

PyLith

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



June 14, 2010

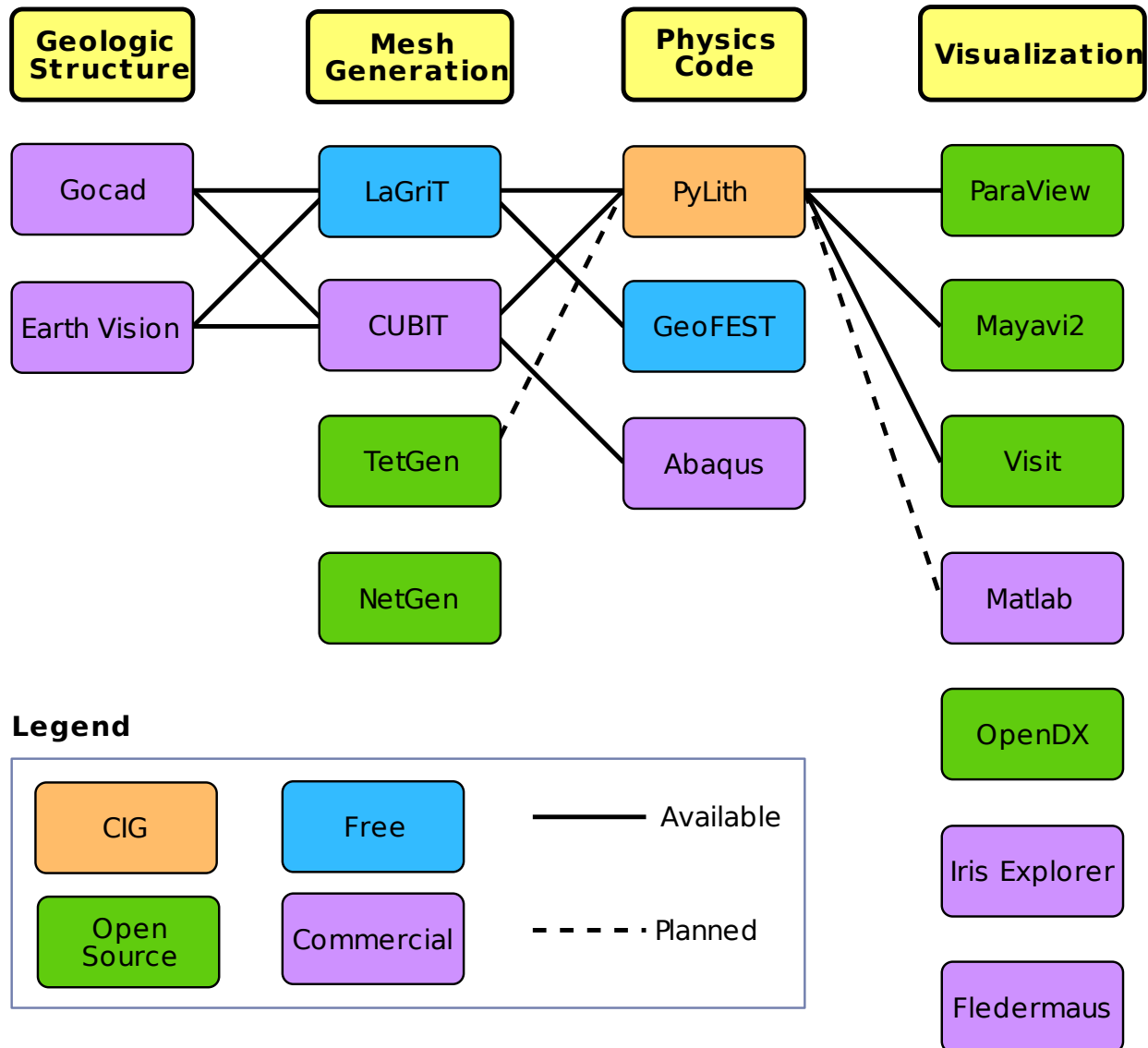
PyLith

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
 - Dynamic (spontaneous) earthquake ruptures
 - Local/regional ground-motion modeling

Crustal Deformation Modeling

Overview of workflow for typical research problem



Features in PyLith 1.5

Enhancements and new features in blue

- Time integration schemes and elasticity formulations
 - Implicit for quasi-static problems (neglect inertial terms)
 - Infinitesimal strains
 - Small strains
 - Explicit for dynamic problems
 - Infinitesimal strains with sparse system Jacobian
 - Infinitesimal strains with lumped system Jacobian
 - Small strains with sparse system Jacobian
- 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)
 - Linear Maxwell viscoelastic model (2-D)
 - Drucker-Prager elastoplastic model (3-D)

Features in PyLith 1.5 (cont.)

