Progress, Current Status, and Development Plans for PyLith/LithoMop

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Other People Involved in Code Development

- **Brad Aagaard (USGS)**

  - *External packages, merging of LithoMop and EqSim into PyLith.*

- **Matt Knepley (CIG/ANL)**

  - *PETSc implementation, parallelization.*

- **Michael Aivazis (CIG/CACR)**

  - *Pyre/pythia.*

What Is LithoMop?

- Finite element code for modeling quasi-static problems in tectonics.

- Includes faults ('split' nodes and 'slippery' nodes.

- Includes rheologies appropriate for earth materials (elastic, viscoelastic, elasto-plastic, viscoelastic-plastic).

- Integration into Pyre framework facilitates coupling/interaction with other codes.

Timeline of Code Development

- **Fall, 2003:** Initial integration of TECTON into Pyre framework. Performance on SCEC benchmarks ~1-2% slower than standalone TECTON.

- **Fall, 2003 - March, 2004:** Code renamed PyCrust. Reworking of code logic in anticipation of future changes, and more use made of Pyre features such as automatic unit conversions.

- **March, 2004 - July, 2004:** Code renamed Lithomop due to name conflict with existing software package. Extensive code modifications to allow for multiple element types and new modular methods of defining material models. Reworking of code logic to increase efficiency and to prepare for the task of code parallelization.

- **August, 2004:** Release of preliminary version of Lithomop3d for testing, primarily by the SCEC Crustal Deformation modeling group. This is an 'alpha' version, with some missing features and a few unresolved bugs. Performance ~2-20% faster than standalone TECTON.

- **Fall, 2004:** Release of beta version of Lithomop3d.

# Timeline of Code Development (cont.)

- September, 2004 - February, 2005: Added automatic computation of gravitational prestresses. These were implemented for elastic and linear Maxwell viscoelastic materials, and equations have been worked out for power-law viscoelastic materials. Complete reworking of force vector setup, improving efficiency and facilitating eventual use of PETSc.

- March - June, 2005: Upgraded code for pythia-0.8 (previously used pythia-0.5). Initial usage of PETSc for linear solution, resulting in a factor of 2 performance improvement (code is still serial). Code logic changed so that looping is now performed over element families, reducing the amount of indexing, simplifying structure, and increasing performance. Major reworking of python driver for more modular code structure. Fixed problems associated with split nodes, slippery nodes, Winkler elements, and local coordinate rotations.

