PyLith

Brad Aagaard, Charles Williams, Matthew Knepley,
Sue Kientz and Leif Strand

Computational Infrastructure for
Geodynamics

June 22, 2009

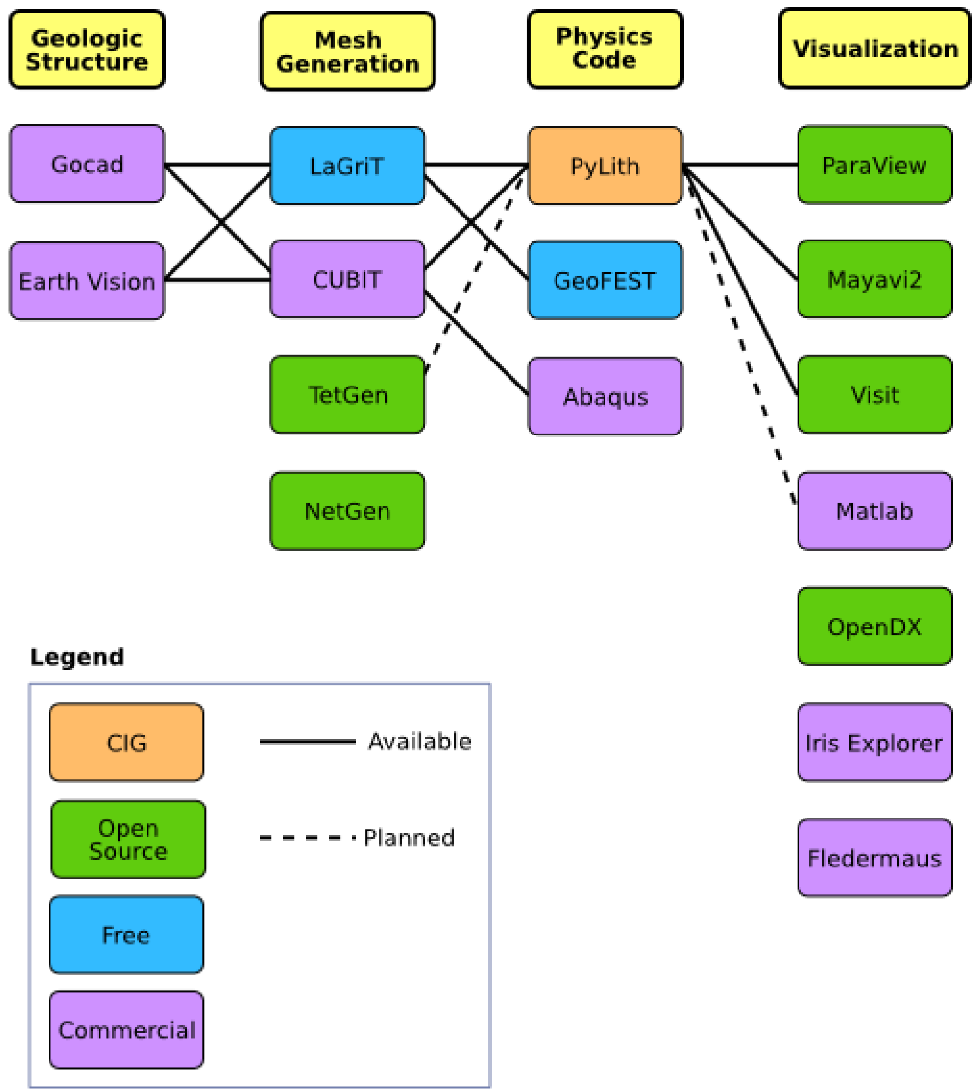
PyLith

What is it good for?

- Elasticity problems where geometry does not change significantly
- Quasi-static crustal deformation
  - Strain accumulation associated with interseismic deformation
  - Post-seismic relaxation of the crust
  - Volcanic deformation associated with magma chambers and/or dikes
- Dynamic rupture and wave propagation
  - Kinematic (prescribed) earthquake ruptures
  - Local/regional ground-motion modeling