Enhancements and new features in blue

- 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
 - **Dynamic (friction) fault interfaces**
 - Time-dependent point forces
 - Gravitational body forces
- Fault constitutive models
 - **Static friction**
 - **Linear slip-weakening**
 - **Dieterich-Ruina rate and state friction w/ageing law**

Features in PyLith 1.5 (cont.)

Enhancements and new features in blue

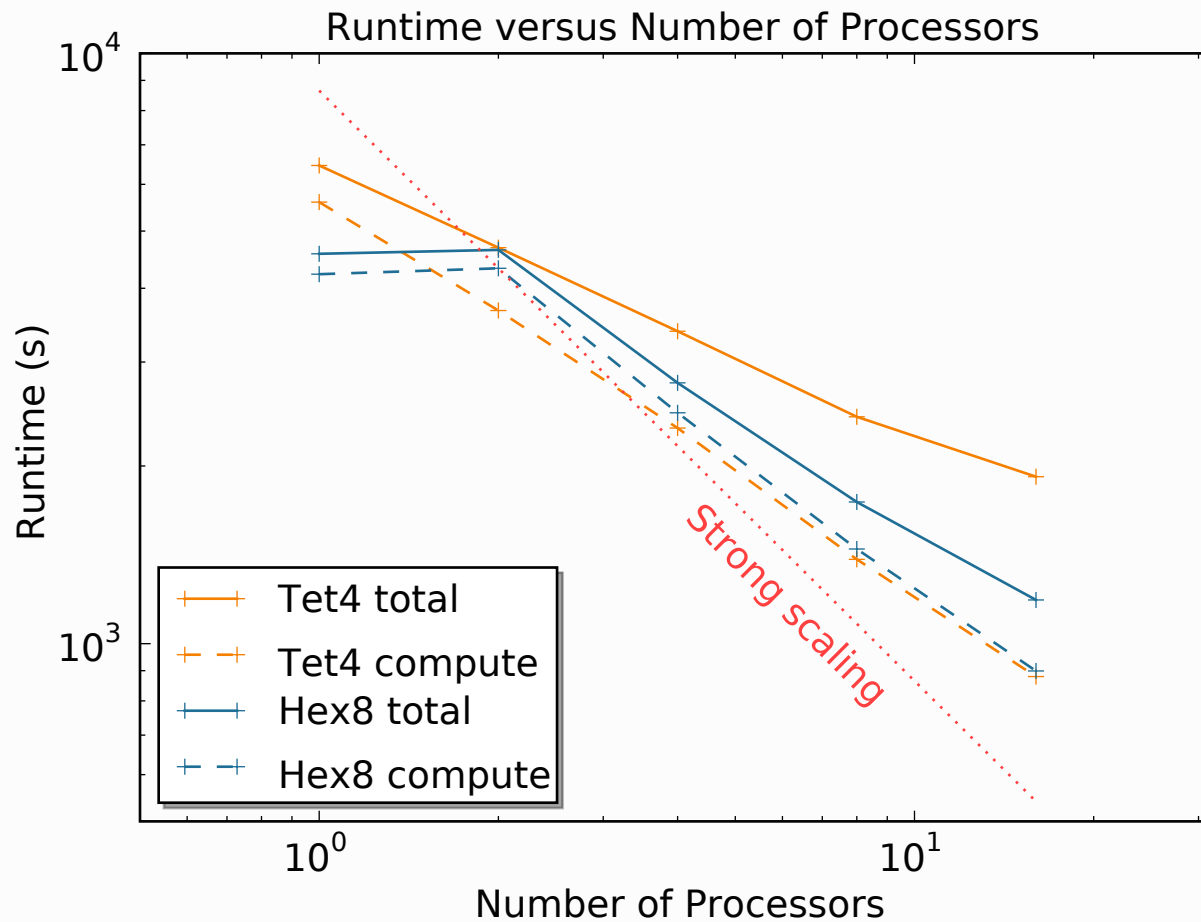
- Automatic and user-controlled time stepping
- Ability to specify initial stress state
- Importing meshes
 - LaGriT: GMV/Pset
 - CUBIT: Exodus II
 - ASCII: PyLith mesh ASCII format (intended for toy problems only)
- Output: VTK files
 - Solution over volume
 - Solution over surface boundary
 - State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

PyLith 1.5: Under-the-hood Improvements

- Additional cleanup of C++ code
- Optimization of several modules
 - Mesh distribution among processors
 - Integration of elasticity terms
- Ability to use algebraic multigrid preconditioners

