GeoFramework: Example of using frameworks in geophysics

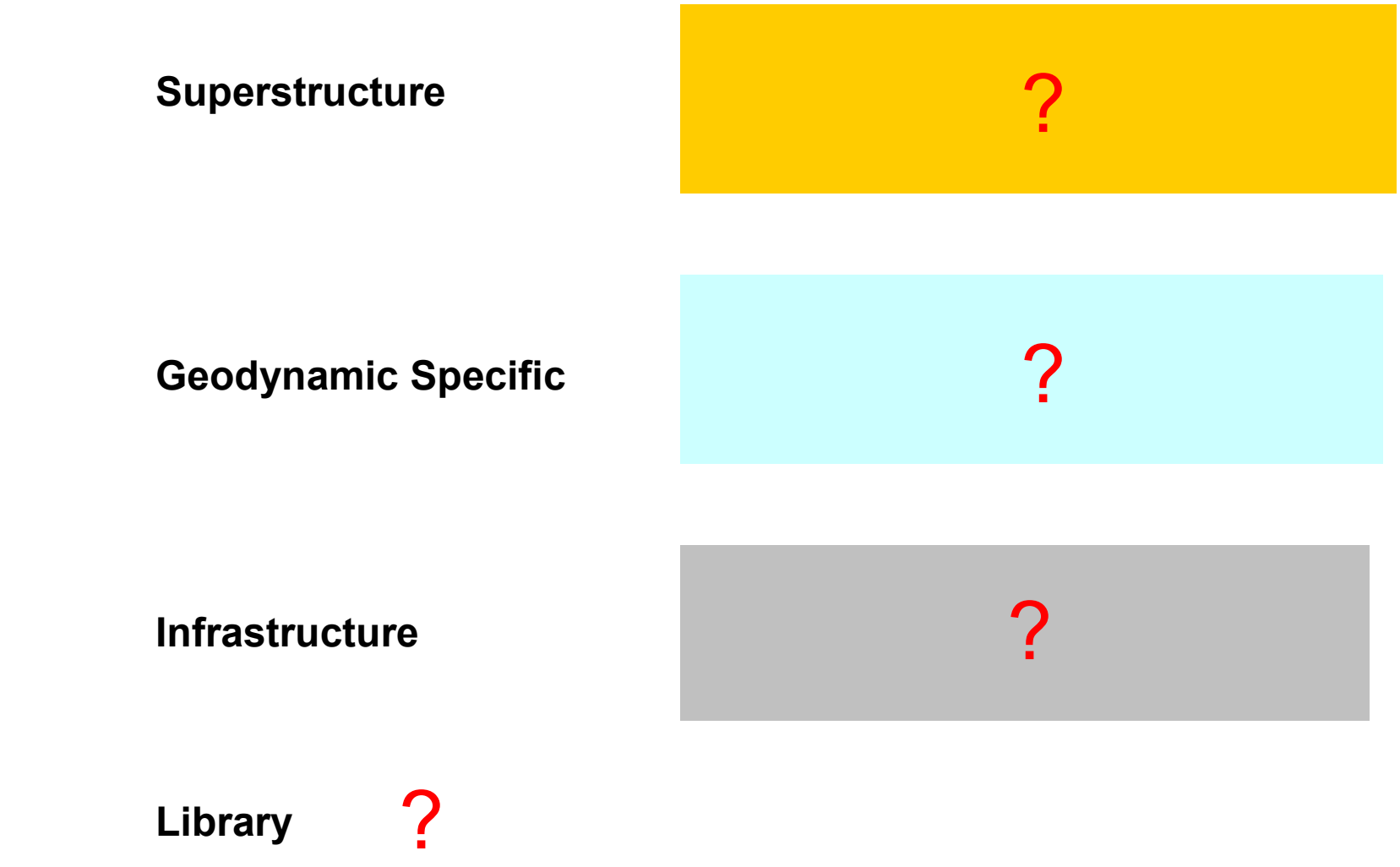
Mike Gurnis
Caltech

CIG/IRIS Computational Seismology Workshop
June, 2005

Topics

- Scientific Rationale
  - *Natural accommodation of boundary conditions*
  - *Multi-scale models*
  - *Multi-physics models*
  - *Data assimilation and prediction*
- GeoFramework project
  - *Builds upon Pyre – A Science Neutral Framework*
  - *New codes with the infrastructure framework StGermain*
  - *Repository/Web site – GeoFramework.org*
- Reengineering & Coupling Codes with Pyre
  - *Made substantial progress:*
    - *Global Mantle Convection – Local convection (CitcomS-CitcomS)*
    - *Viscous Mantle flow – elastic plate (CitcomS-SNAC)*
  - *Still working on:*
    - *Full Seismic Wave field - Global Mantle Convection (SpecFEM3D, CitcomS)*
    - *Plate Tectonic Stresses – Earthquake Rupture (TECTON-eqsim)*
    - *Mantle flow -- petrologic phase relations (ConMan-pHMELTS)*

A hierarchy of software components



Superstructure and Geodynamic Specific Layers

Superstructure

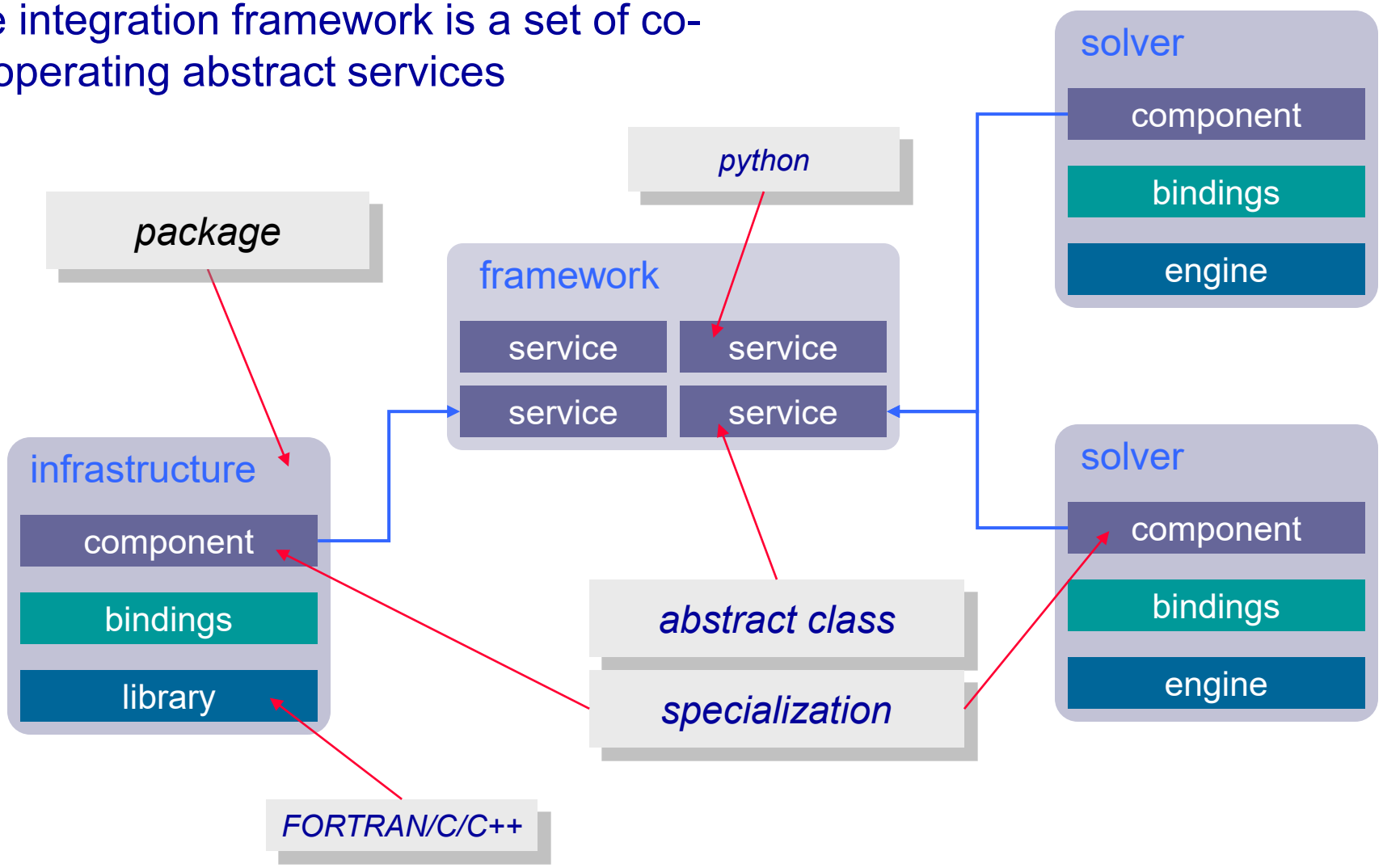
- Simulation controller
- Monitor Simulation
- Couple Fluid to Solid

