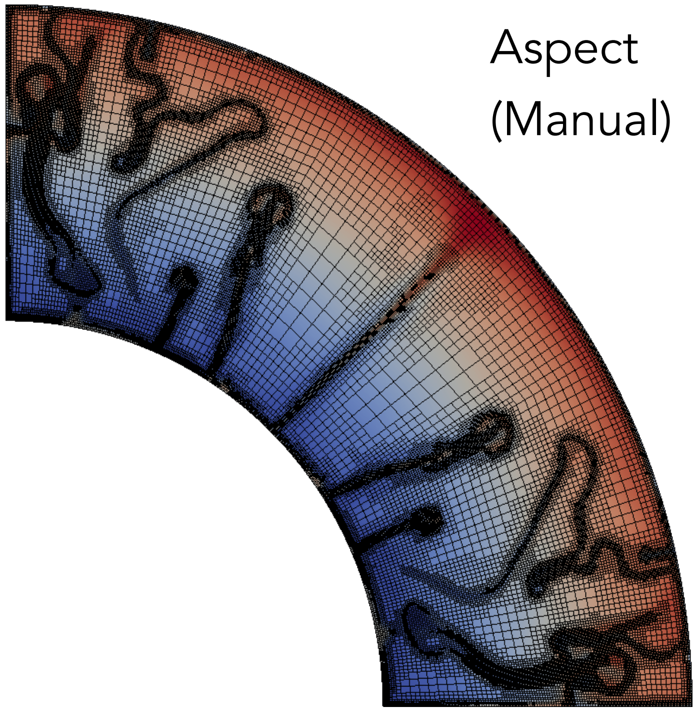




Near Future — 5 to 10 years

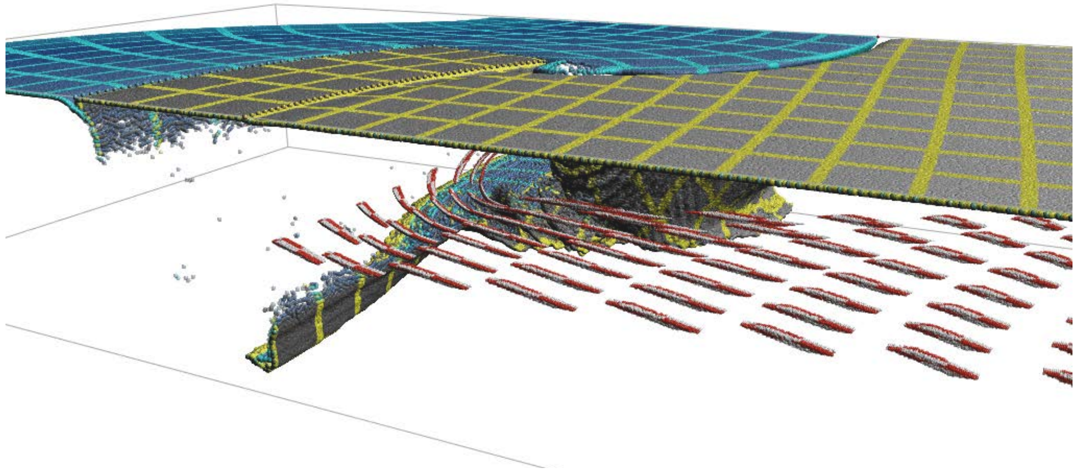
- Integrated workflows
- Documentation
- Reliability
- Installation

- Simulations not Models
  - Data assimilation / model steering
  - Robust & extensible physics
  - Coupled models
  - Respecting small scale / large-scale interactions
  - Data and models on equal footing
- Robust solution methods
- Flexible geometry
  - Unstructured meshes
  - Free surfaces
  - Adaptivity
- Parallel scaling
- Lightweight layers, building on libraries

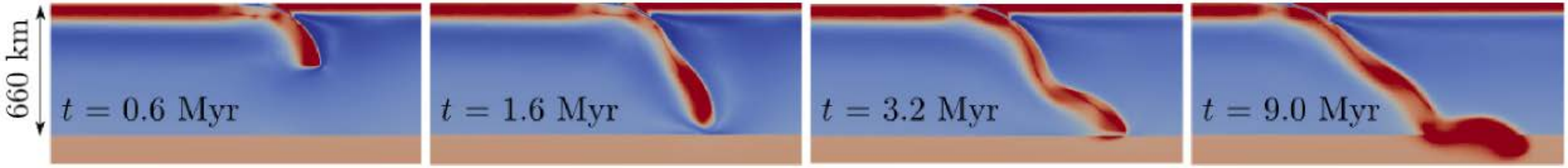


Aspect (Manual)