PyLith 1.5 Performance

PyLith 1.5 is up to ~??% faster than PyLith 1.4



PyLith 1.x: Planned Releases

Current productivity is about 2 feature releases per year

- PyLith 1.6: anticipate release in late 2010 or early 2011
 - Additional fault constitutive models
 - Additional optimization
- PyLith 1.7: Automation of 4-D Green's functions
- PyLith 1.8: Coupling of quasi-static and dynamic simulations
- Long-term objectives
 - Adaptive mesh refinement and adjoint methods
 - Easier discretization (ability to use structured meshes, meshless methods)

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

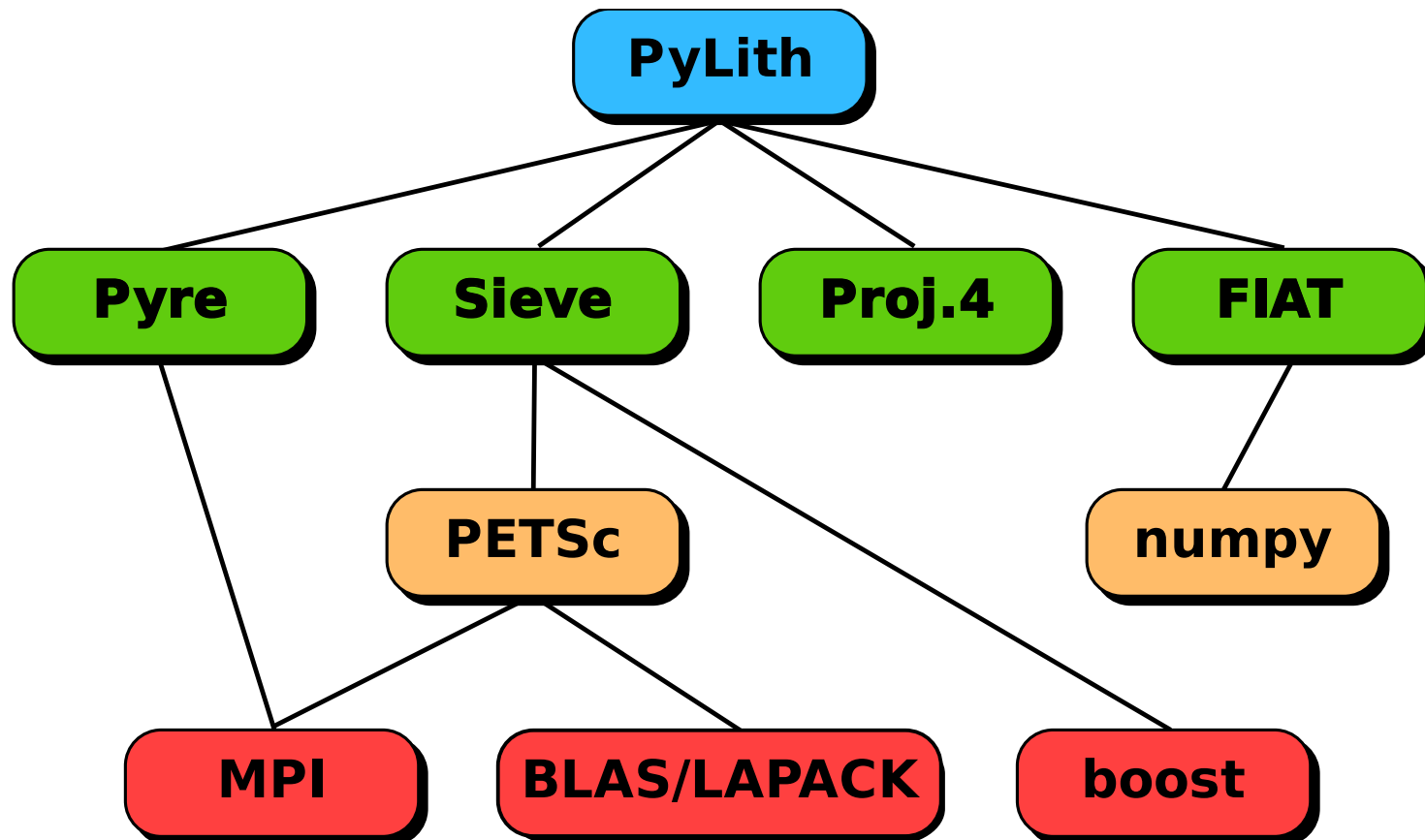
PyLith is a Community Code

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

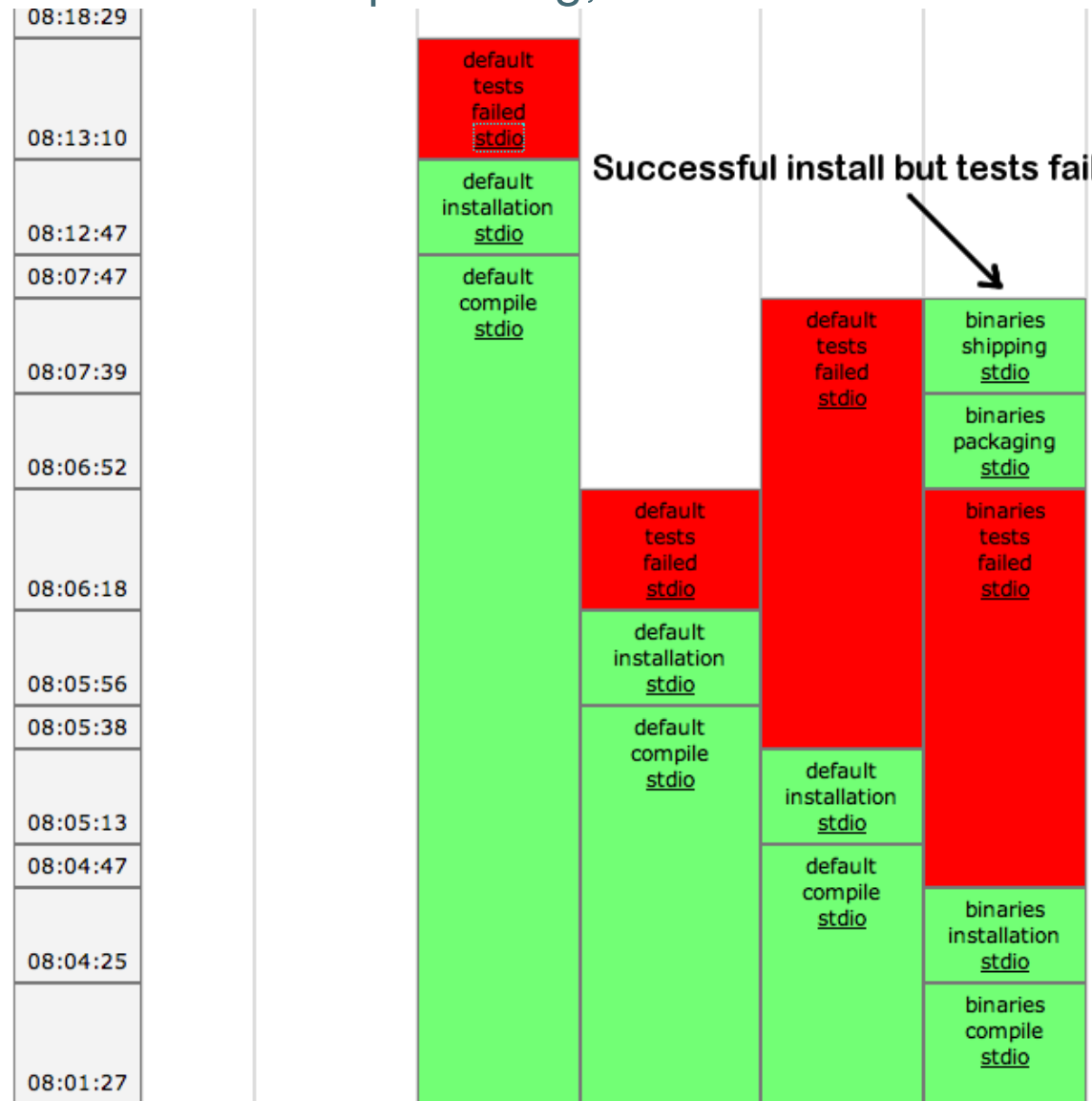
PyLith Design

Tests, tests, and more tests (>1800 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