- June - July, 2005: Added output option for binary UCD format, resulting in much smaller file sizes. Debugging and packaging of code. Entire package consisting of PETSc, MPICH2, pythia-0.8, and LithoMop now available as a tarball. Posted installation and testing instructions on web. Tutorial using SCEC BM 5 posted on web.
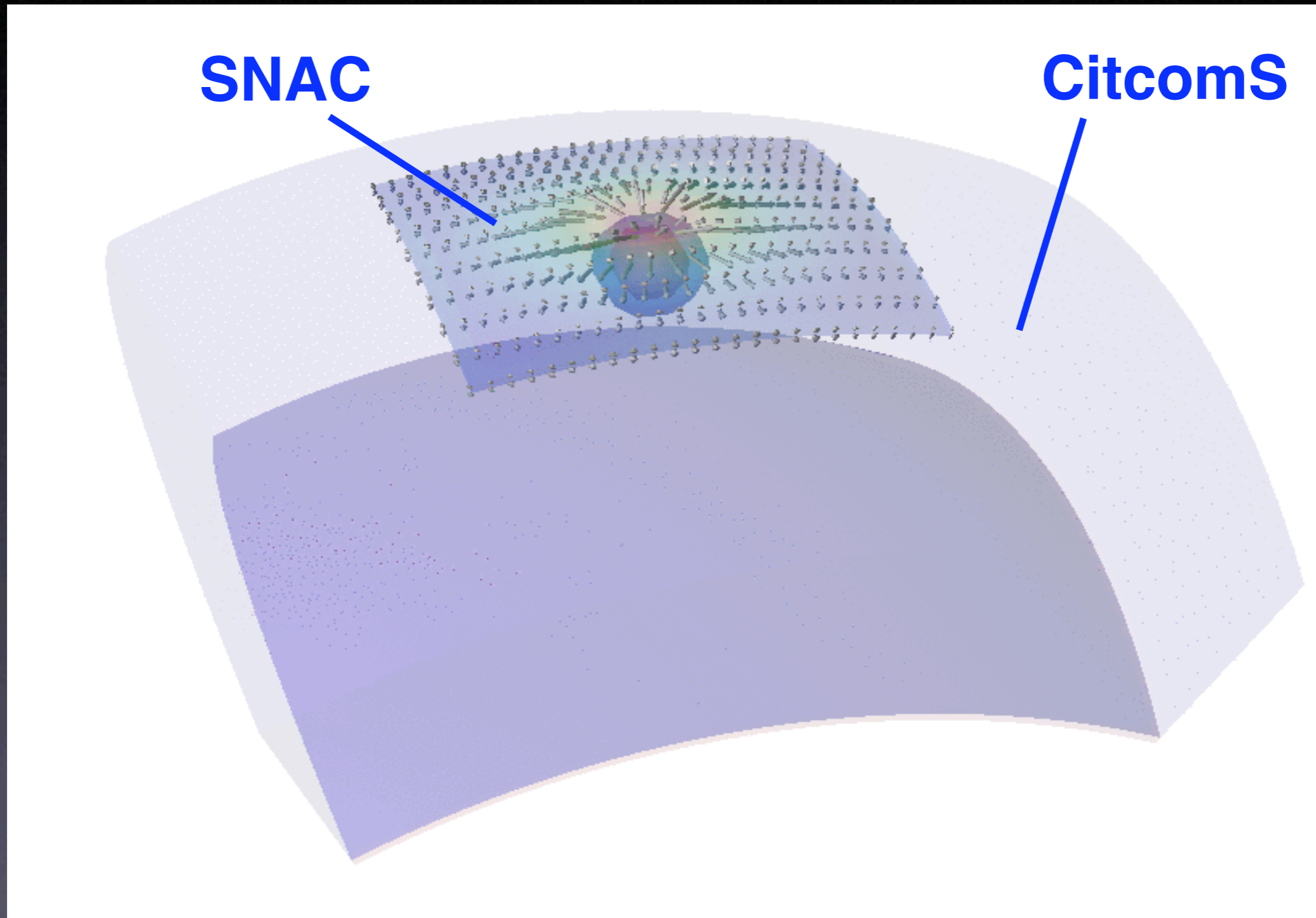
Pyre Architecture
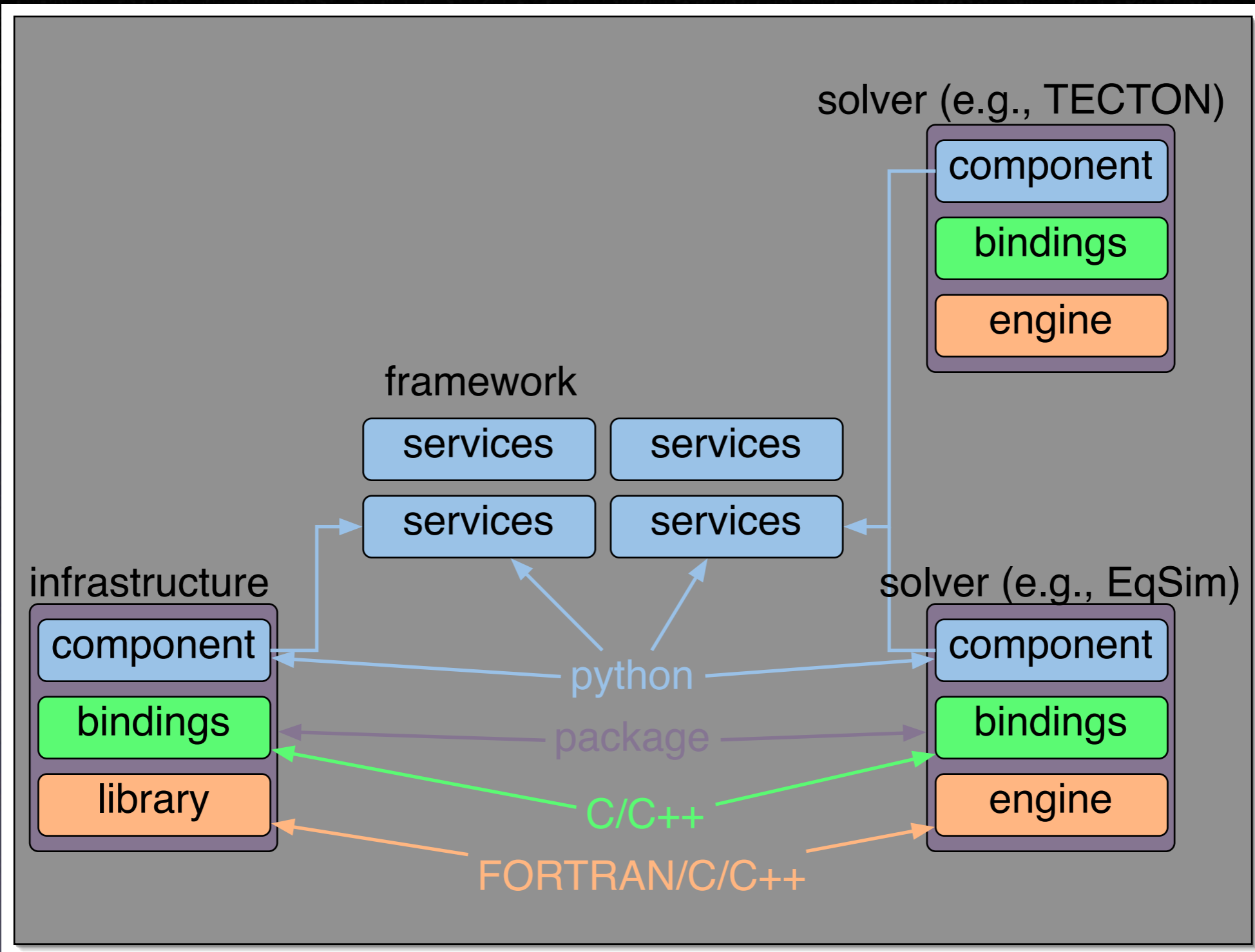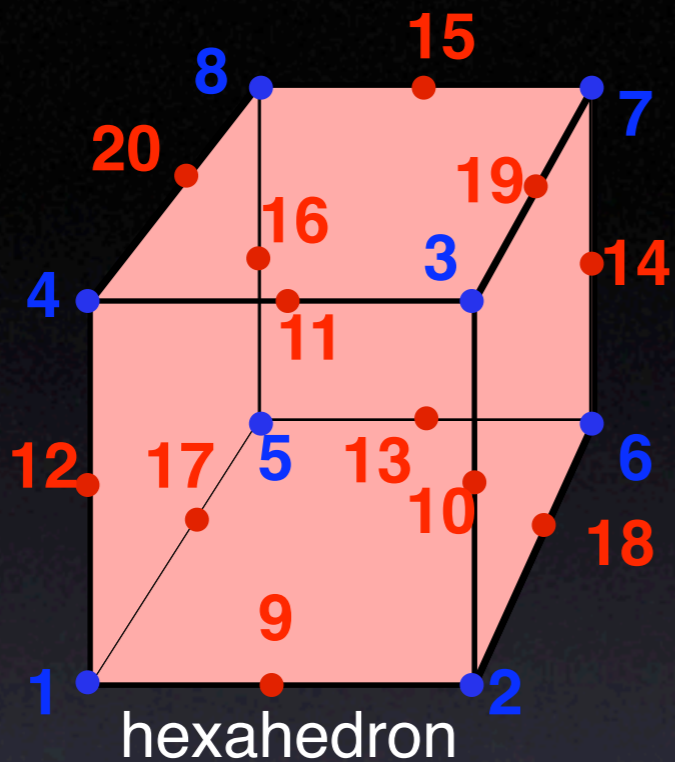
Examples of Code Coupling Using Pyre
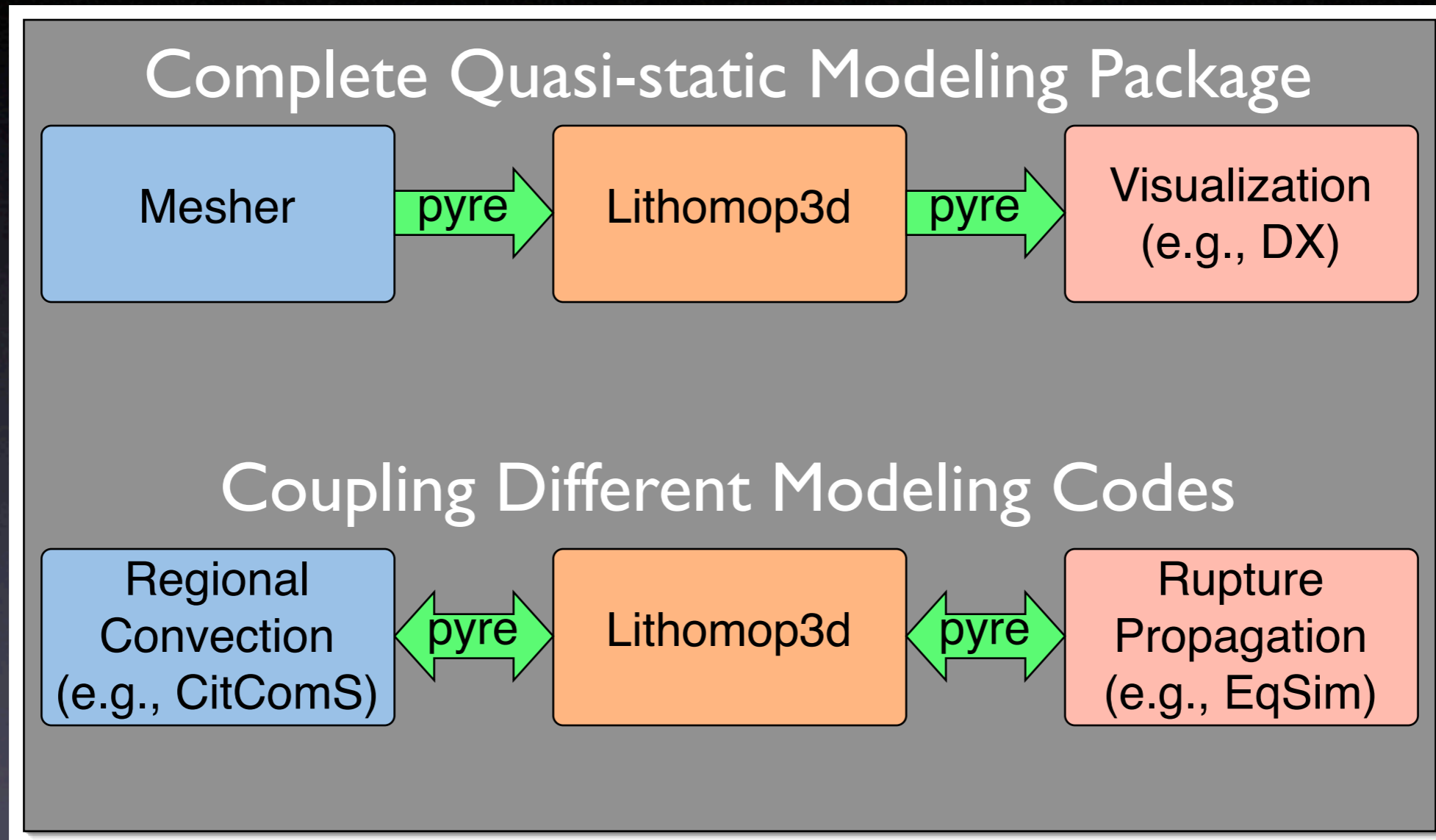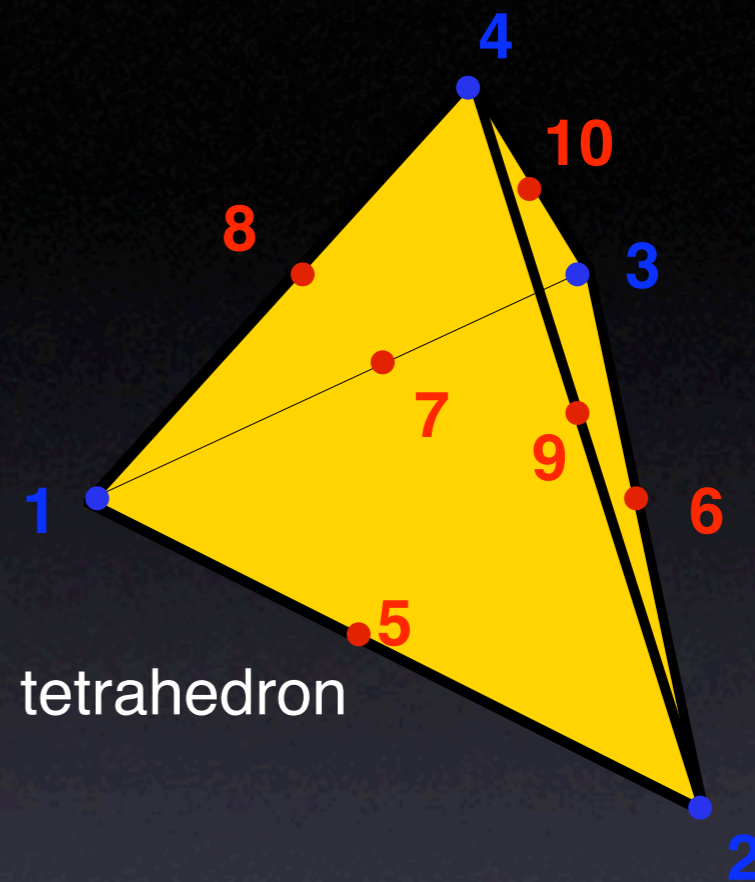
CitcomS Coupled With SNAC via Pyre

SNAC

CitcomS

E. Choi, August, 2004

Current Element Types in Lithomop3d
10 Types Total (Linear + Quadratic)