Underworld 2

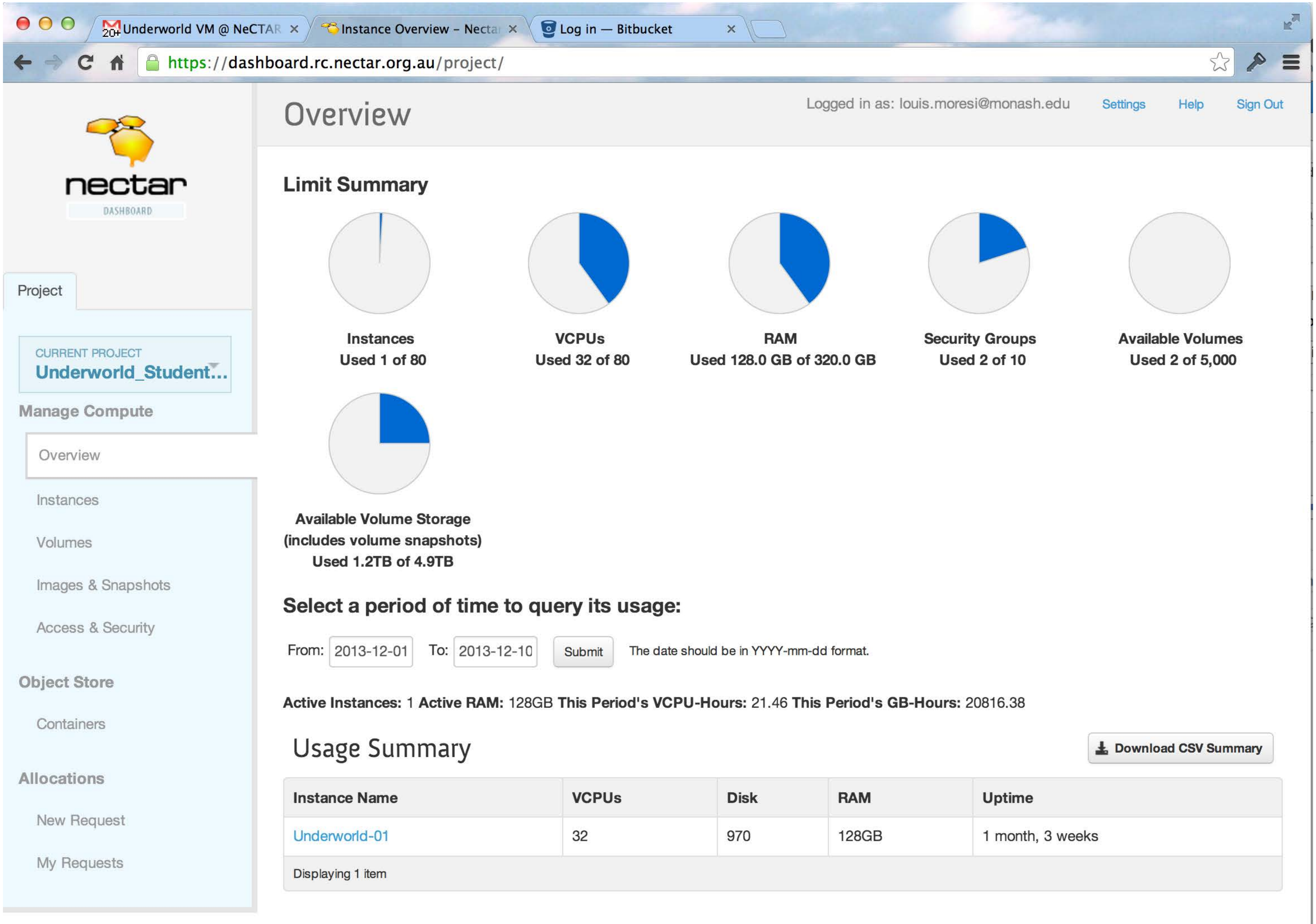


Fluidity (Garel, 2014)