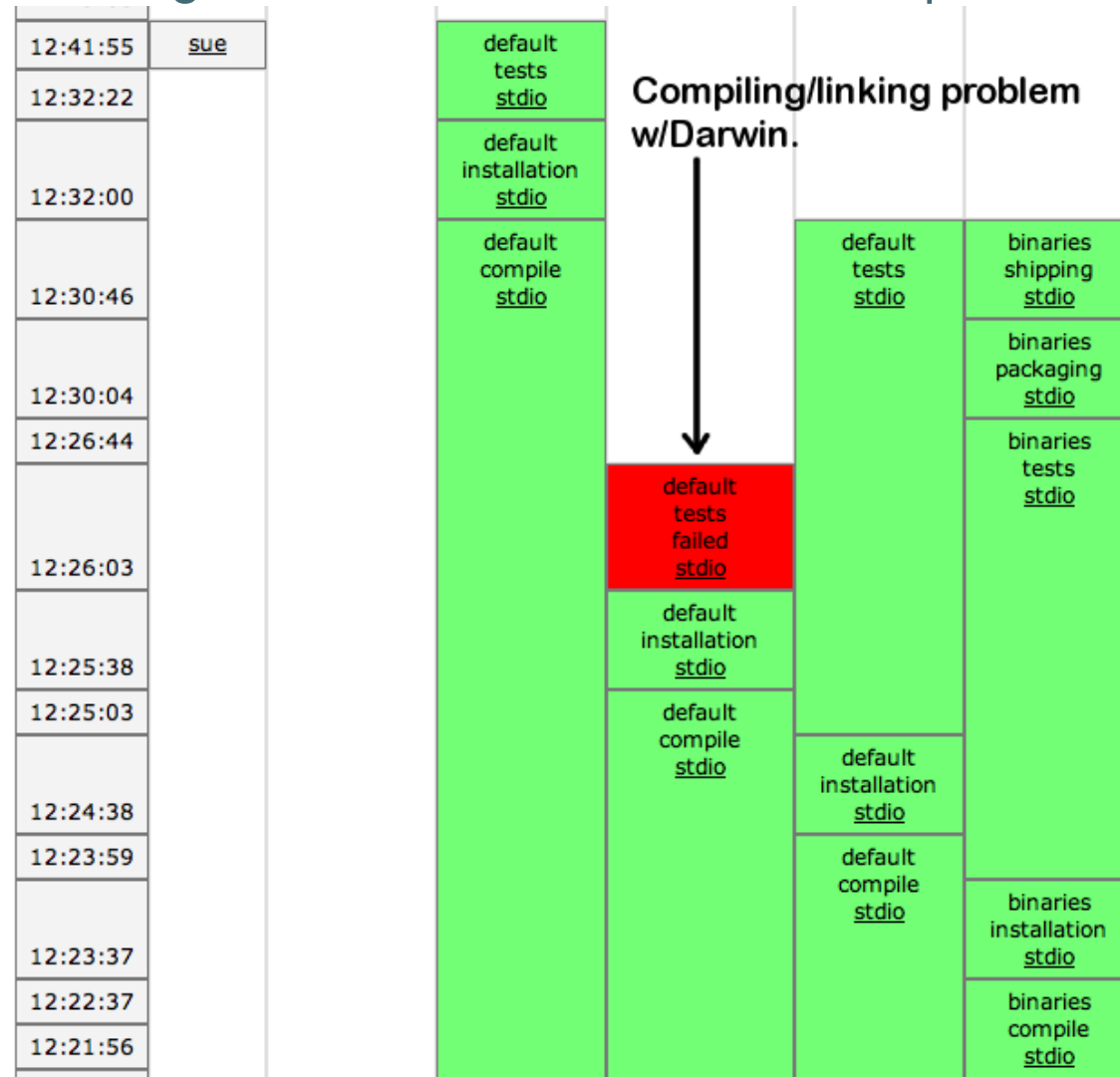
Example of Automated Building and Testing

Test written to expose bug, buildbot shows tests fail



Automated Building and Testing

Bug is fixed, buildbot shows tests pass



Implementation: Finite-Element Data Structures

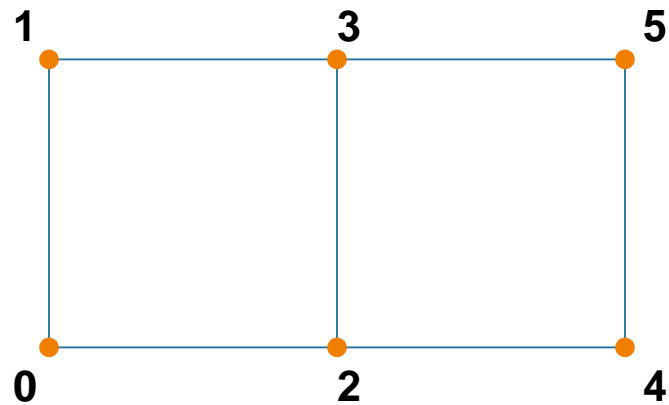
Use Sieve for storage and manipulating mesh information