Primary Elements

hexahedron
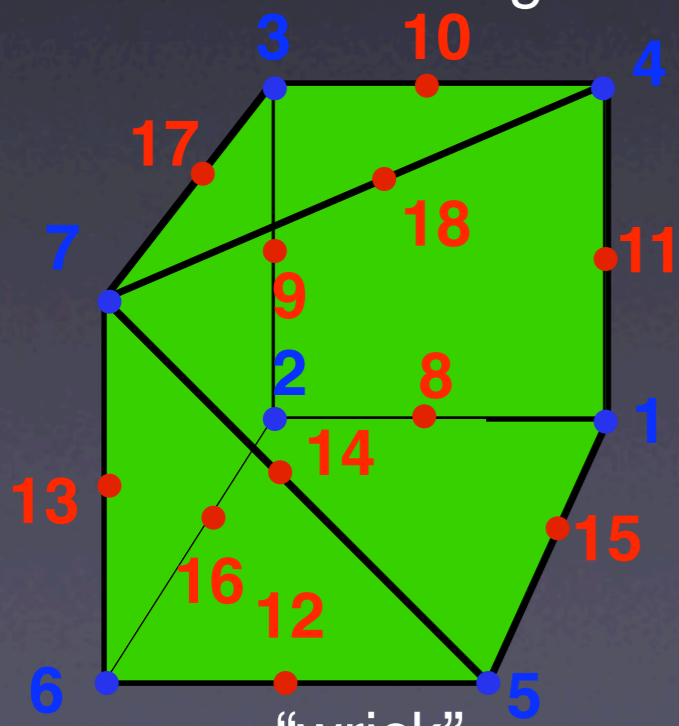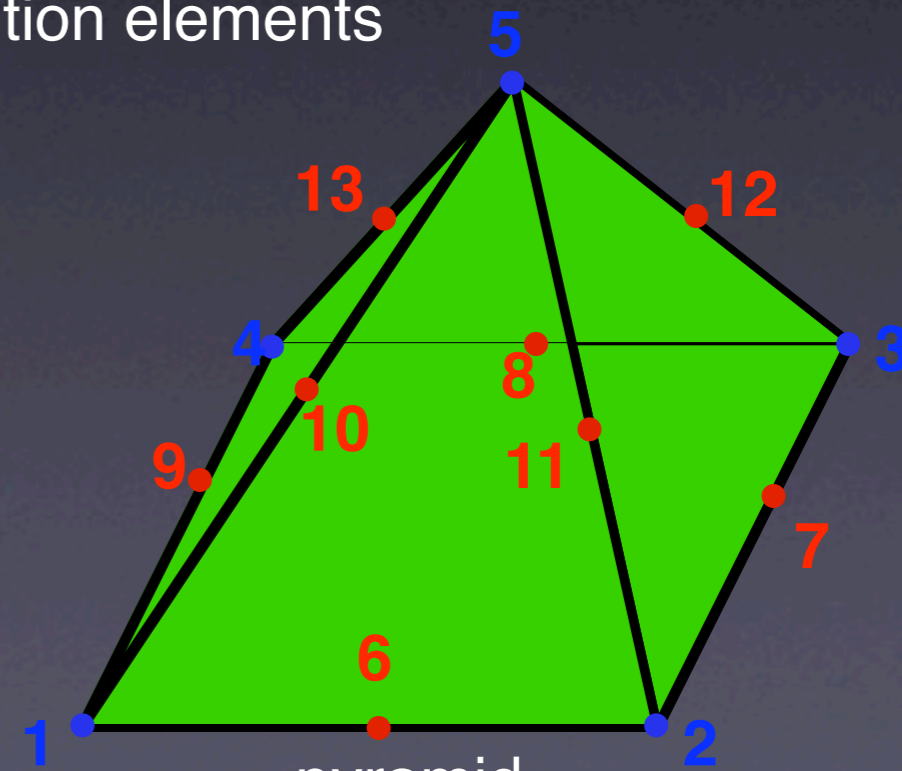
tetrahedron

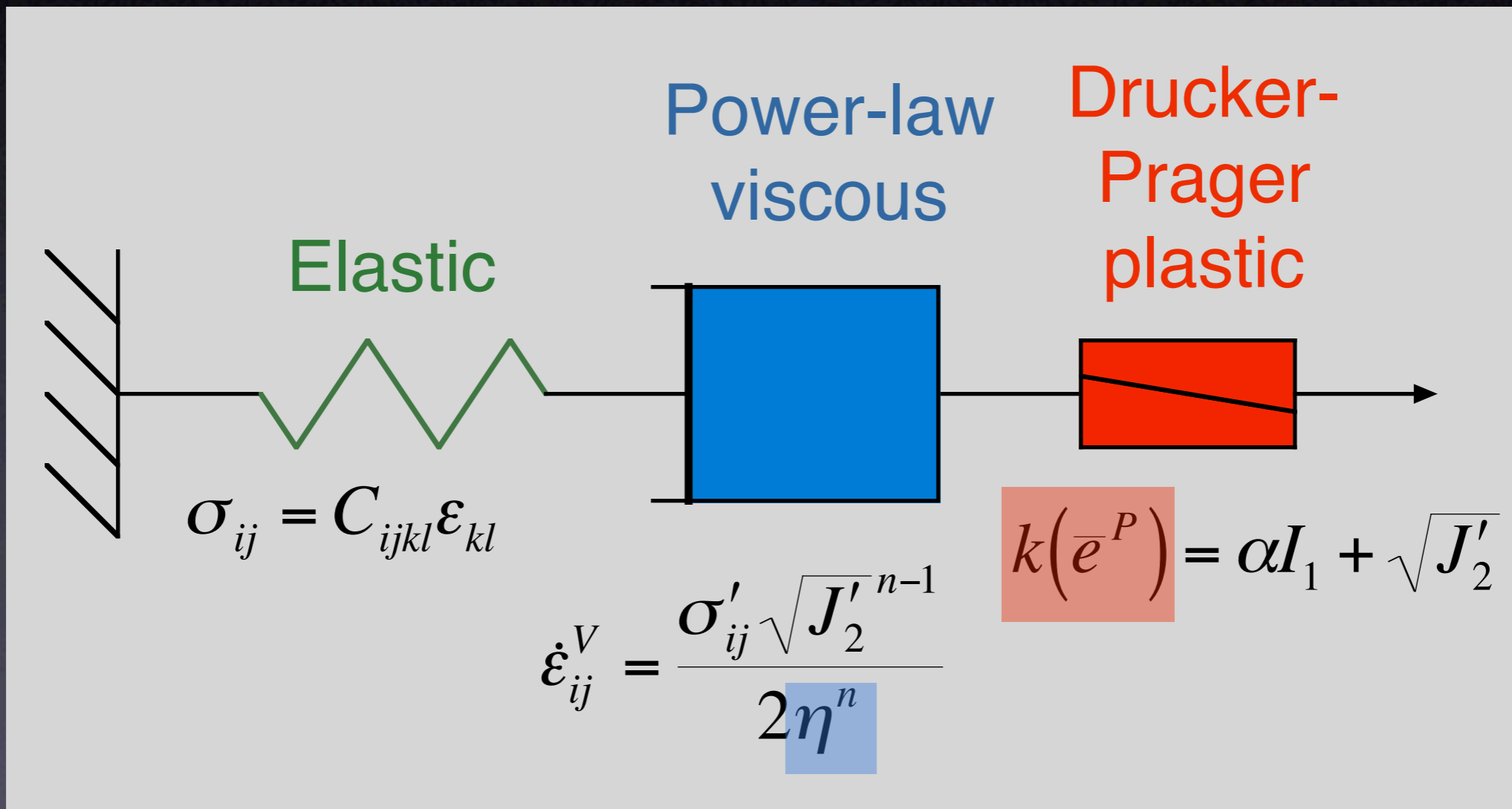Degenerate Hexahedra -- Used as transition elements

"wrick"

wedge

pyramid

TECTON 1.0 Material Property Specification

Elastic

Power-law viscous

Drucker-Prager plastic

$$\sigma_{ij} = C_{ijkl}\varepsilon_{kl}$$

$$\dot{\varepsilon}_{ij}^{V} = \frac{\sigma_{ij}'\sqrt{J_2'}^{\,n-1}}{2\eta^{n}}$$

$$k\left(\bar{e}^{P}\right) = \alpha I_1 + \sqrt{J_2'}$$

Lithomop Material Property Specification

Elastic

Viscoelastic

Elasto-plastic

Viscoelastic/plastic
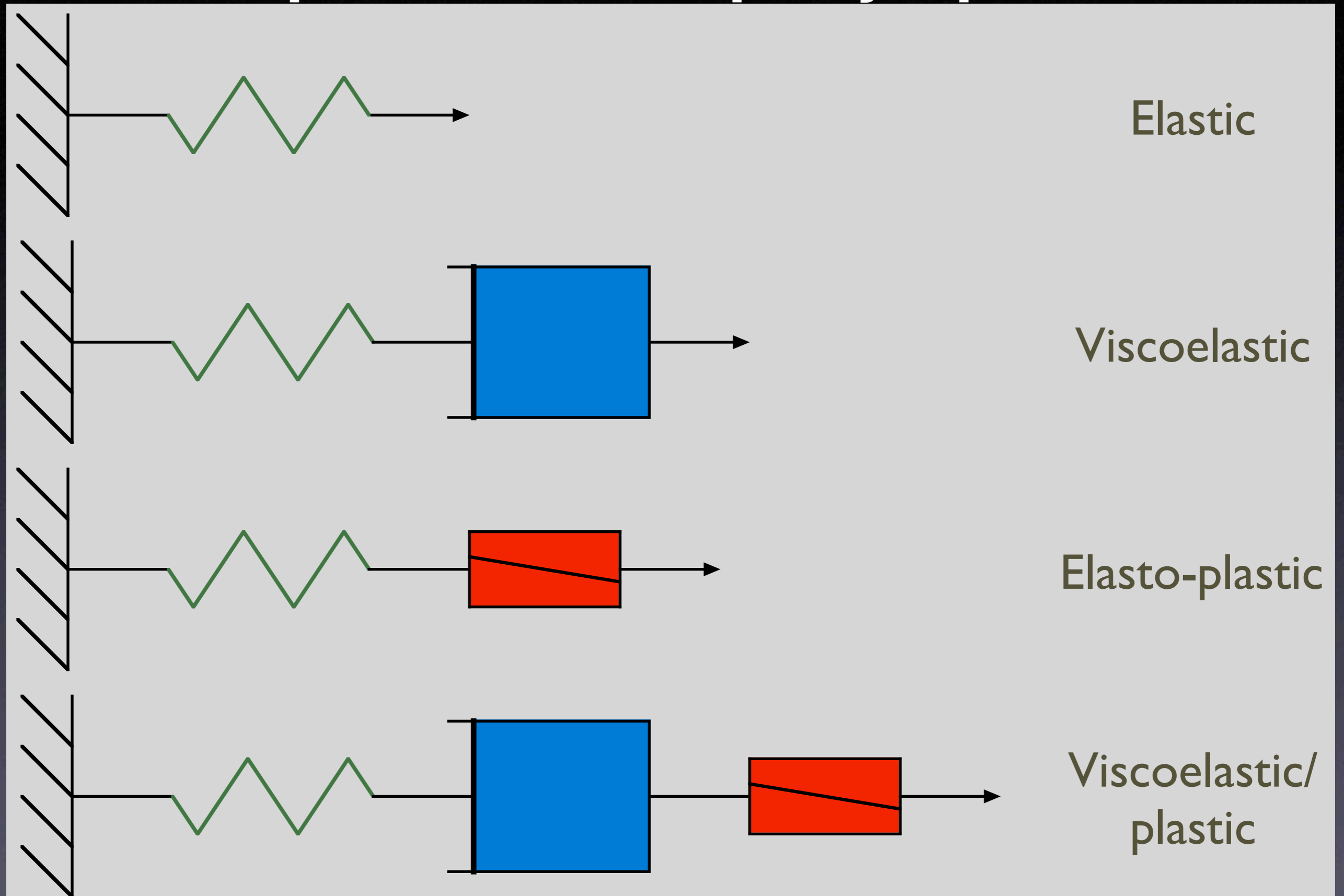
Planned Material Models for LithoMop3d