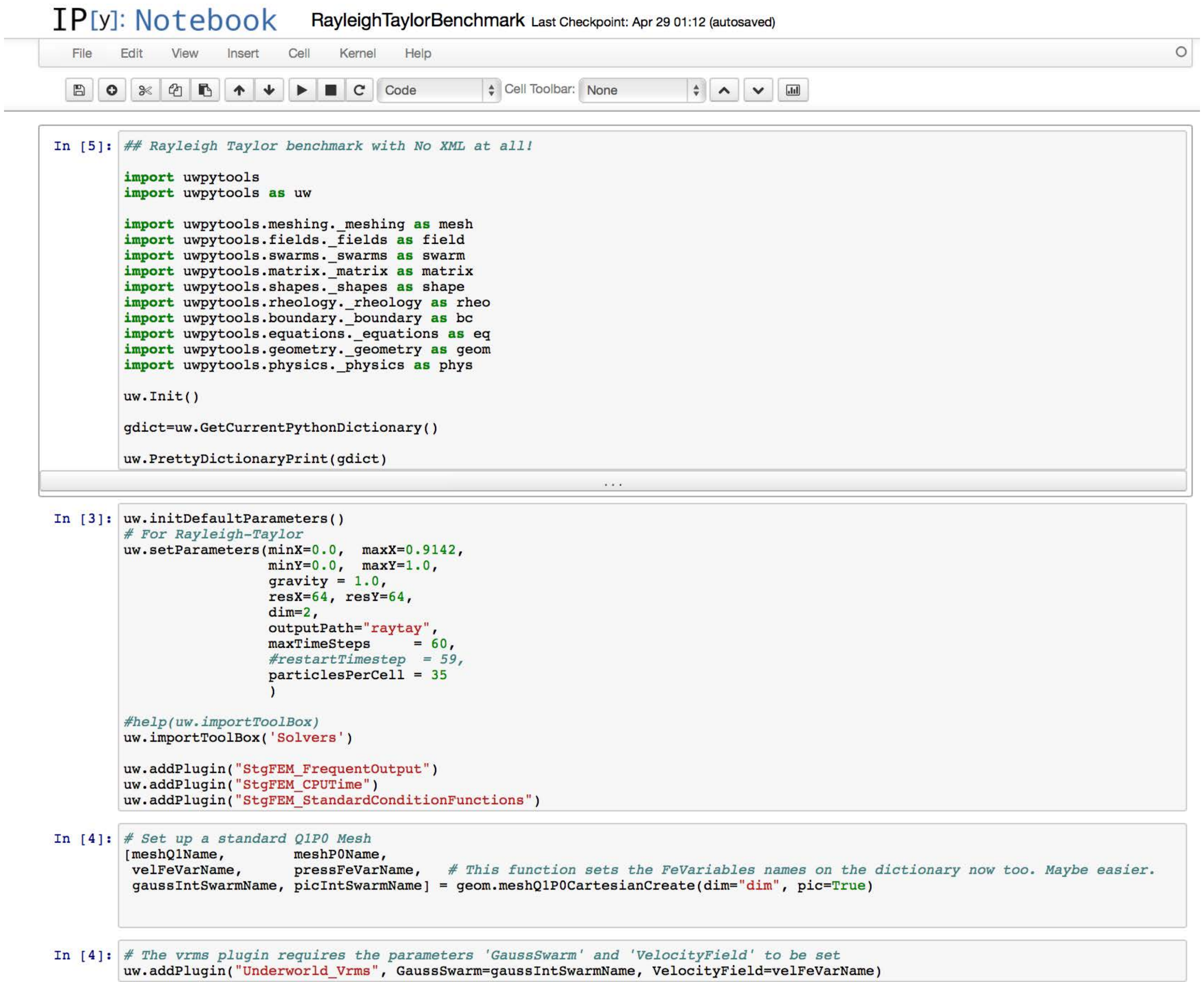
Virtual machines

steve.quenette@monash.edu



Smart front end (e.g. python / Underworld)