Geodynamic Specific

- Component A
- Component B
- ….

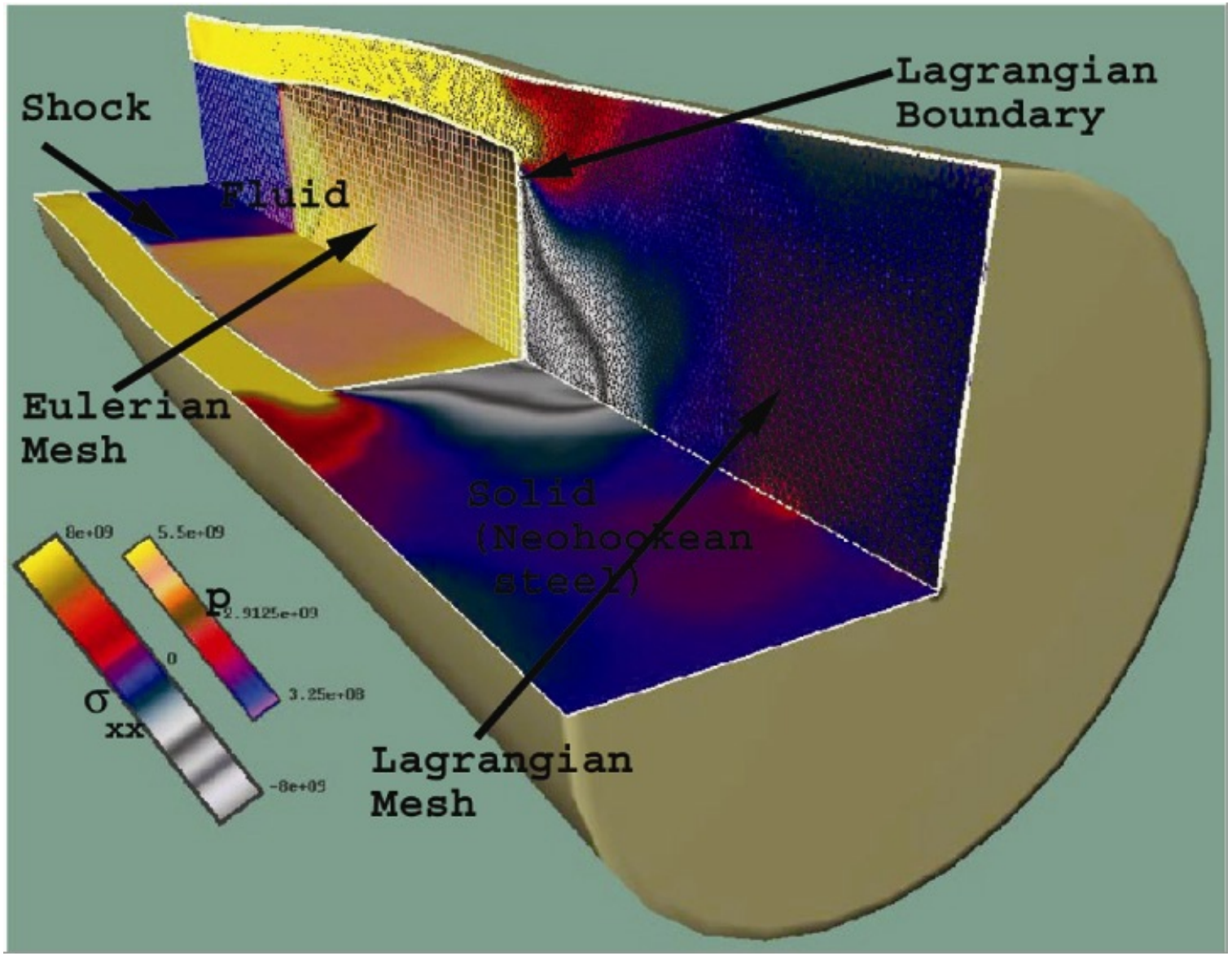
Pyre Framework (Science Neutral)