Model	TECTON 1.0	Lithomop3d
1. Isotropic Elastic	Yes	Yes
2. Transversely Isotropic Elastic	No	Planned
3. Orthotropic Elastic	No	Planned
4. Anisotropic Elastic	No	Planned
5. Maxwell Linear Viscoelastic	Yes	Yes
6. Maxwell Power-Law Viscoelastic	Yes	Planned
7. Drucker-Prager Elasto-Plastic	Yes	Planned
8. Model 5 + Model 7	Yes	Planned
9. Model 6 + Model 7	Yes	Planned

Advantages of Using PETSc

- Easy access to a number of fast solution algorithms.

- Can easily set most options from command line.

- Debugging facilities.

- Greatly simplifies the task of code parallelization.

  - High-level interface to MPI routines.

  - High-level interface to parallel data structures and solution algorithms.

Automatic Computation of Prestresses

Initial State	Gravity 'turned on'	Elastic Solution
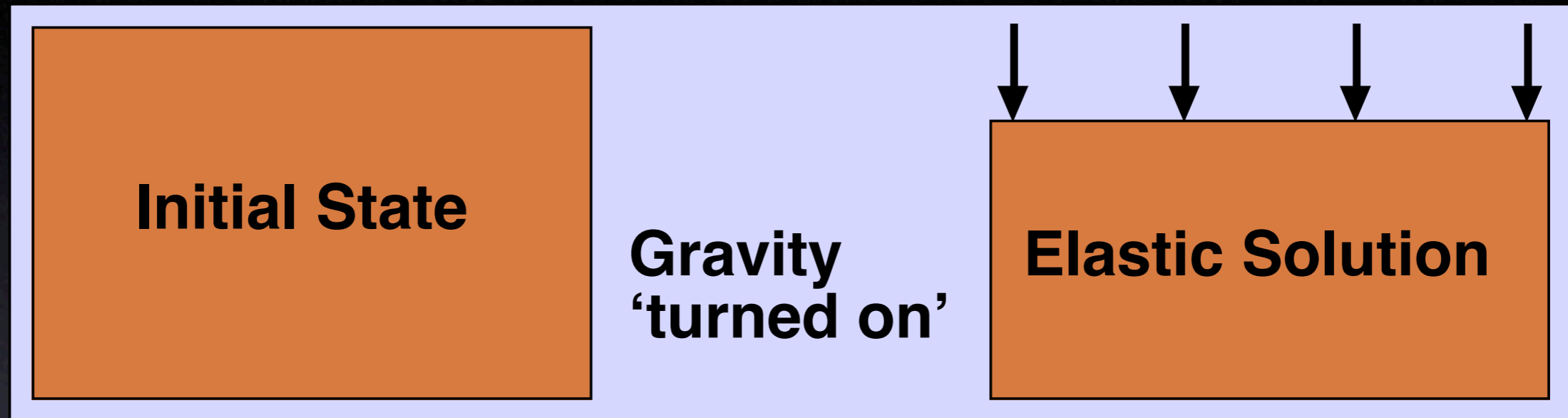
- Application of gravity results in unrealistically large initial deformation.

- Solution is to apply initial stresses to cancel gravity.

- This is now done automatically in LithoMop.

- Using this method, it is also possible to avoid the Poisson's ratio problem with gravity.