Particle Density




```
In [5]: ## Rayleigh Taylor benchmark with No XML at all!

        import uwpytools
        import uwpytools as uw

        import uwpytools.meshing._meshing as mesh
        import uwpytools.fields._fields as field
        import uwpytools.swarms._swarms as swarm
        import uwpytools.matrix._matrix as matrix
        import uwpytools.shapes._shapes as shape
        import uwpytools.rheology._rheology as rheo
        import uwpytools.boundary._boundary as bc
        import uwpytools.equations._equations as eq
        import uwpytools.geometry._geometry as geom
        import uwpytools.physics._physics as phys

        uw.Init()

        gdict=uw.GetCurrentPythonDictionary()

        uw.PrettyDictionaryPrint(gdict)
```

```
In [3]: uw.initDefaultParameters()
        # For Rayleigh-Taylor
        uw.setParameters(minX=0.0,  maxX=0.9142,
                         minY=0.0,  maxY=1.0,
                         gravity = 1.0,
                         resX=64, resY=64,
                         dim=2,
                         outputPath="raytay",
                         maxTimeSteps      = 60,
                         #restartTimestep  = 59,
                         particlesPerCell = 35
                         )

        #help(uw.importToolBox)
        uw.importToolBox('Solvers')

        uw.addPlugin("StgFEM_FrequentOutput")
        uw.addPlugin("StgFEM_CPUTime")
        uw.addPlugin("StgFEM_StandardConditionFunctions")
```

```
In [4]: # Set up a standard Q1P0 Mesh
        [meshQ1Name,        meshP0Name,
         velFeVarName,      pressFeVarName,   # This function sets the FeVariables names on the dictionary now too. Maybe easier.
         gaussIntSwarmName, picIntSwarmName] = geom.meshQ1P0CartesianCreate(dim="dim", pic=True)
```

```
In [4]: # The vrms plugin requires the parameters 'GaussSwarm' and 'VelocityField' to be set
        uw.addPlugin("Underworld_Vrms", GaussSwarm=gaussIntSwarmName, VelocityField=velFeVarName)
```

StGermain component / class structure matches flexibility given by high-level front end (better than XML, that's for sure !)

Flexible composition of problems / equations / initial conditions using 3rd party libraries

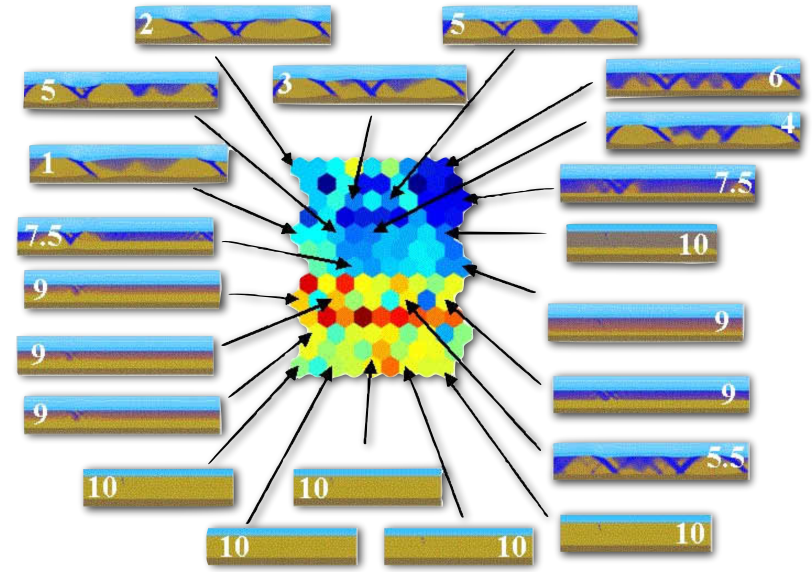
Direct access to data structures from numpy arrays.

Analysis using 3rd party libraries

gLucifer as WebGL tool (can be embedded in iPython)

Challenge to handle parallelism / HPC well at the highest level

The “flying car future” — 20 years



- Unrecognisable environments —
  - unlimited resources
  - unlimited streams of data
  - unfamiliar ways to interact with models and data

- Algorithmic priorities will be very different
  - Assume any equations can be solved efficiently at sufficient resolution (?)
    (We are much less neurotic about loop unrolling etc than we were — let’s not look back !)
  - Composing at the conceptual level of datasets / modelsets rather than operations

- “A Model” will be an ensemble of models of today’s definition
  - To propagate errors, uncertainties etc, it is much better to think of a single model being a whole swarm of individual realisations
  - We can create **metrics** and **comparison operators** with this approach

- Models (ensembles) will be richly tagged with evolving metadata
  - Google-style searches on models will be trivial
    (We probably couldn’t imagine how to automatically search text for arbitrary concepts 20 years ago)
  - Libraries / Catalogues of models will be possible / searchable given metrics etc