The integration framework is a set of co-operating abstract services

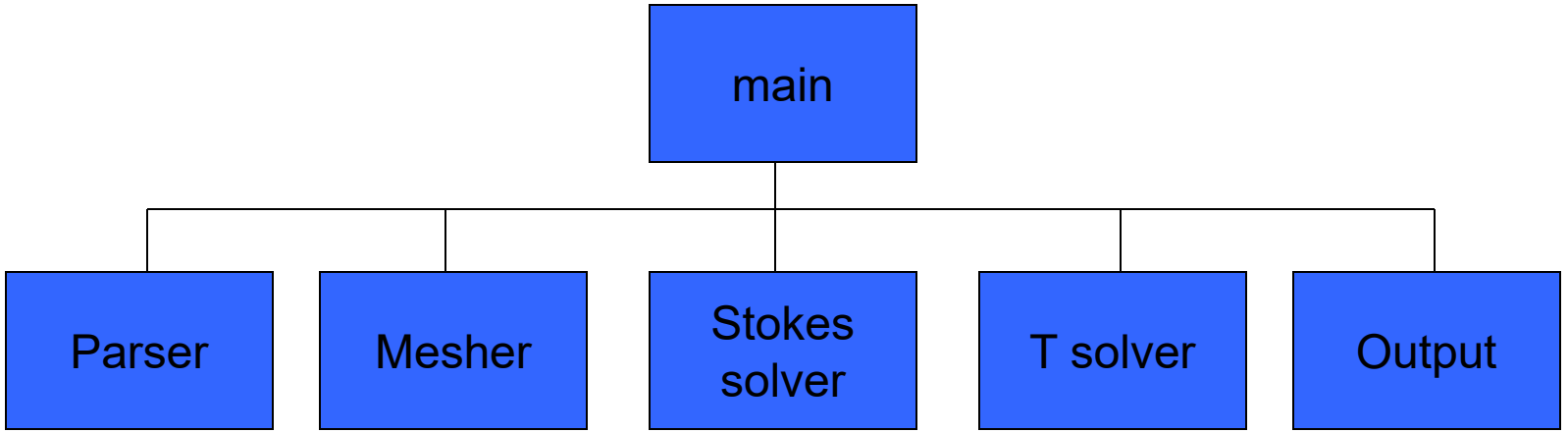


Developed by Michael Aivazis

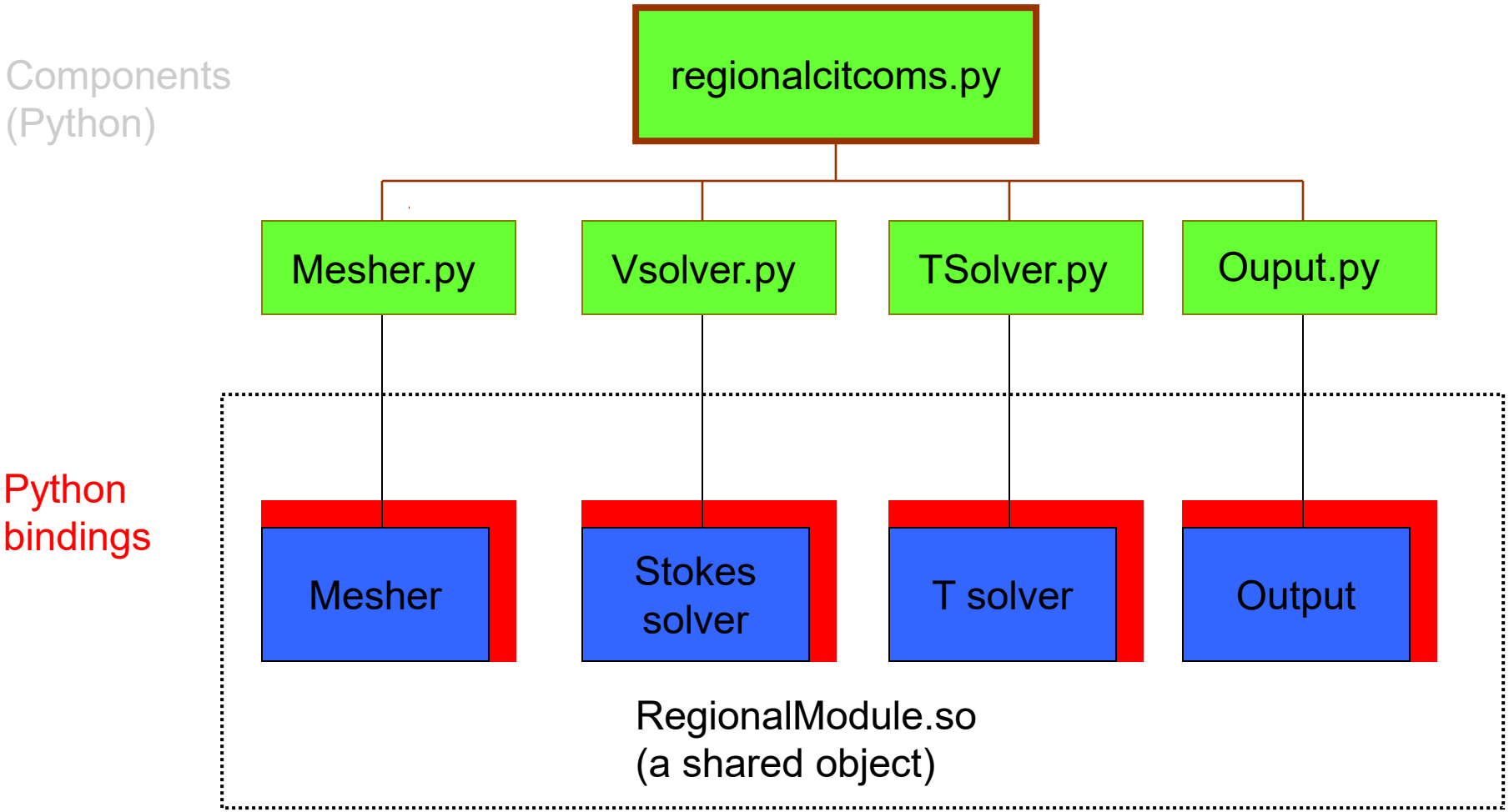
Virtual Test Facility (VTF): Example From Pyre