Code Usage - SCEC Benchmarks

BM5
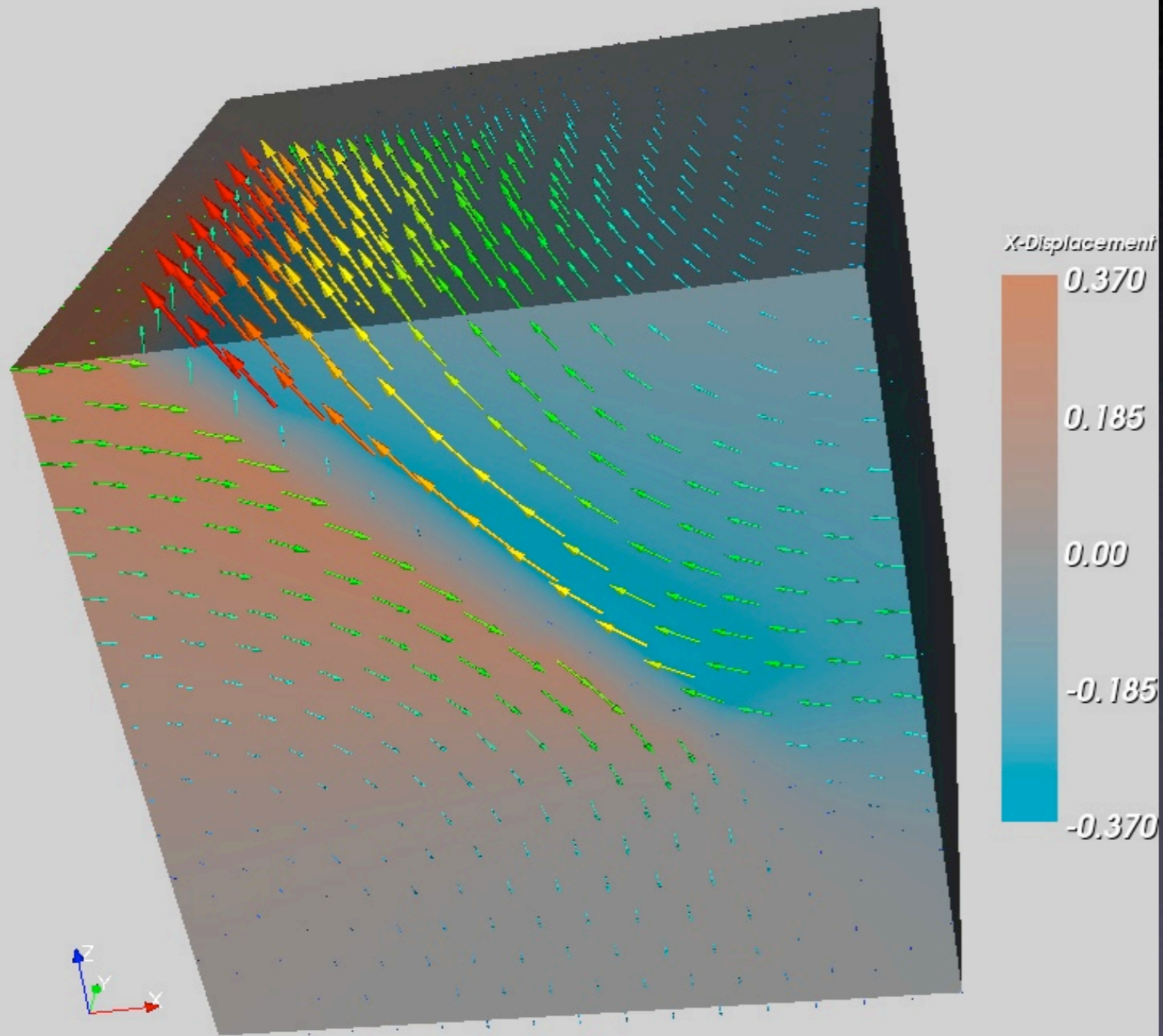
X-Displacement

0.370

0.185

0.00

-0.185
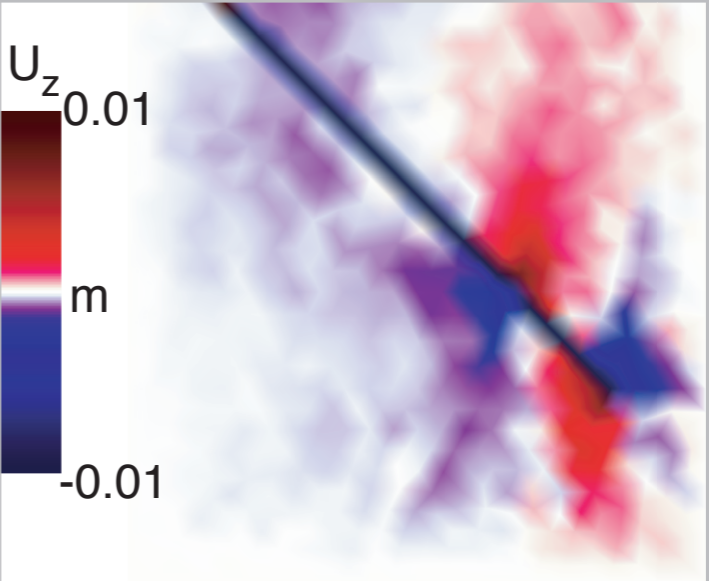
-0.370

BM7
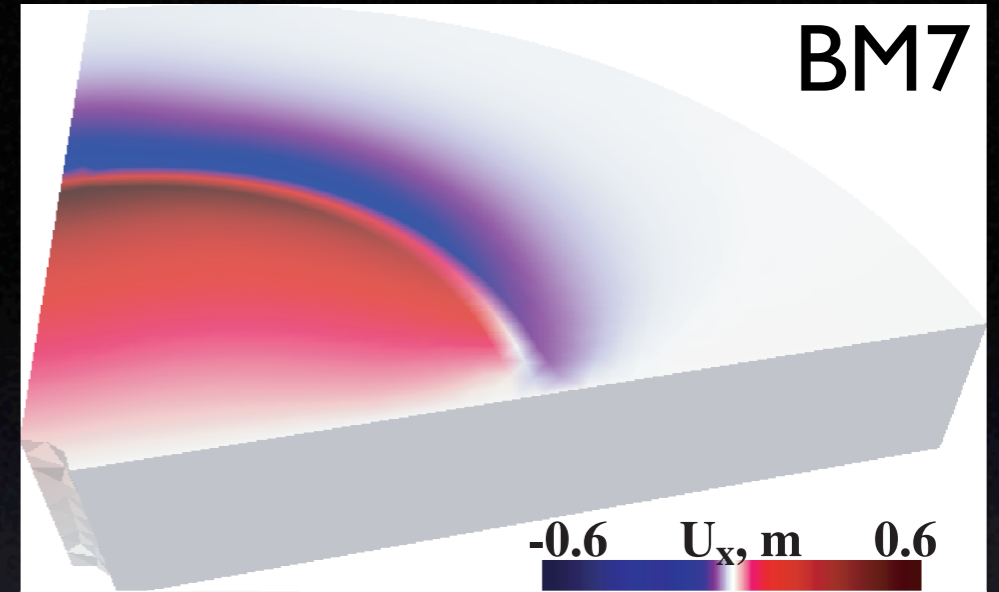
-0.6 U_x, m   0.6
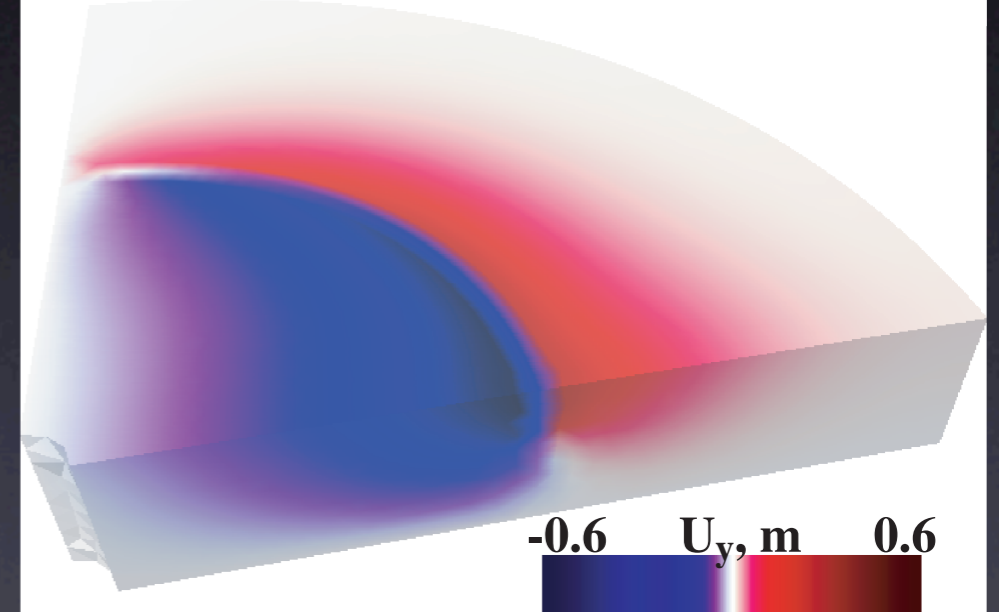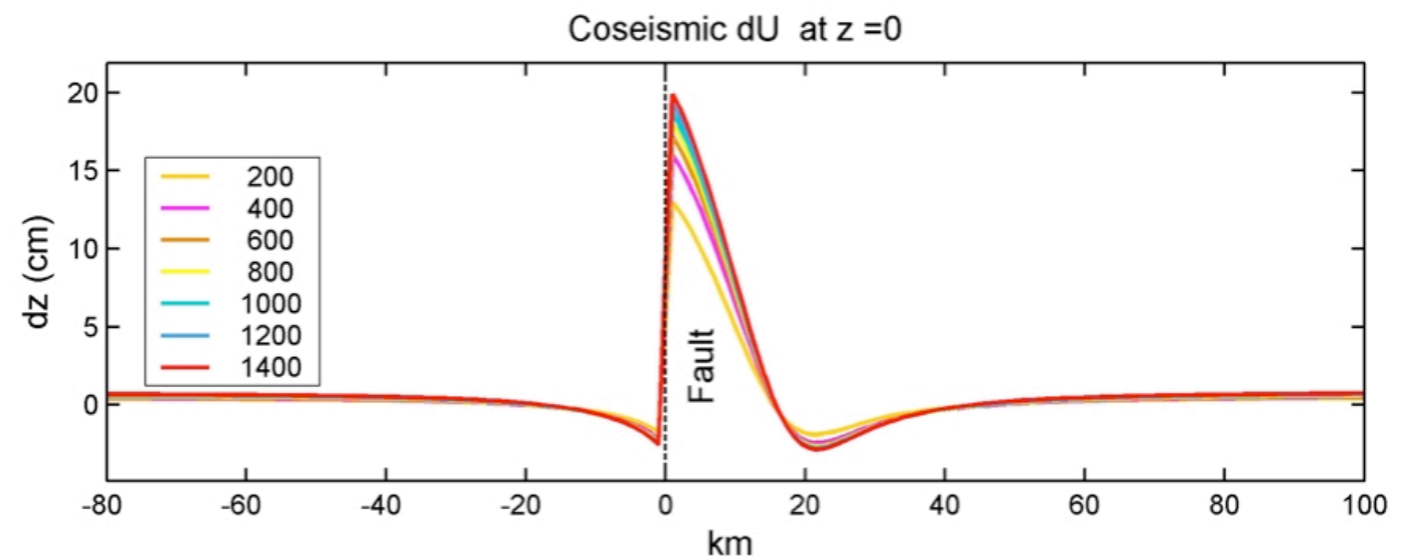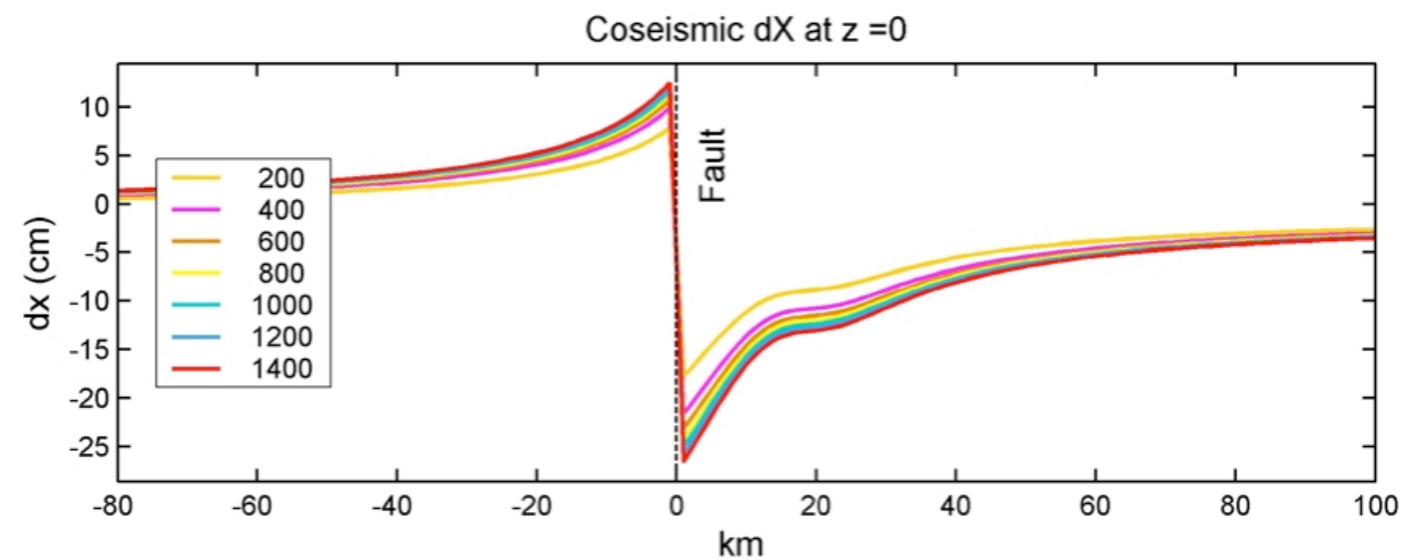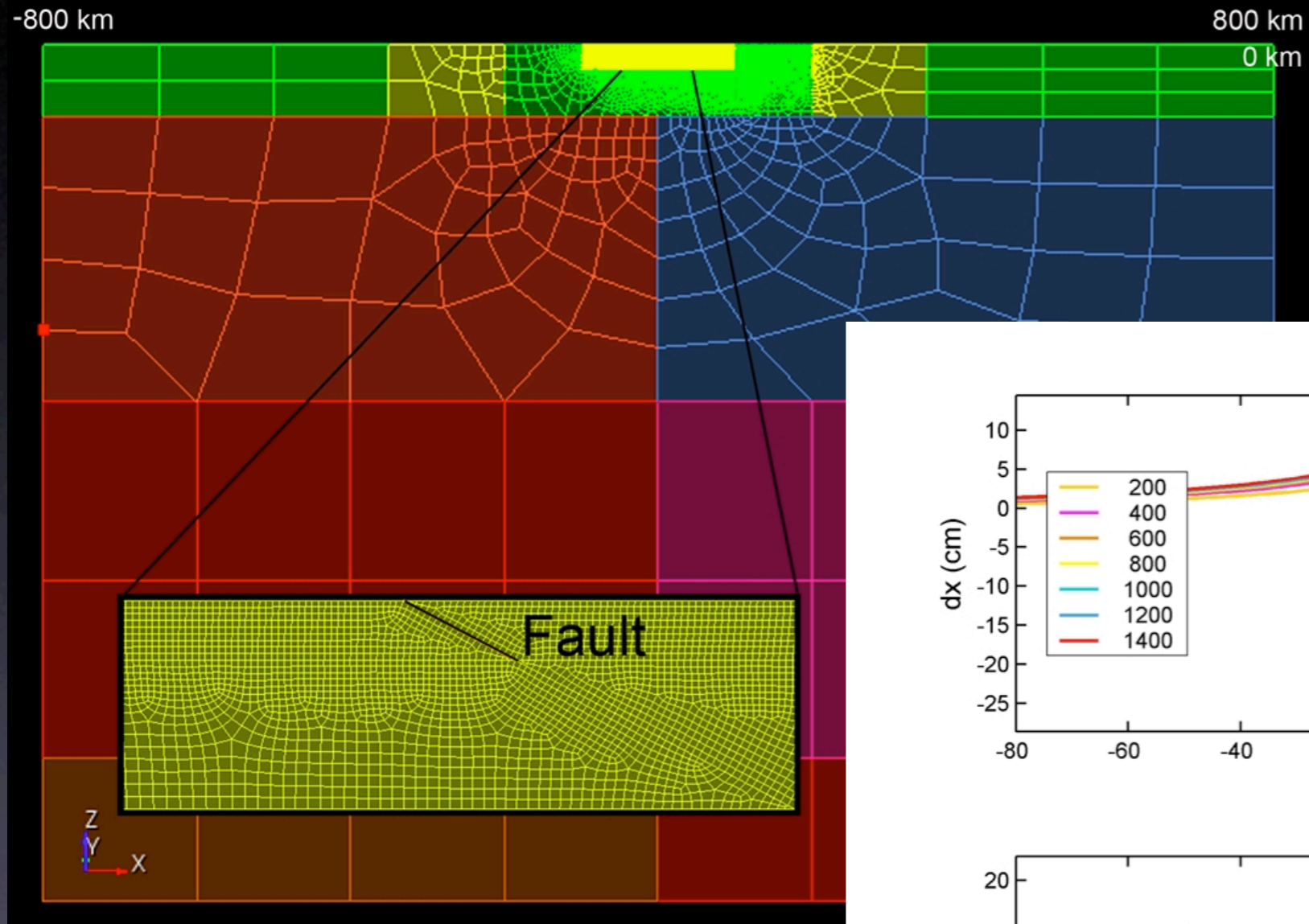
-0.6 U_y, m   0.6
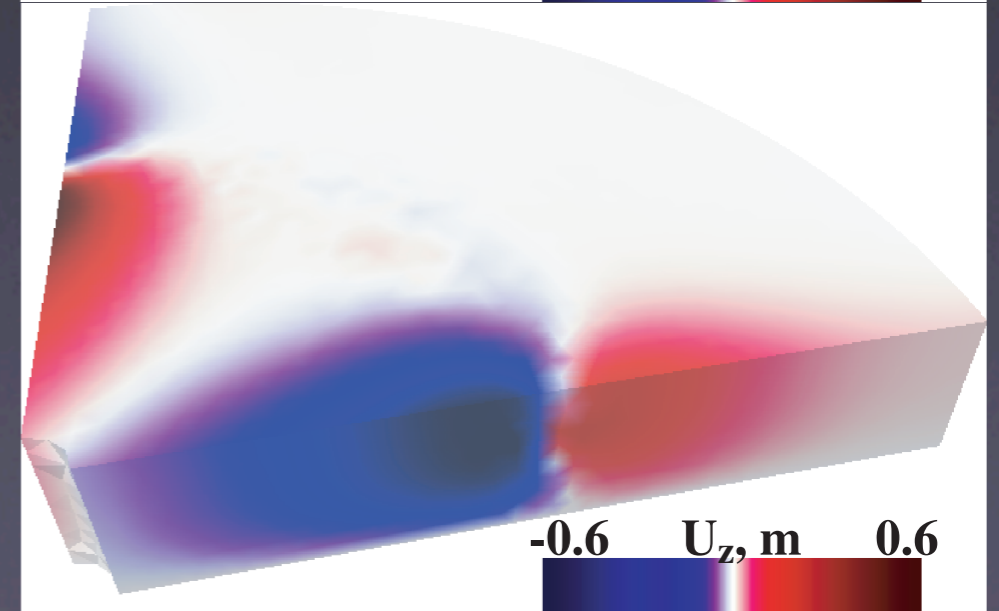
-0.6 U_z, m   0.6