Crustal Deformation Modeling

Overview of workflow for typical research problem



Computational Infrastructure for Geodynamics

Features in PyLith 1.4

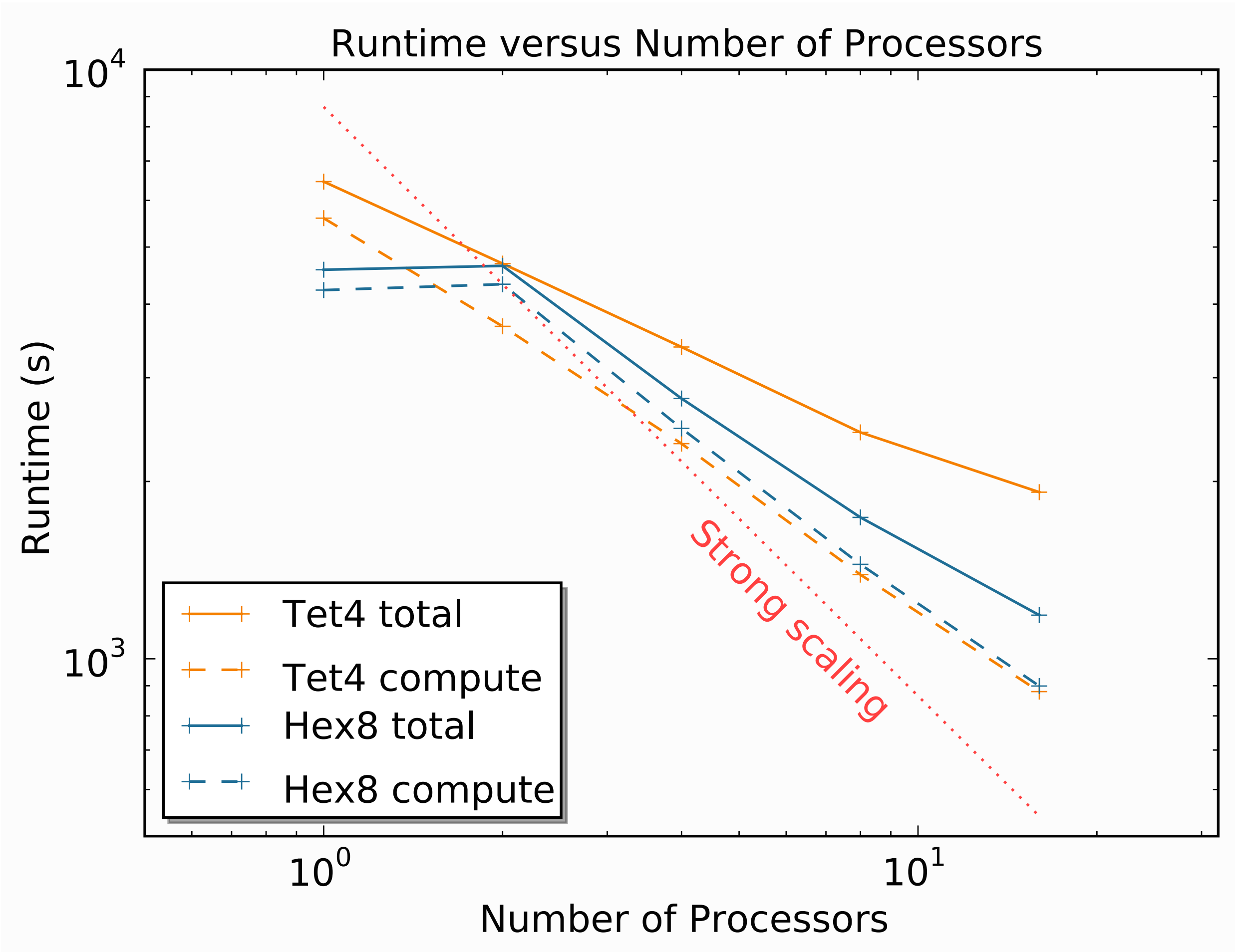
- Time integration schemes
  - Implicit time stepping for quasi-static problems
  - Explicit time stepping for dynamic problems
- Bulk constitutive models
  - Elastic model (1-D, 2-D, and 3-D)
  - Linear and Generalized Maxwell viscoelastic models (3-D)
  - Power-law viscoelastic model (3-D)
- Boundary and interface conditions
  - Time-dependent Dirichlet boundary conditions
  - Time-dependent Neumann (traction) boundary conditions
  - Absorbing boundary conditions
  - Kinematic (prescribed slip) fault interfaces w/multiple ruptures
  - Time-dependent point forces
  - Gravitational body forces

Features in PyLith 1.4 (cont.)