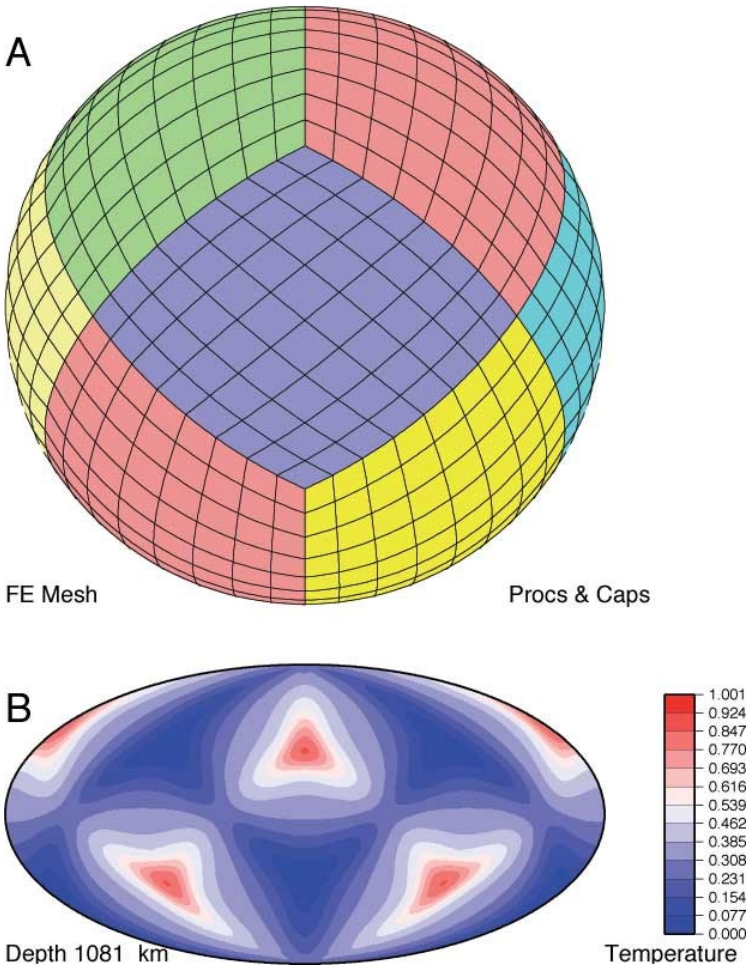
CitcomS



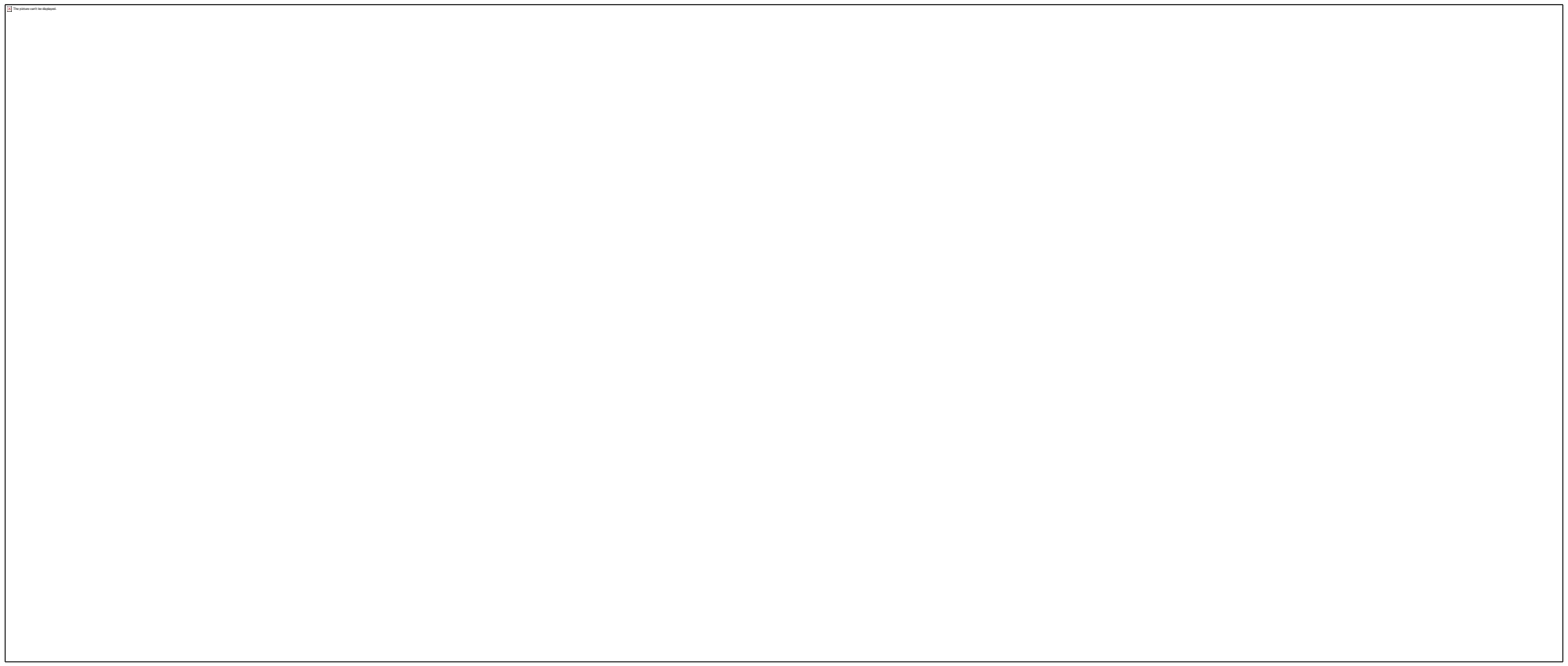
Pyre version of CitcomS

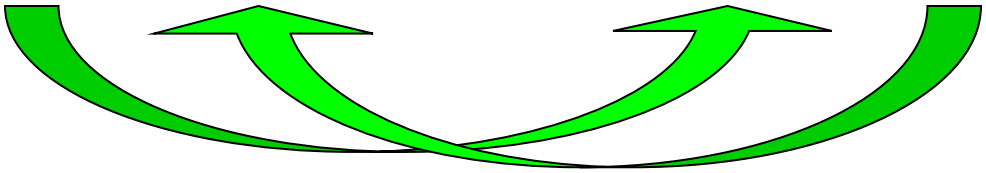


CitcomS.py as a single component