Misfits for SCEC BM 5
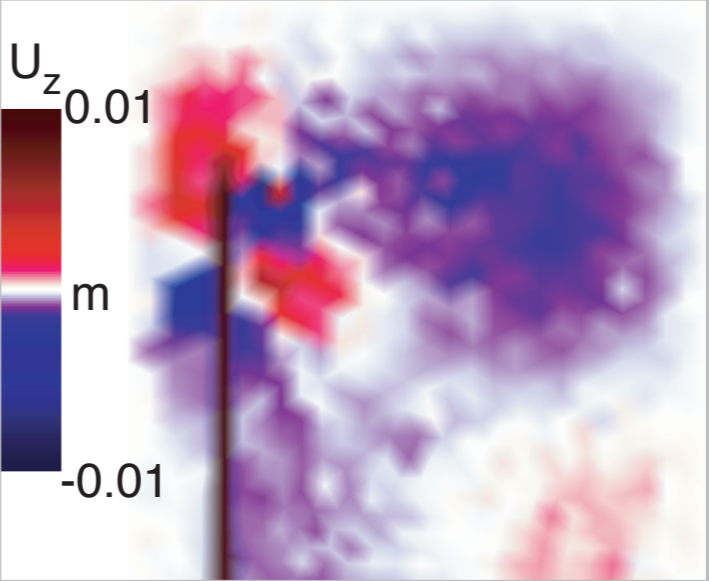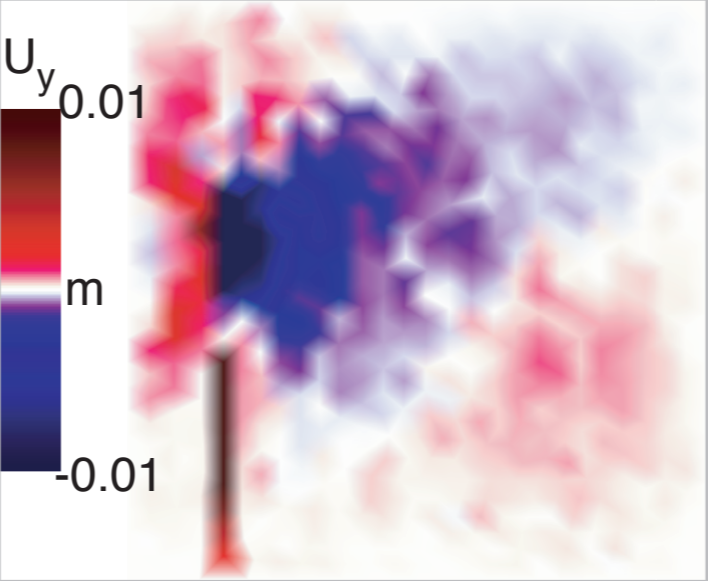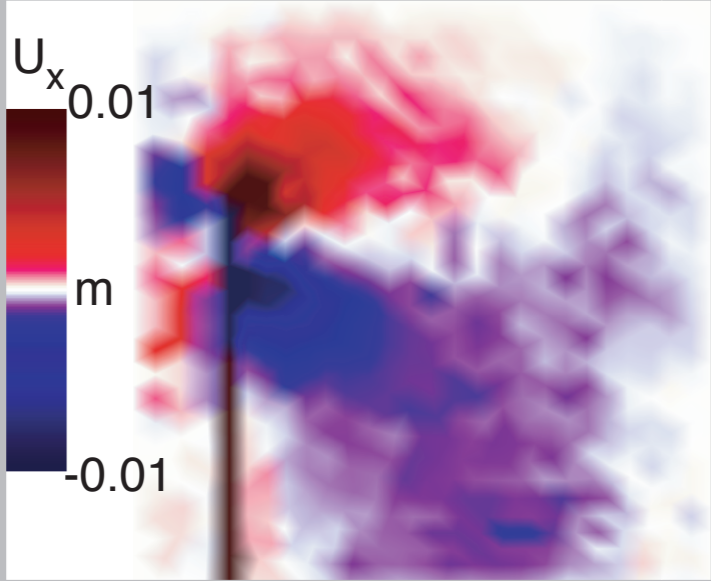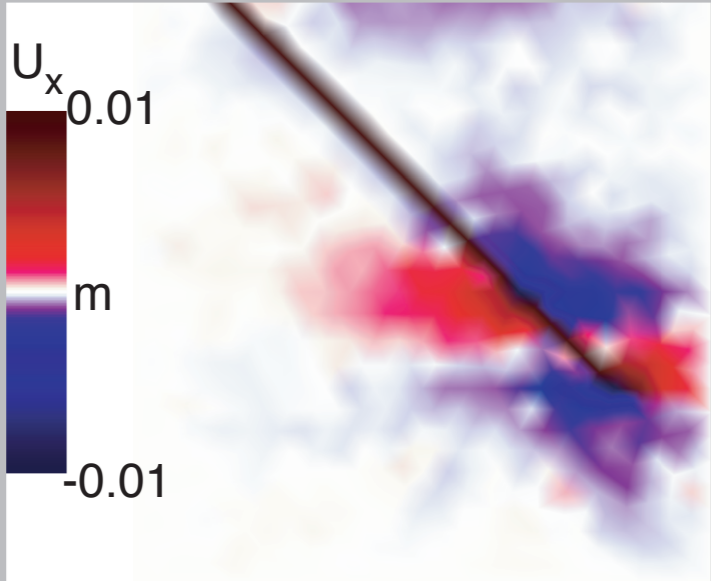
Code Usage - Multiple Earthquake Simulations for Taiwan