- 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

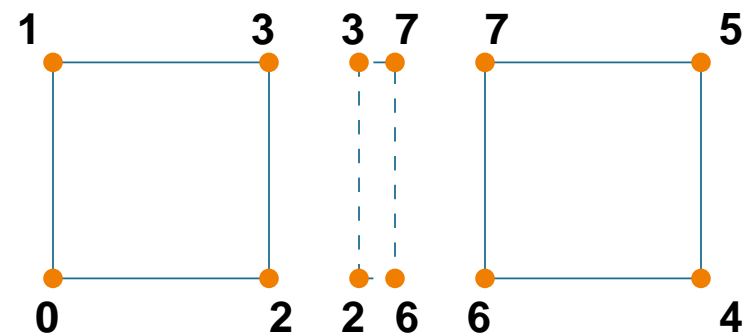
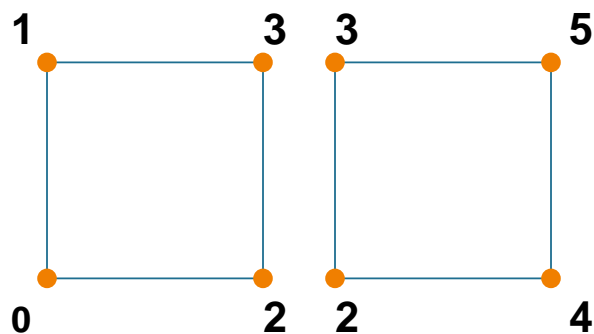
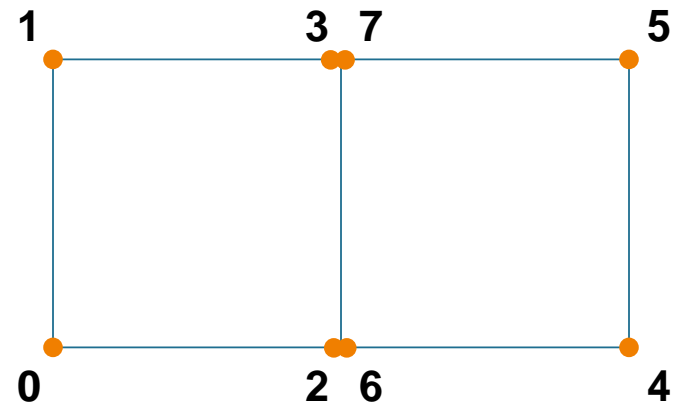
Implementation: Fault Interfaces

Use cohesive cells to control fault behavior

Original Mesh



Mesh with Cohesive Cell



Exploded view of meshes

Implementation: Fault Interfaces

Use Lagrange multipliers to specify slip/tractions

- System without cohesive cells

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

- System with cohesive cells

$$\begin{pmatrix} \underline{A} & \underline{C}^T \\ \underline{C} & 0 \end{pmatrix} \begin{pmatrix} \vec{u} \\ \vec{l} \end{pmatrix} = \begin{pmatrix} \vec{b} \\ \vec{d} \end{pmatrix}$$

- Kinematic slip: specify $\vec{d}(t)$.
- Dynamic slip: fault constitutive model places bounds on $\vec{l}(t)$

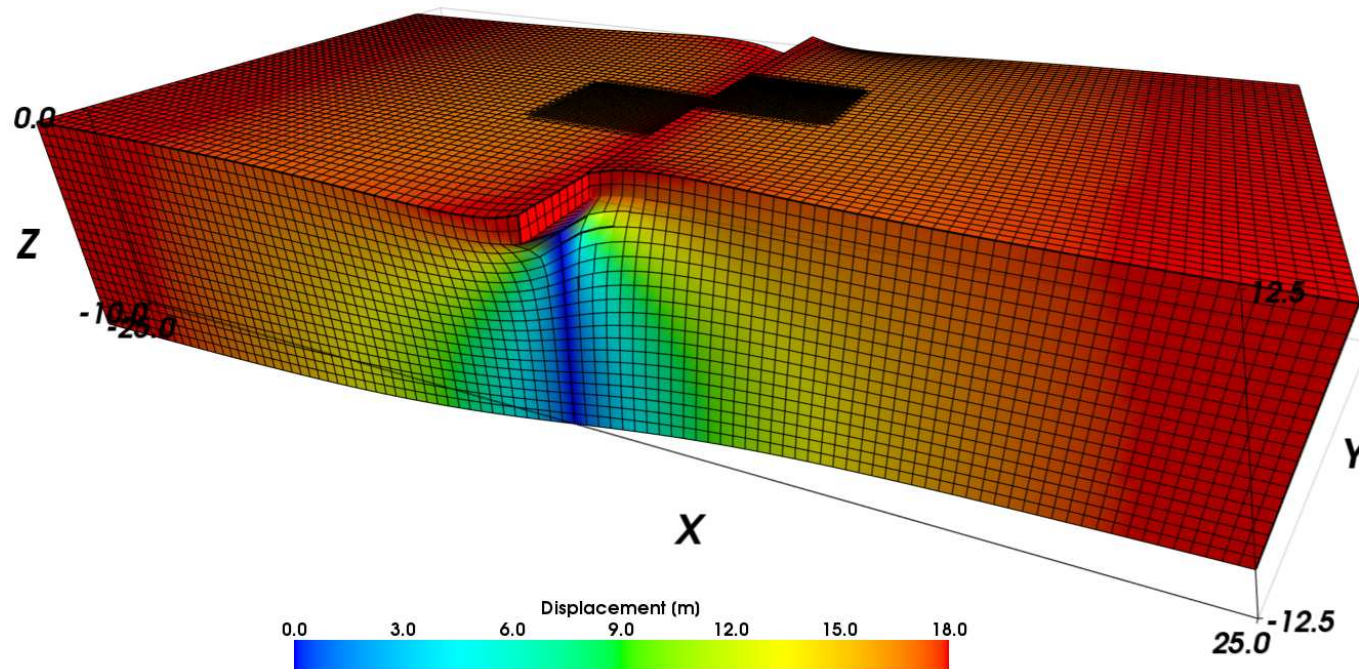
Implementing Fault Slip with Lagrange multipliers