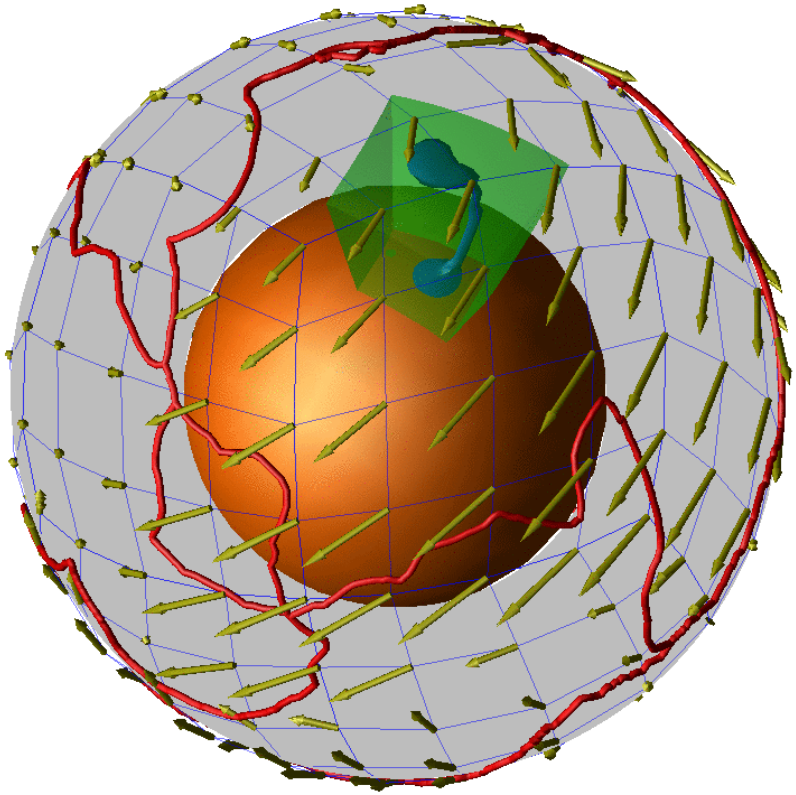


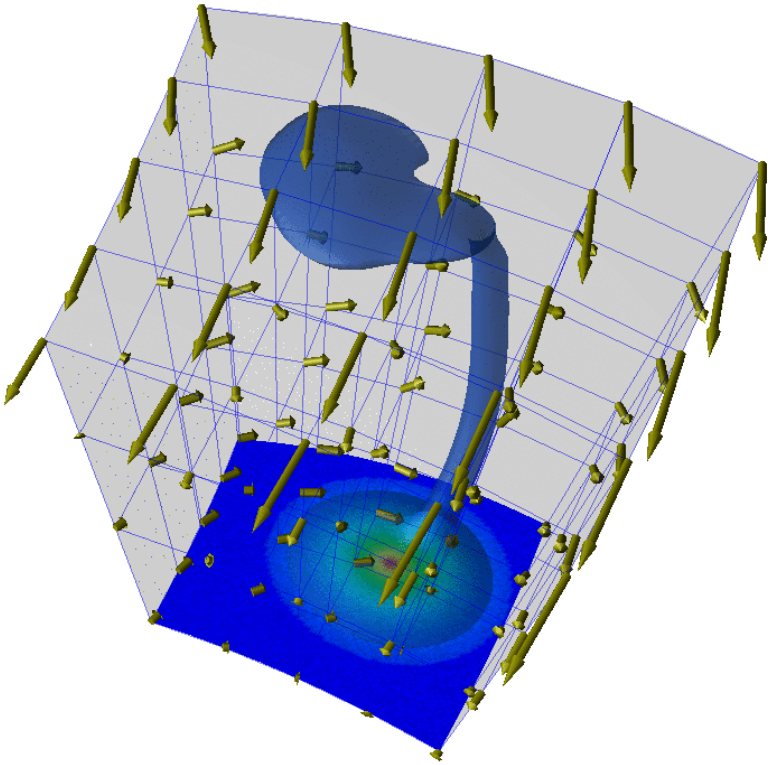
Coupling With Pyre





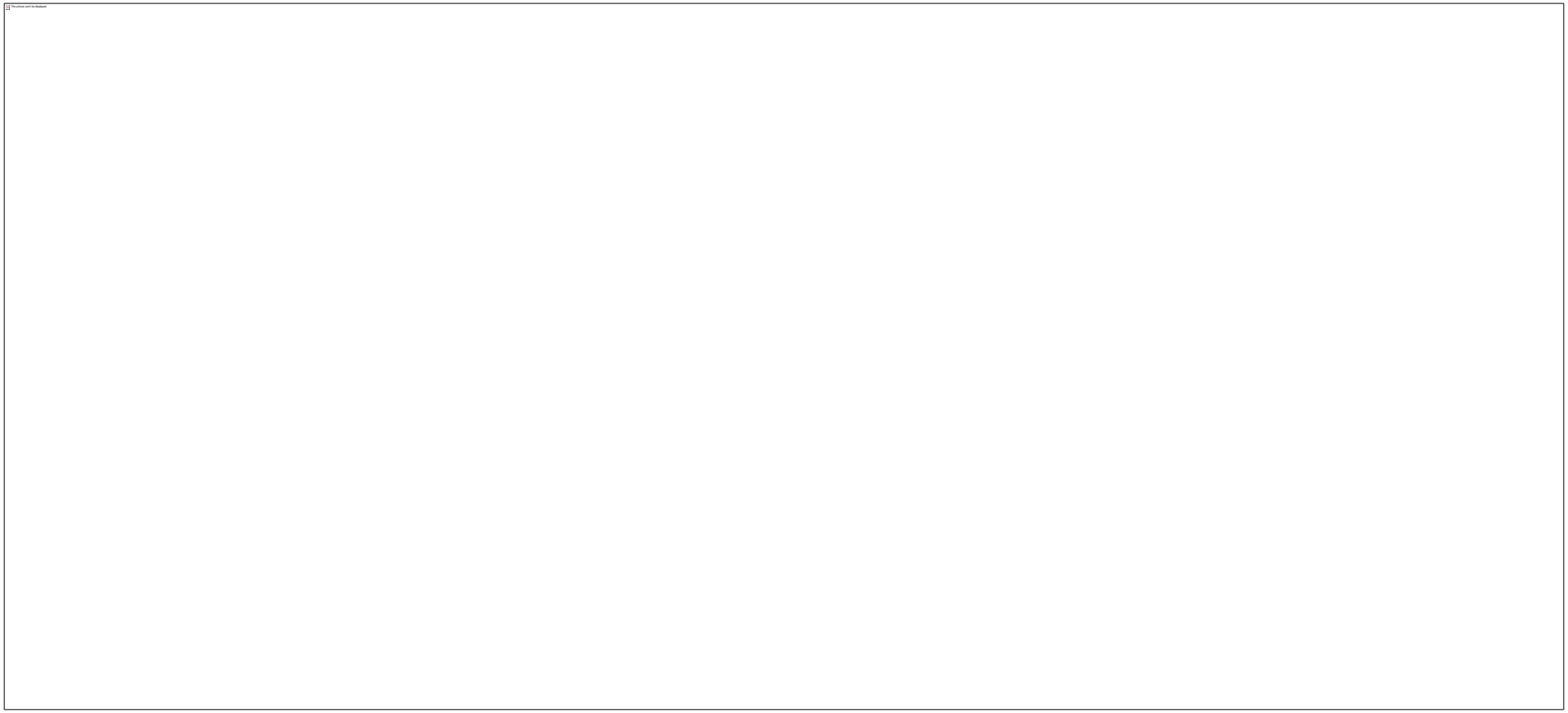
Regional and Global Mantle Flow Coupled with Pyre