From Ya-Ju Hsu [2005]

What's Next?

- Code parallelization, making use of CIG package for mesh partitioning and refinement.

- Use of spatial database for specification of boundary conditions and material properties.

- Use of cohesive elements to represent faults.

- Improved use of Pyre, such as Simulation Controller.

- Addition of new material models, missing features, etc.

- Eventual merging of LithoMop and EqSim (dynamic rupture propagation code) into PyLith.

- Comprehensive set of benchmarks, set up for both serial and parallel computation.
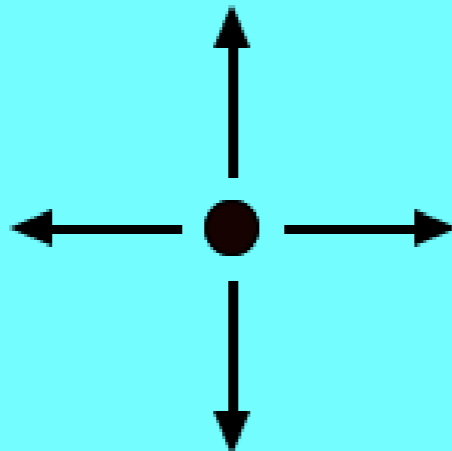
Cohesive Elements

- Kinematic case: Specified Slip on nodes.

- 'Dynamic' case: Slip determined by element constitutive relationship.

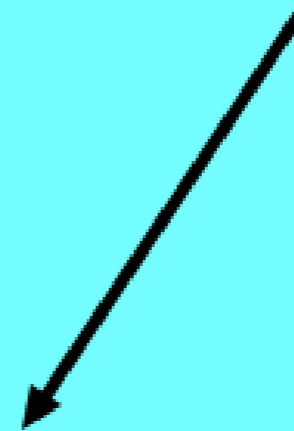From WARP3D Manual

inter_8

trint6

trint12
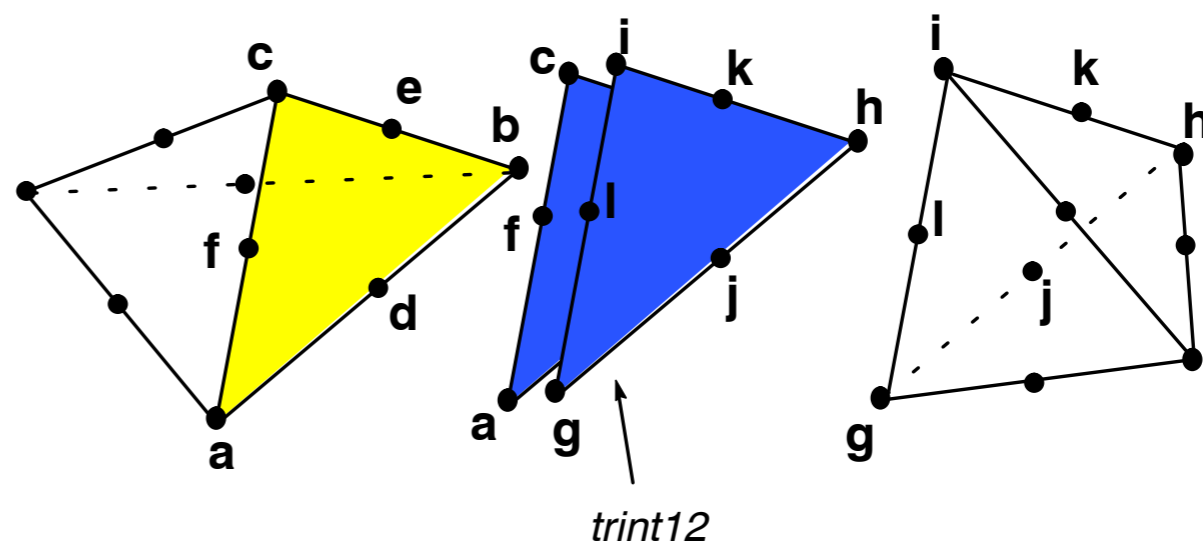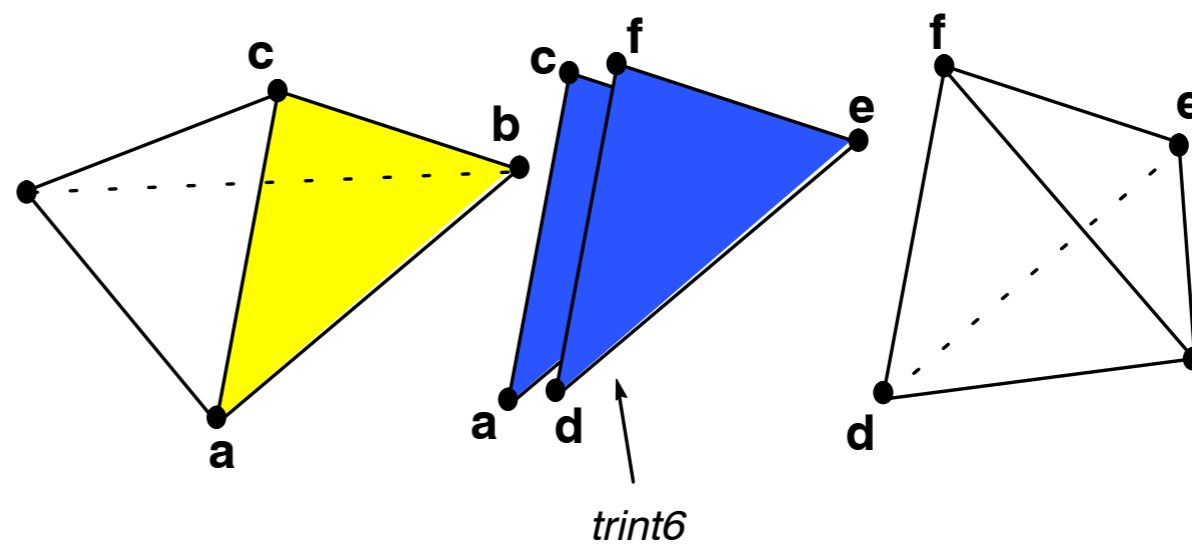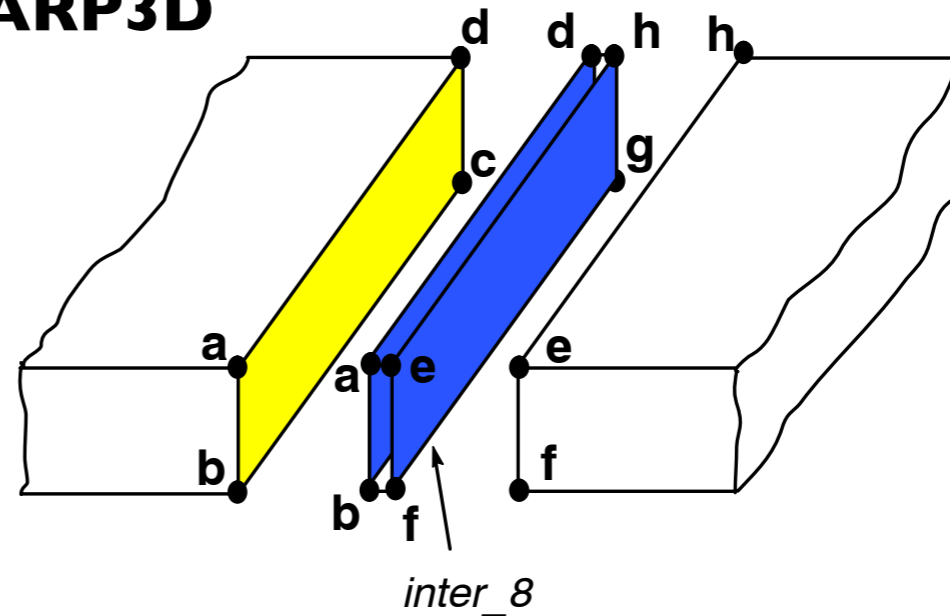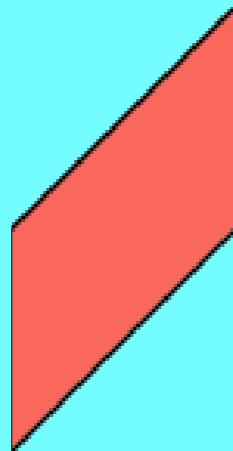
Simple Spatial Database

Point

Constant material properties
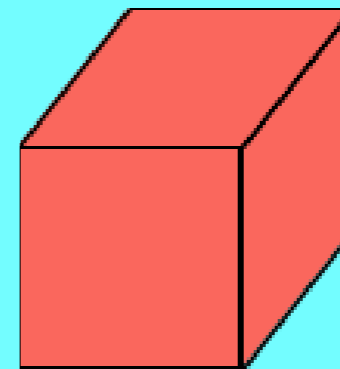Uniform boundary conditions

Line

Depth-varying material properties
Linearly-varying boundary conditions

Plane

Fault slip distribution
BC on external boundary

Volume

Heterogeneous material properties

Mesh Creation

Meshing Package
LaGriT, CUBIT,
NetGen, etc.