- Automatic and user-controlled time stepping
- Ability to specify initial stress state
- Importing meshes
  - LaGriT: GMV/Pset
  - CUBIT: Exodus II
  - ASCII: PyLith mesh ASCII format (intended for toy problems only)
- Output: VTK files
  - Solution over volume
  - Solution over surface boundary
  - State variables (e.g., stress and strain) for each material
  - Fault information (e.g., slip and tractions)
- Automatic conversion of units for all parameters

PyLith 1.4 Performance

PyLith 1.4 is ~5% faster and uses ~50% less memory than PyLith 1.3



Computational Infrastructure for Geodynamics

PyLith 1.x: Planned Releases

Current productivity is about 2 feature releases per year

- PyLith 1.5: anticipate release in late 2009 or early 2010
  - Fault constitutive behavior with several widely used friction models
  - Ability to specify initial strain and state variables
- PyLith 1.6: Large deformations and finite strain
- PyLith 1.7: Automation of 4-D Green's functions
- PyLith 1.8: Coupling of quasi-static and dynamic simulations

PyLith Design Objective

Want a code developed for and by the community

- Modular
  - Users can swap modules to run the problem of interest
- Scalable
  - Code runs on one to a thousand processors efficiently
- Extensible
  - Expert users can add functionality to solve their problem without polluting main code