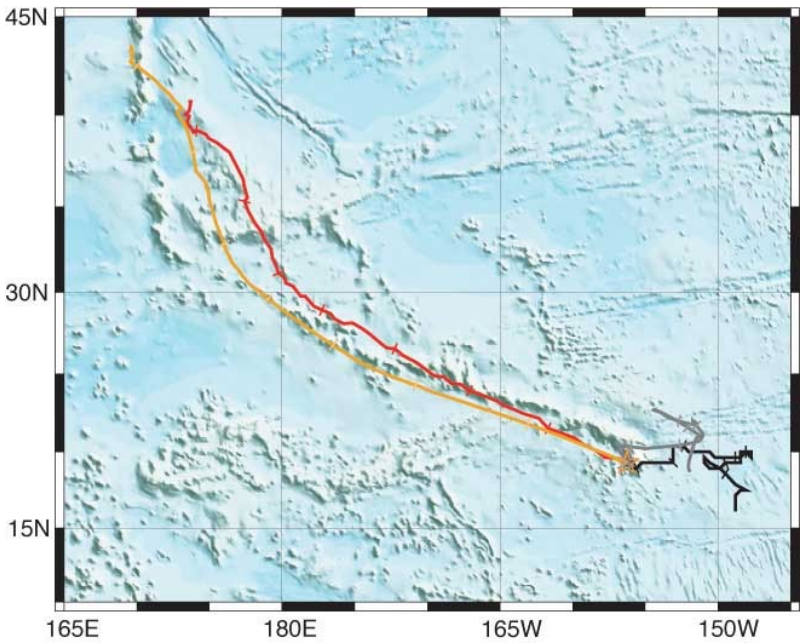


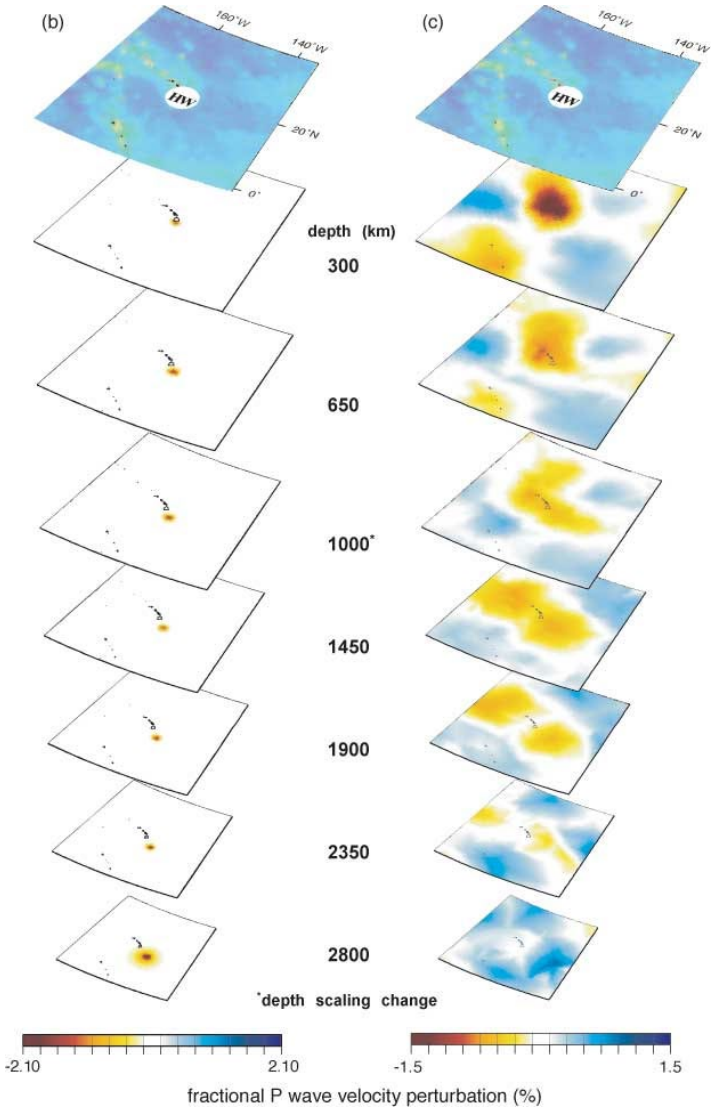
CitcomS.py, Eh Tan

Regional CitcomS coupled to full CitcomS



Predictions: Hot-spot track & synthetic tomography





Example: Mantle convection coupled to lithosphere

Superstructure

- Monitor Simulation
- Couple Fluid to Solid
- Visualization

Geodynamic Specific

- Self-contained geophysics (single phyiscs)
- Rheology modules

Infrastructure

- Mesher: Solid & Fluid
- Solver: Solid & Fluid

Library: PETSc, BLAS, MPI

Example of Geodynamic Specific & Infrastructure Layers

Geodynamic Specific

- SNARK -- particle based FEM with implicit solver
- SNAC -- Lagragian explicit FEM

Infrastructure

- StGermain: A framework with entry points & plugins for: building meshes, advecting particles, calling solvers, I/O…..

Library: PETSc, MPI

Example of Geodynamic Specific & Infrastructure Layers

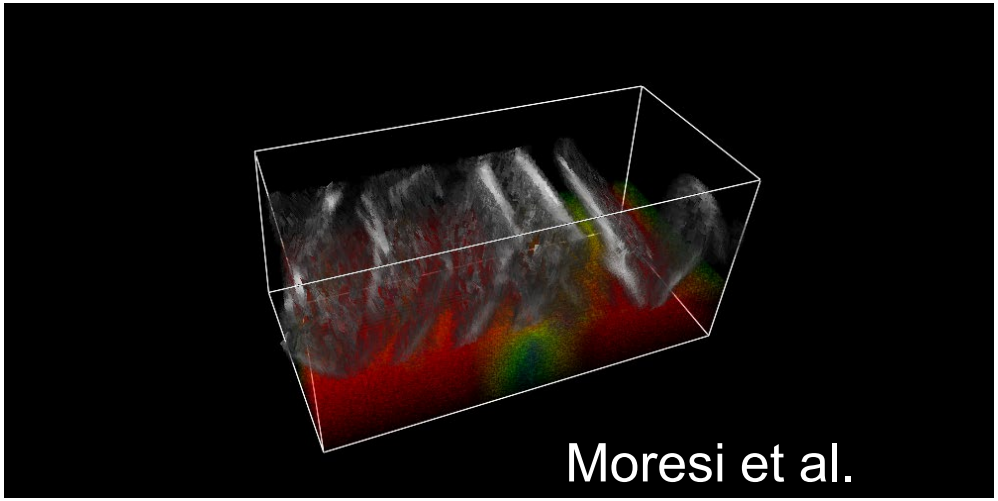
- SNARK -- particle based FEM with implicit solver
- SNAC -- Lagragian explicit FEM

Geodynamic Specific
SNARK: Monash group (Moresi)
SNAC: Caltech/Texas groups (Gurnis, Lavier)

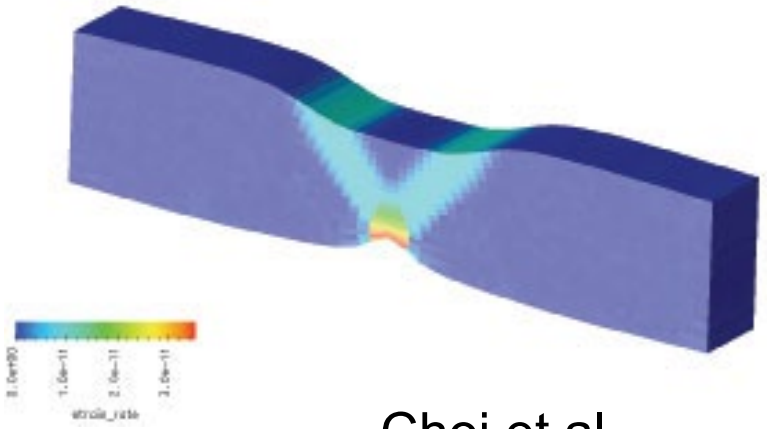
- StGermain: A framework with entry points & plugins for: building meshes, advecting particles, calling solvers, I/O…..

Infrastructure:
Software Engineers at the Victorian Partnership for Advanced Computing (Steve Quenette Team Leader)

SNARK & SNAC



Moresi et al.

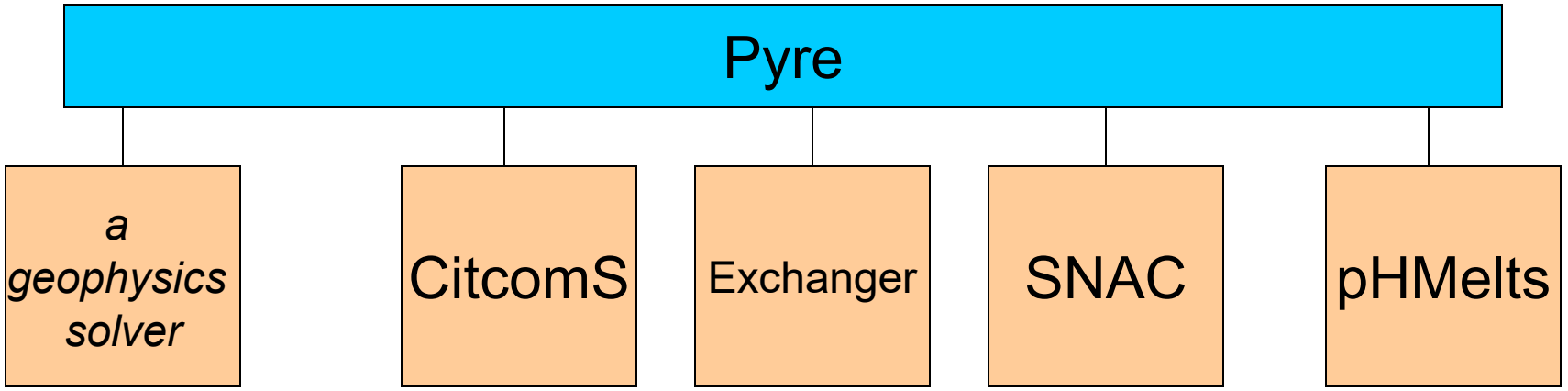


Choi et al.