- 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

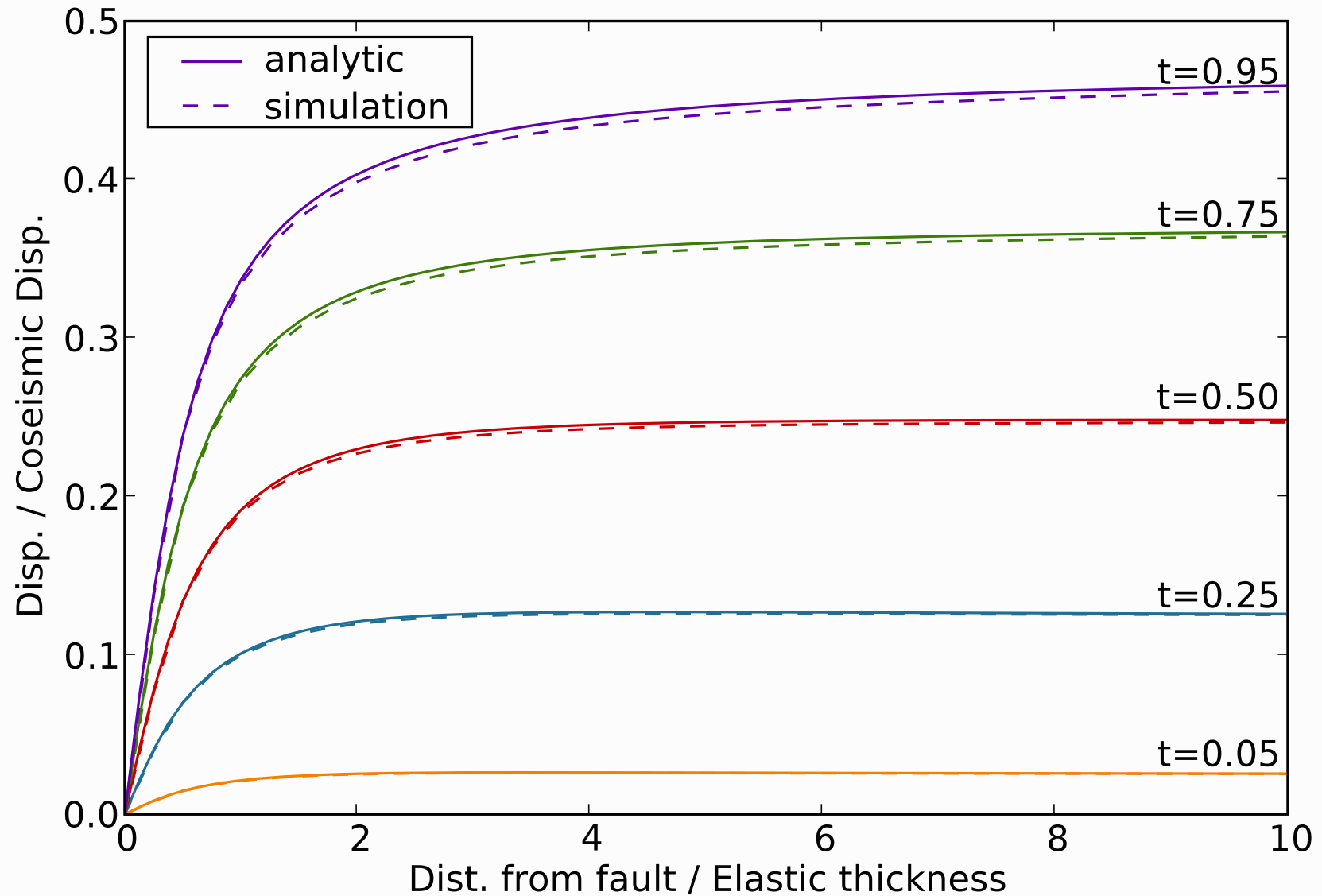
Analytical solution from Savage and Prescott (1978)