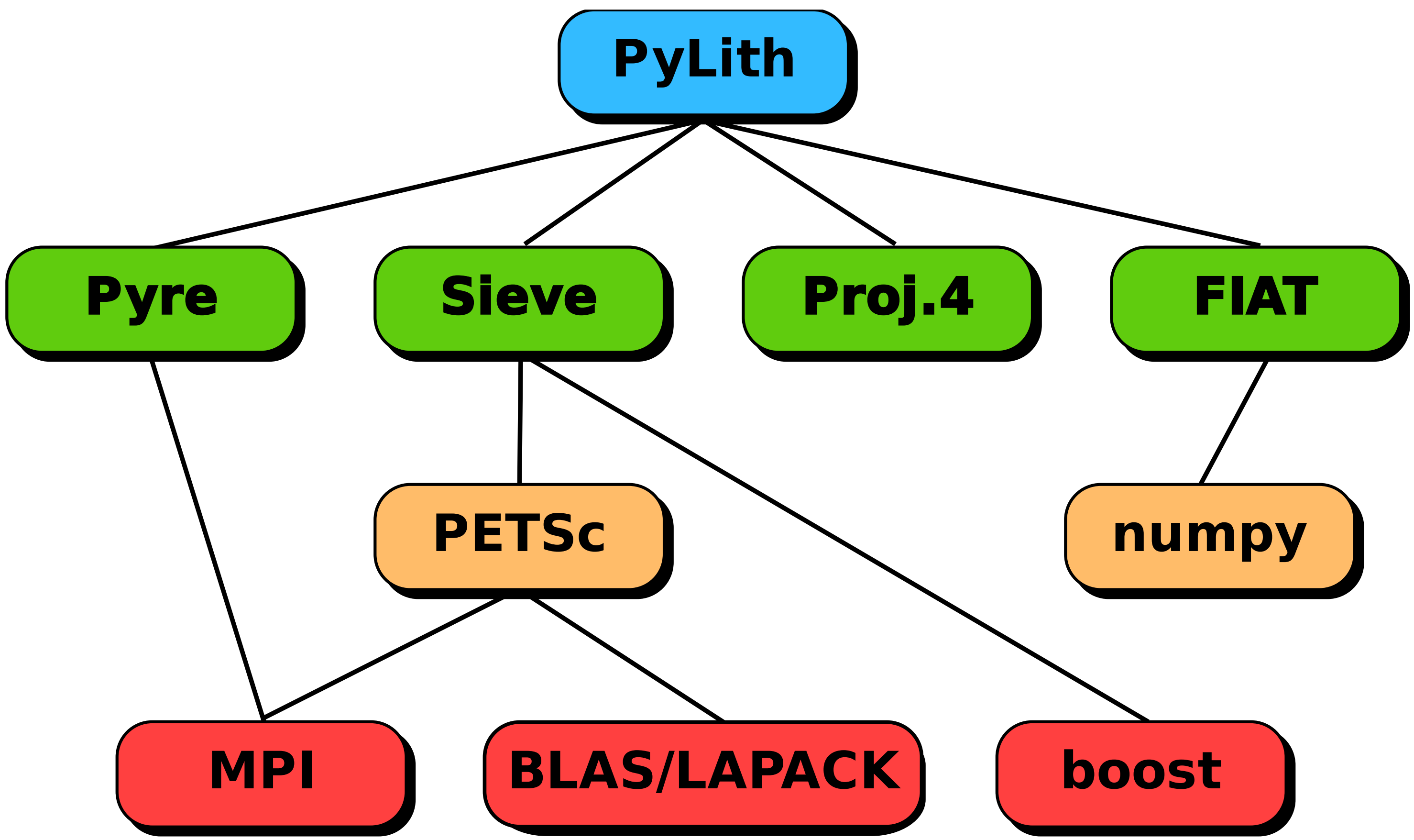
PyLith is a Community Code

Success of code depends on community participation

- End-users (anyone who uses the code)
  - Help define and prioritize features that should be added
  - Report bugs/problems and suggest improvements
- Expert users
  - Help test alpha versions of releases
  - Run benchmarks and report results
  - Contribute meshing and visualization examples to documentation
  - Add features following template (e.g., constitutive models)
- Developer
  - Define development strategy
  - Implement new features and tests
  - Write documentation

PyLith Design: Focus on Geodynamics

Leverage packages developed by computational scientists



PyLith Design: Code Architecture

Flexible and modular with good performance

- Top-level code written in Python
  - Expressive, high-level, object-oriented language
  - Dynamic typing allows adding additional modules at runtime
  - Convenient scripting
- Low-level code written in C++
  - Compiled (fast execution), object oriented language
- Bindings to glue Python & C++ together
  - SWIG generates code for calling C++ functions from Python