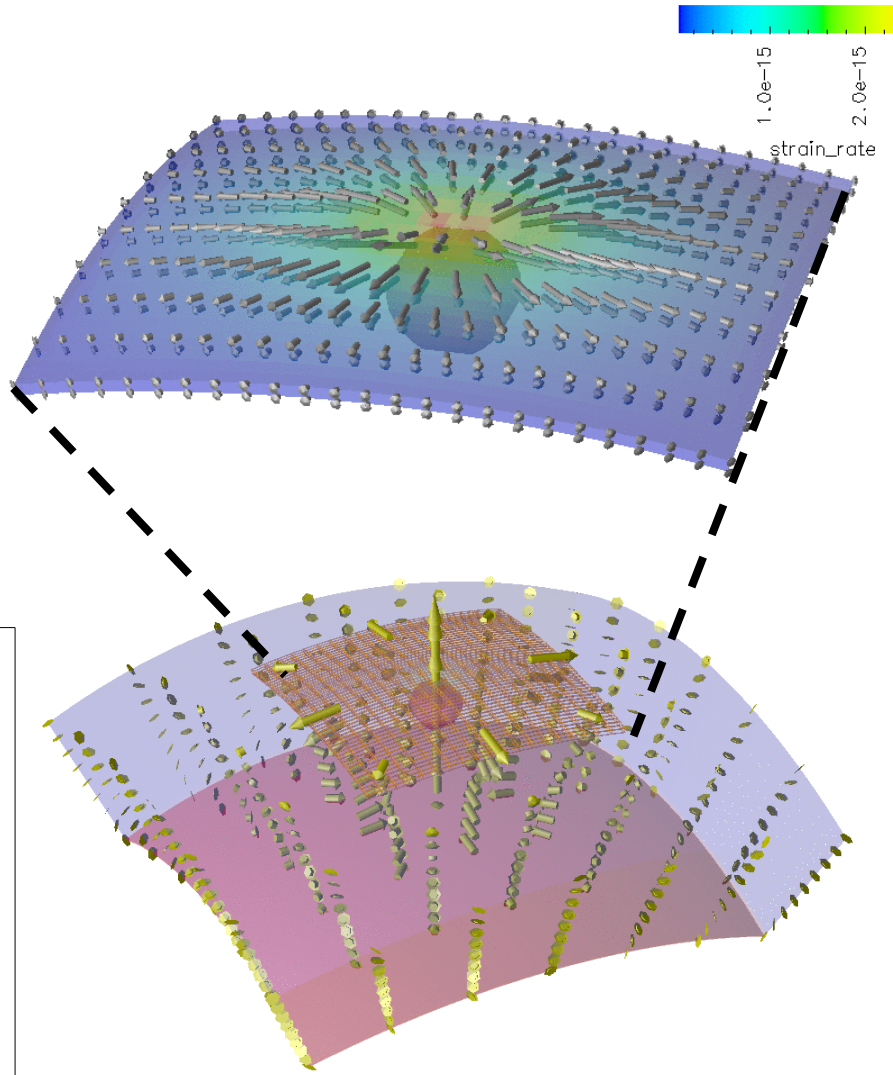
StGermain: A framework with entry points & plugins for: building meshes, advecting particles, calling solvers, I/O…..

Quenette et al.

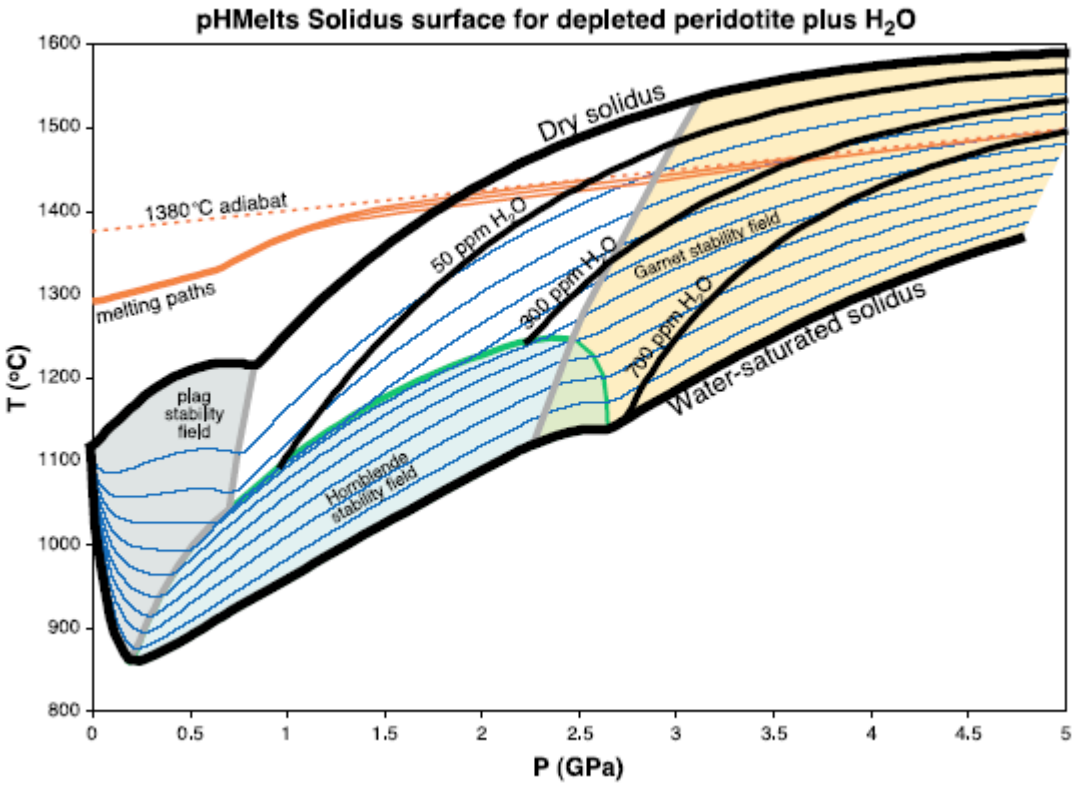
Examples of coupling codes with Pyre (“superstructure” framework): GeoFramework



SNAC CitcomS coupling (Crust-Mantle Interaction)



Eun-seo Choi et al.



pHMelts petrological model

(Asimow et al., 2004)