- 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

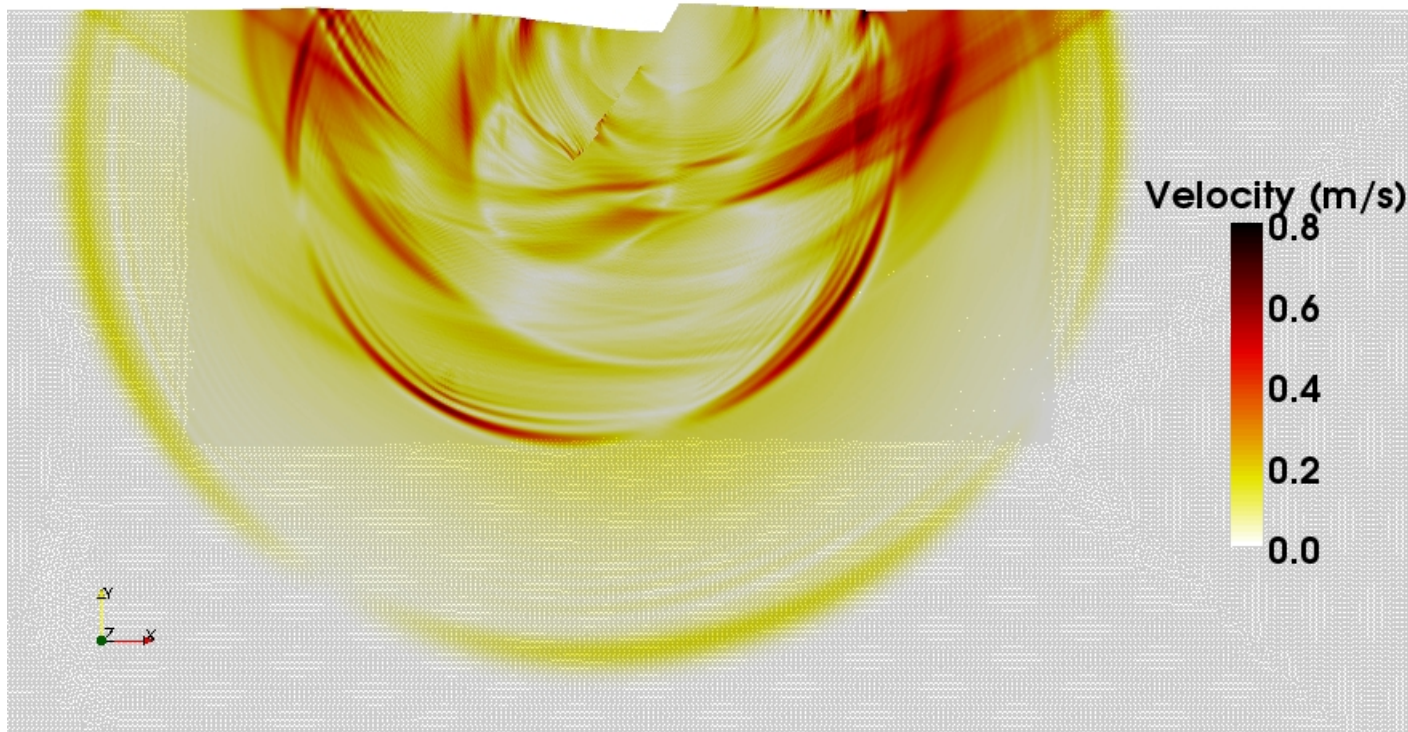
Simulation closely matches analytical solution during 10th eq cycle



Benchmarking PyLith

SCEC Dynamic Rupture Verification Benchmarks

- Rupture on a 60 degree normal fault
- Initial tractions proportional to overburden pressure
- Linear slip-weakening friction



Benchmarking PyLith

Close agreement with other dynamic rupture codes