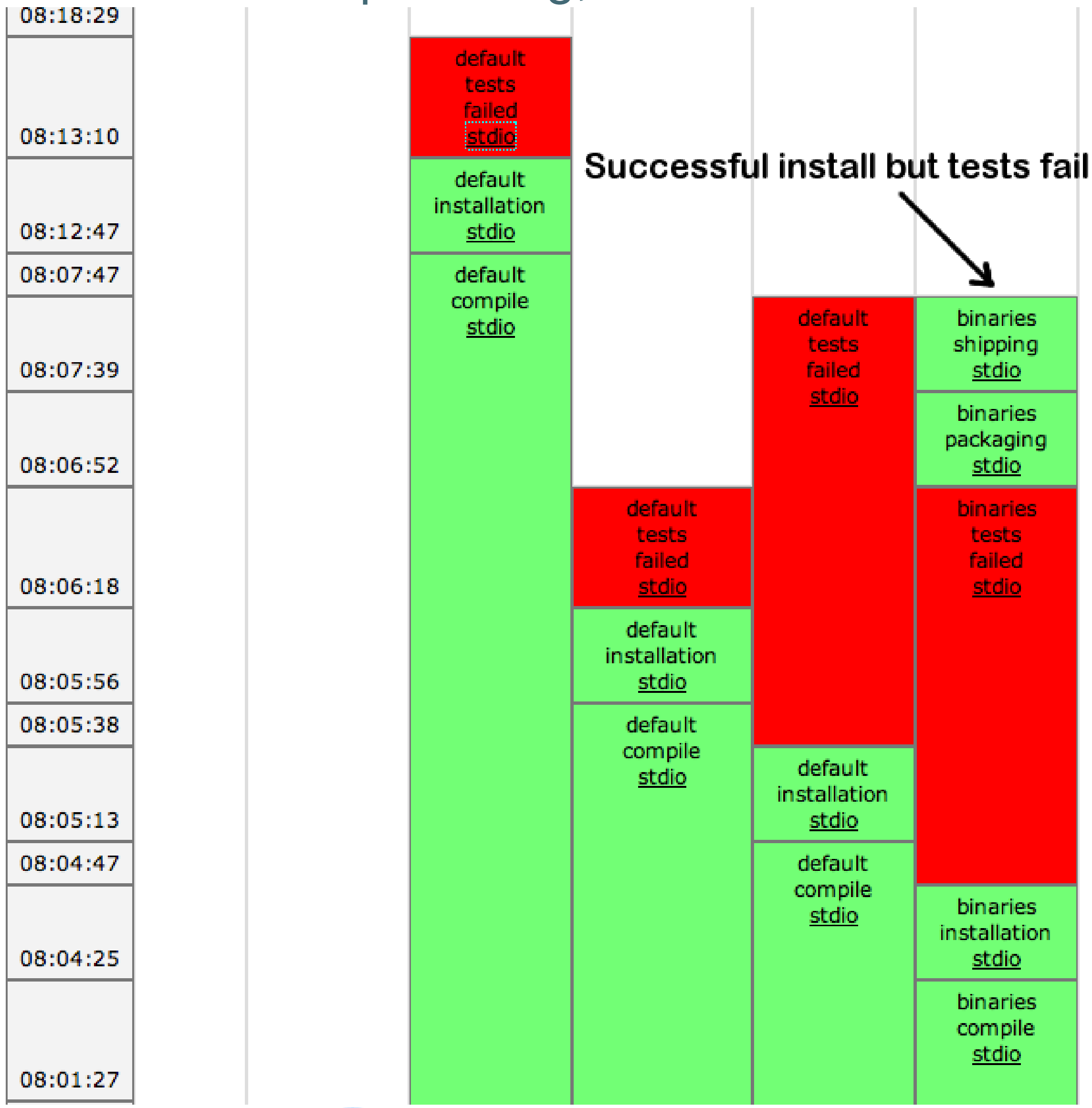
PyLith Design

Tests, tests, and more tests ($>$1100 in all)

- Create tests for nearly every function during development
  - Remove most bugs during initial implementation
  - Isolate and expose bugs at origin
- Create new tests to expose bugs reported
  - Prevent bugs from reoccurring
- Rerun tests whenever code is changed
  - Allows optimization of performance with quality control
  - Code continually improves

Example of Automated Building and Testing

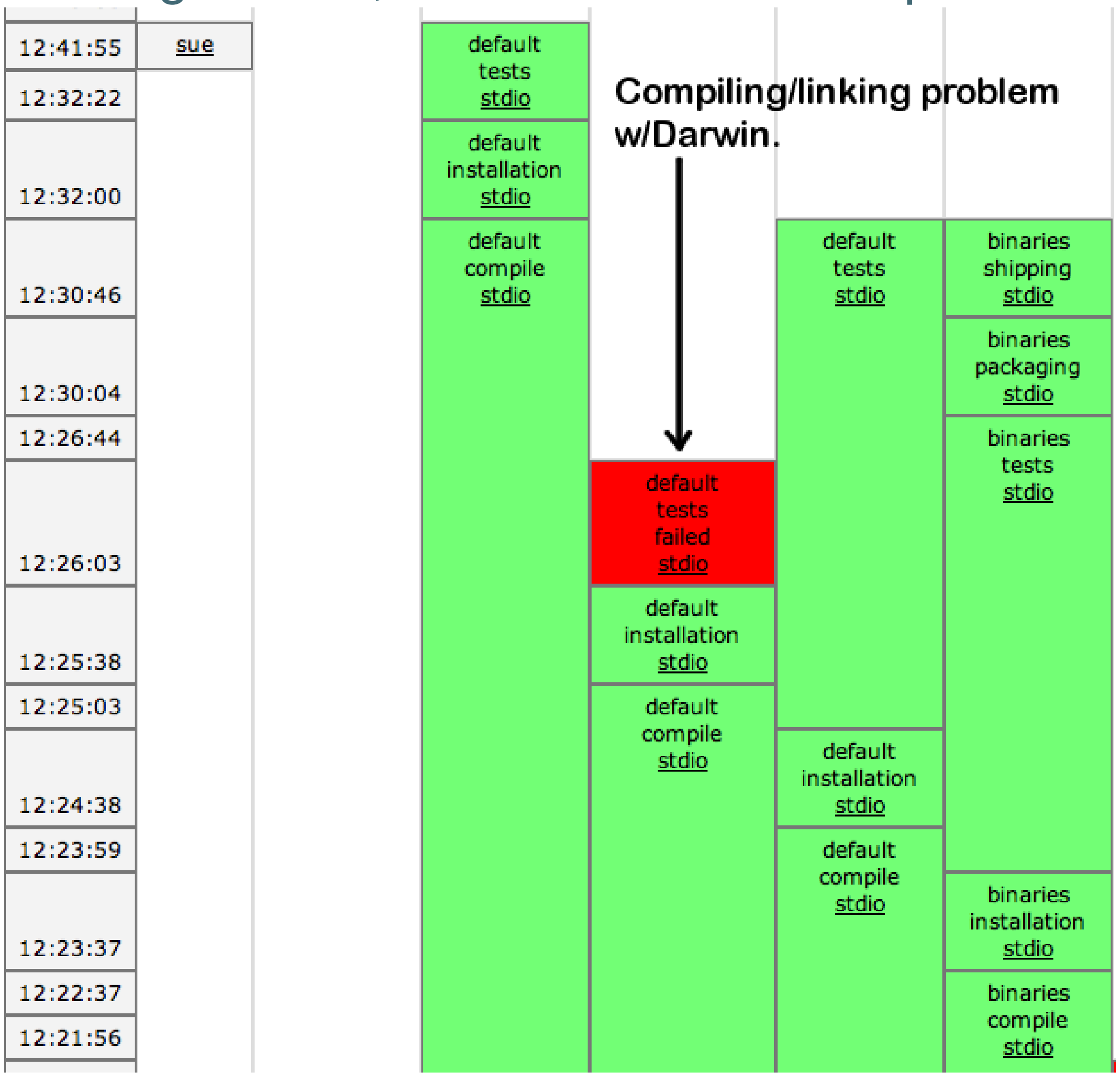
Test written to expose bug, buildbot shows tests fail