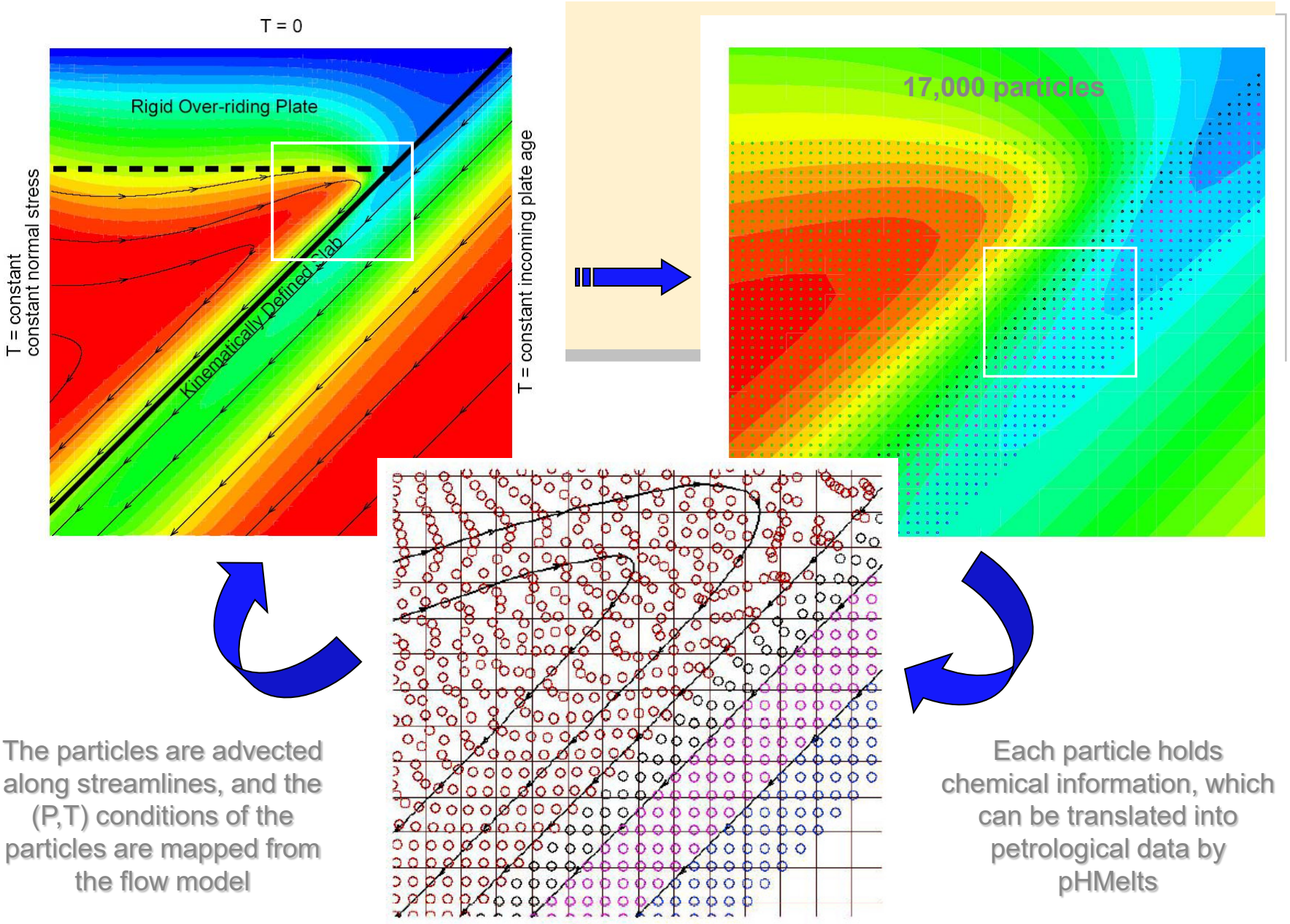
Advantages:

pHMelts uses trace element partitioning to distribute water between the system and the nominally anhydrous minerals (NAM)

Major and trace element information can be collected

Both hydrous and nominally anhydrous phases can be handled in a single model

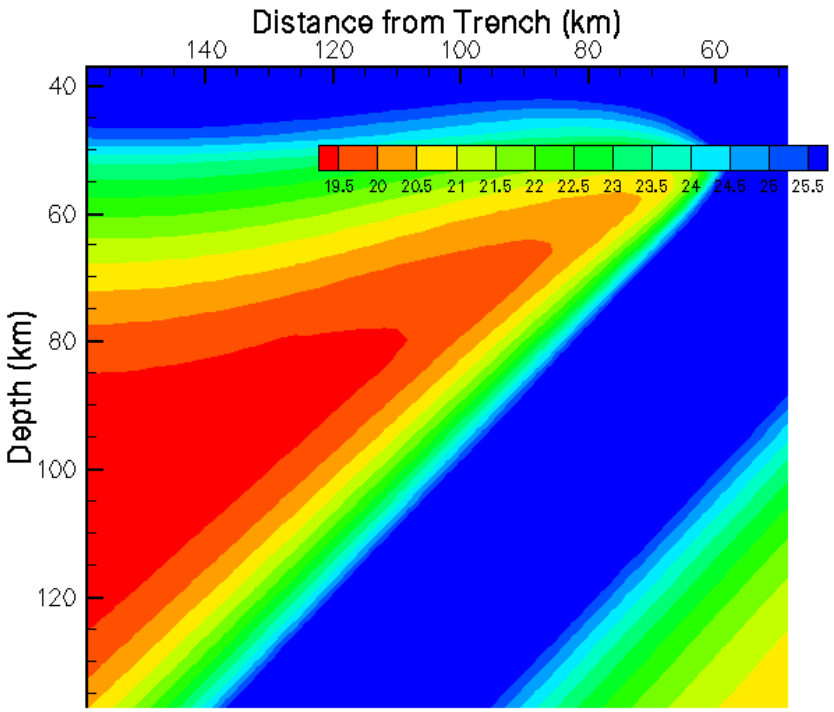
<u>Output</u>: mineral stability, mineral chemistry (major and trace element), melt presence and chemistry, phase proportions, water content in NAM, free water presence and normalized amount



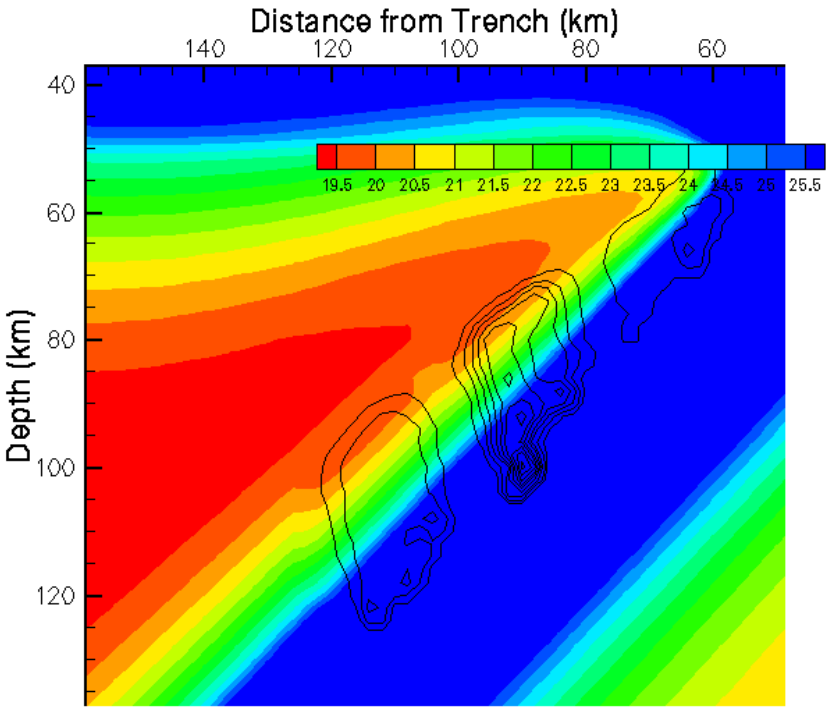
The particles are advected along streamlines, and the (P,T) conditions of the particles are mapped from the flow model

Each particle holds chemical information, which can be translated into petrological data by pHMelts

Baker, Hall, Smith, Asimow, & Gurnis



(1) Initial viscosity structure



(2) Viscosity structure calculated after slab-water influx

Some lessons for other geophysicists

- Frameworks, both higher level like Pyre and lower level like StGermain, show enormous potential for Earth science problems
- We've now been able to start to address more complex multi-physics and multi-scale problems -- problems long recognized to be important but previously intractable
- It is possible, in some cases, to effectively reengineer codes so that they can be used in frameworks
- Working geophysicists can effectively collaborate with software engineers.