CIG Package

Partitioning

Uniform Refinement
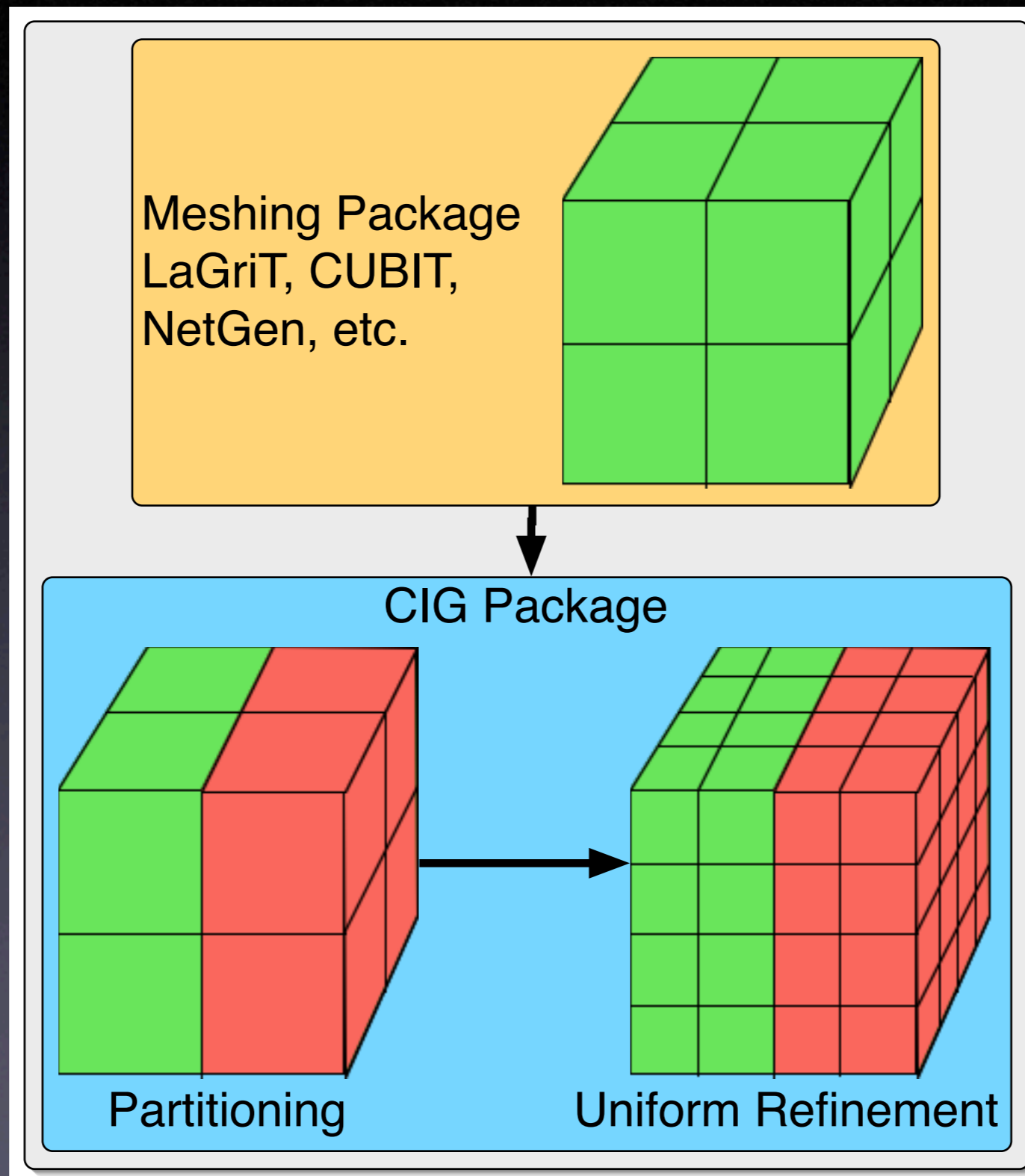
Simpler User Interface

- Meshing package generates nodal coordinates, connectivities, node lists, and element lists.

- Partitioning/refinement package provides partioned mesh, including faults created from node lists.

- BC are applied by associating node lists with a spatial database. Both fault and external BC may be applied in either a global or local coordinate system.

- Material properties are obtained from a spatial database.

Advantages of Using Simulation Controller and Other Pyre Facilities

- Ability to couple codes (e.g., CitComS, EqSim).

- Gathers user input with reasonable defaults.

- User can easily control all high-level functions including time stepping.

- Real-time visualization and simulation monitoring.

- Easier to set up Monte Carlo simulations using, for example, the same mesh and different material properties or boundary conditions.

PyLith: The Merging of LithoMop and EqSim

- LithoMop solves quasi-static problems while EqSim solves dynamic rupture propagation problems.

- Programs share many core features, and they are being reingineered to have even more characteristics in common.

- Within the next year, these codes will be combined into a coherent suite of software packages called PyLith.

- Resulting software will be able to simulate crustal deformation over spatial scales from meters to hundreds of km, and temporal scales from milliseconds to thousands of years.

Structure of PyLith Package
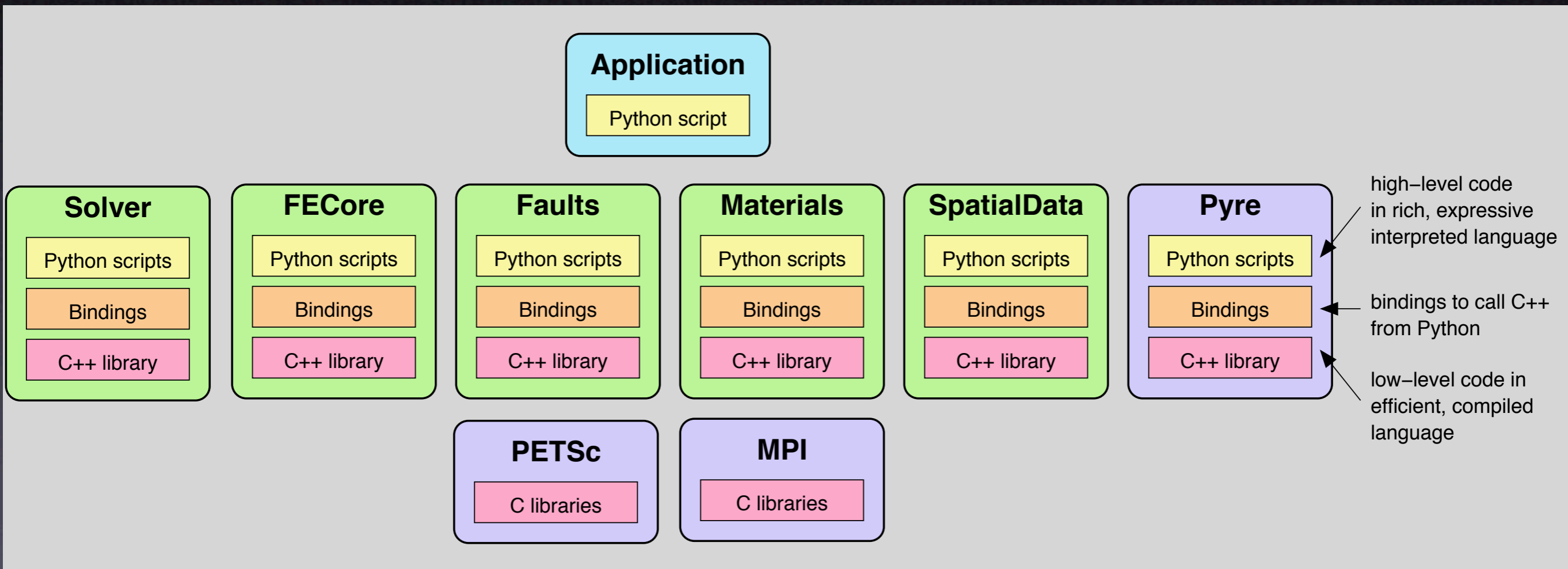
Further Information

- http://www.geodynamics.org
  - Click on 'Software' tab.

LithoMop/PyLith/CIG Code Development Priorities?

- Simple and robust cross-platform build system.

- ????

Interests

- Mesh generation to FE input.

- List of codes.

- Setting up LithoMop.

- How will people use LaGriT?