Computational Infrastructure for Geodynamics

Automated Building and Testing

Bug is fixed, buildbot shows tests pass



Computational Infrastructure for Geodynamics

Implementation: Finite-Element Data Structures

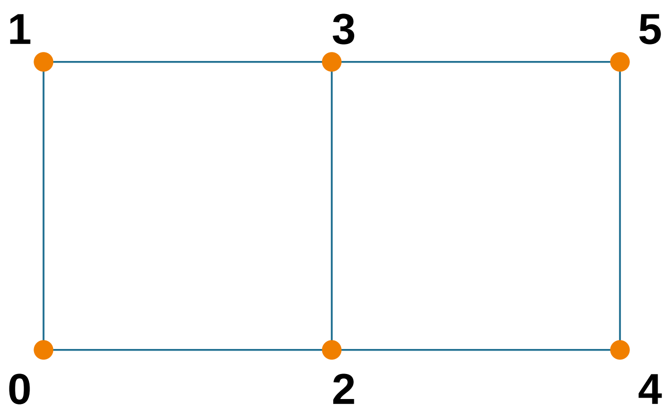
Use Sieve for storage and manipulating mesh information

- PyLith makes only a few MPI calls
- Data structures are independent of basis functions and reference cells
  - Same code for many cell shapes and types
  - Physics implementation limits code, not data structures
- Sieve routines force adhering to finite-element formulation
  - Do not have access to underlying storage
  - Manipulations must be done using Sieve interface
  - Only valid finite-element manipulation is allowed

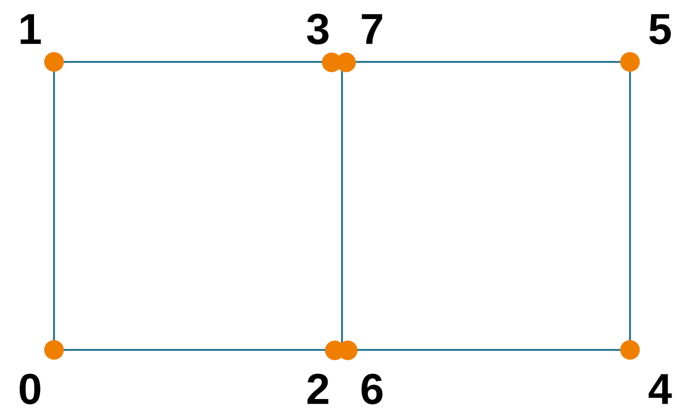
Implementation: Fault Interfaces

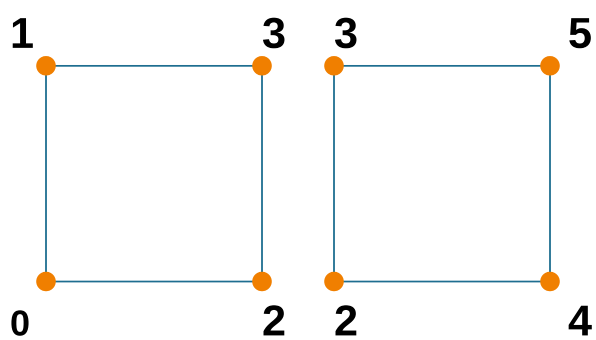
Use cohesive cells to control fault behavior

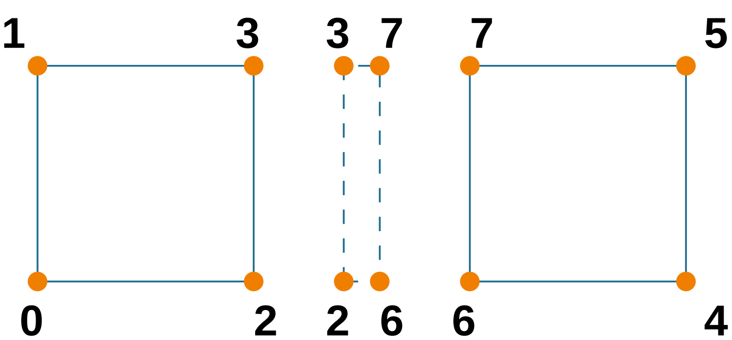
Original Mesh



Mesh with Cohesive Cell







Exploded view of meshes

Kinematic (prescribed) slip earthquake ruptures

Use Lagrange multipliers to specify slip

- System without cohesive cells

$$\underline{\mathsf{A}}\vec{u} = \vec{b}$$

- System with cohesive cells

$$\begin{pmatrix} \underline{\mathsf{A}} & \underline{\mathsf{C}}^T \\ \underline{\mathsf{C}} & 0 \end{pmatrix} \begin{pmatrix} \vec{u} \\ \vec{L} \end{pmatrix} = \begin{pmatrix} \vec{b} \\ \vec{D} \end{pmatrix}$$

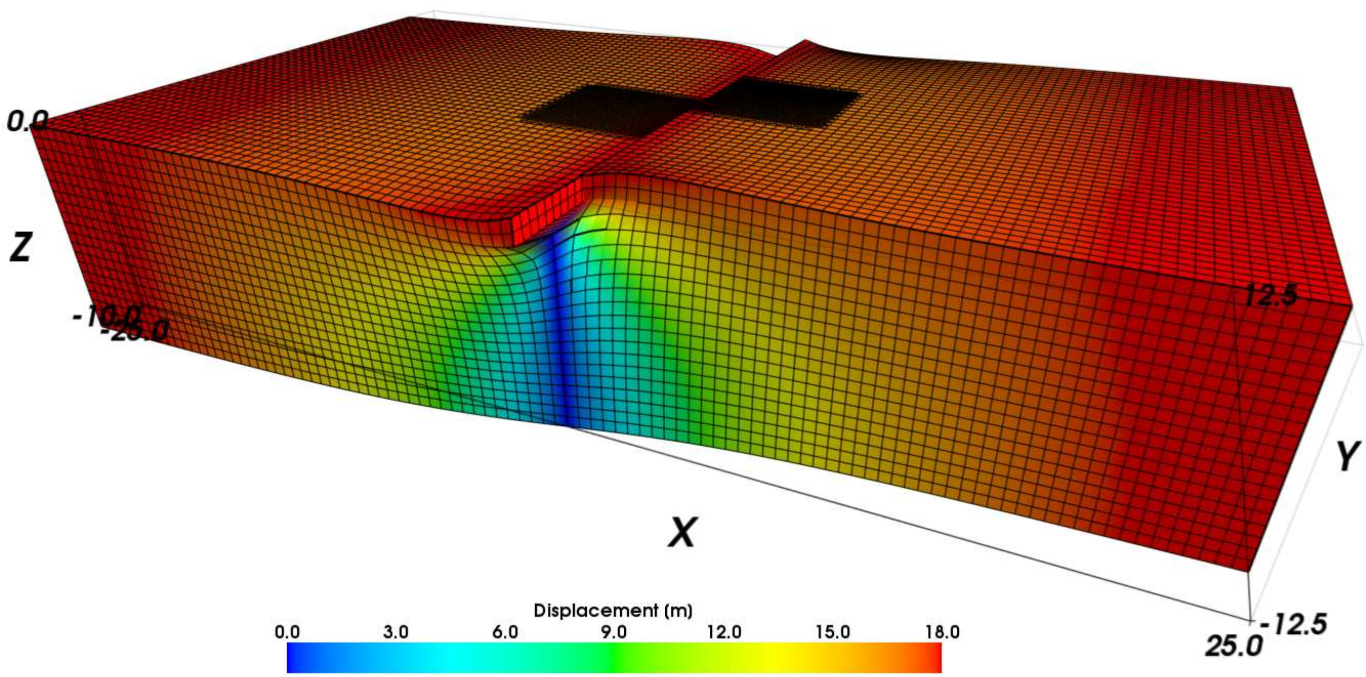
Implementing Fault Slip with Lagrange multipliers

- Advantages
  - Fault implementation is local to cohesive cell
  - Solution includes forces generating slip (Lagrange multipliers)
  - Retains block structure of matrix (same number of DOF per vertex)
  - Offsets in mesh mimic slip on natural faults
- Disadvantages
  - Creates a saddle point problem (slower convergence)
  - Mixes displacements and forces in solution

Benchmarking PyLith

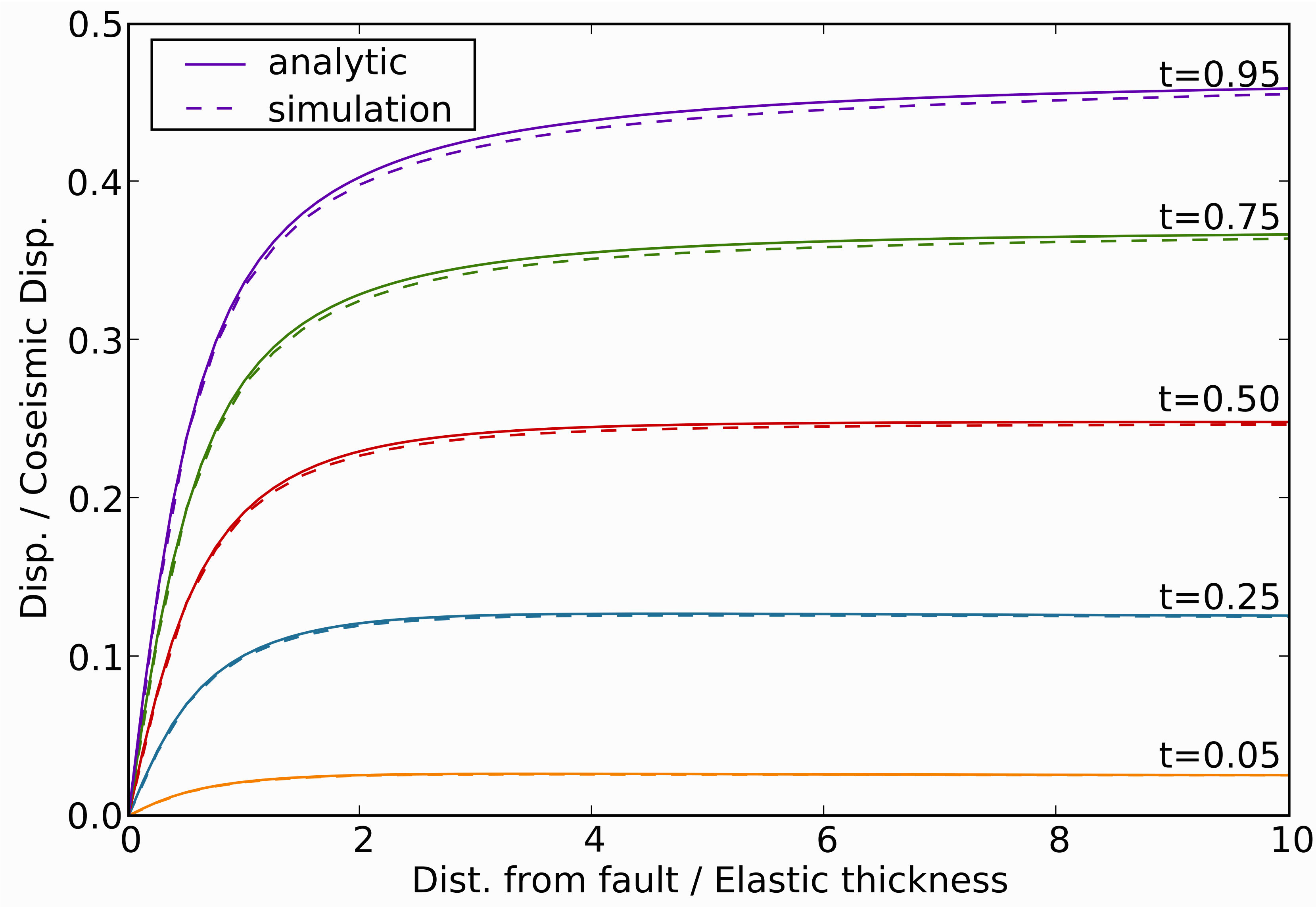
Analytical solution from Savage and Prescott (1978)

- Repeated rupture on a vertical, strike-slip fault
- Elastic layer over a linear Maxwell viscoelastic half-space
- Steady creep over bottom half of the elastic layer



Benchmarking PyLith

Simulation closely matches analytical solution during 10th eq cycle



Computational Infrastructure for Geodynamics