PyLith

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Computational Infrastructure for Geodynamics

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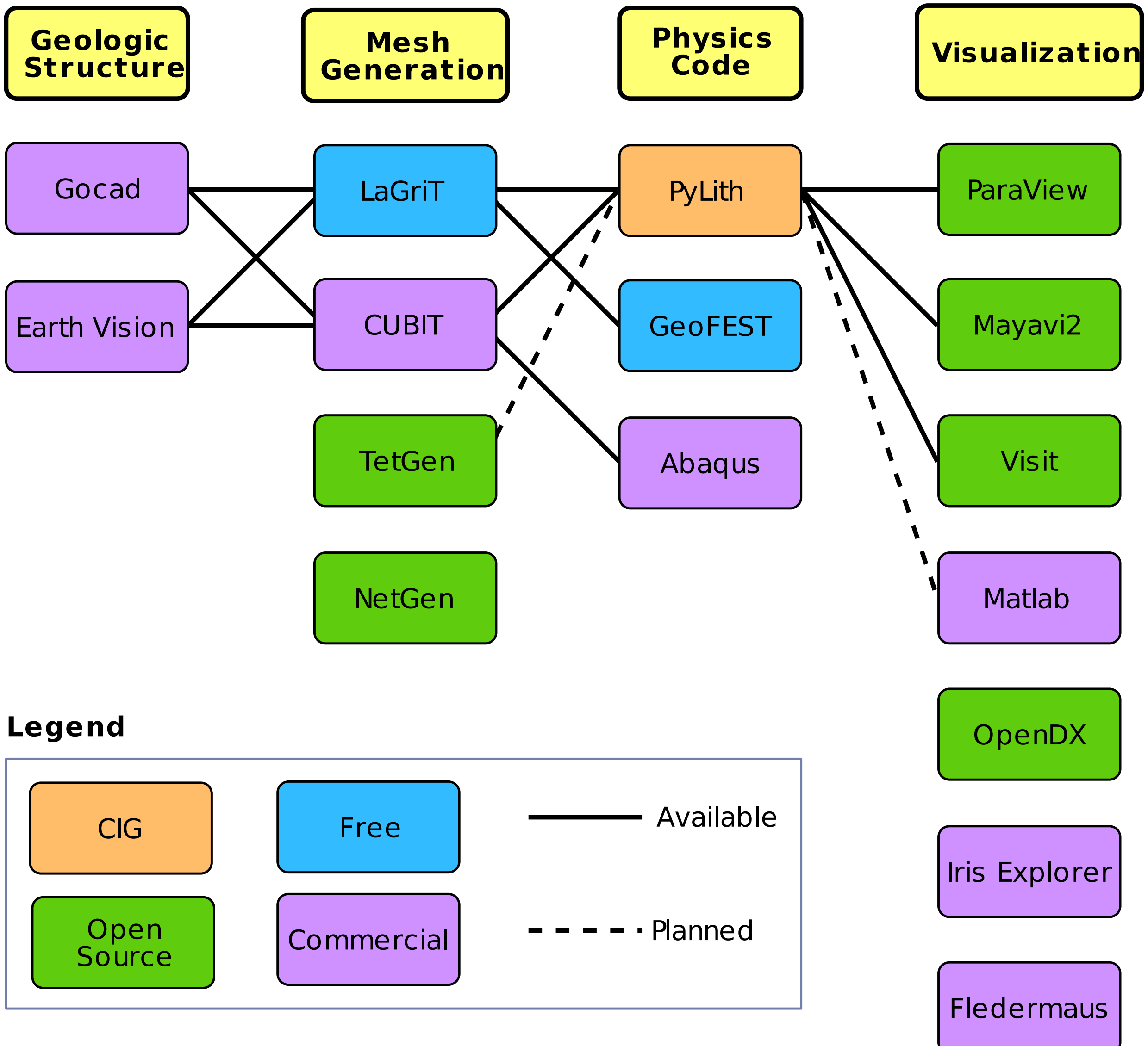
PyLith

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

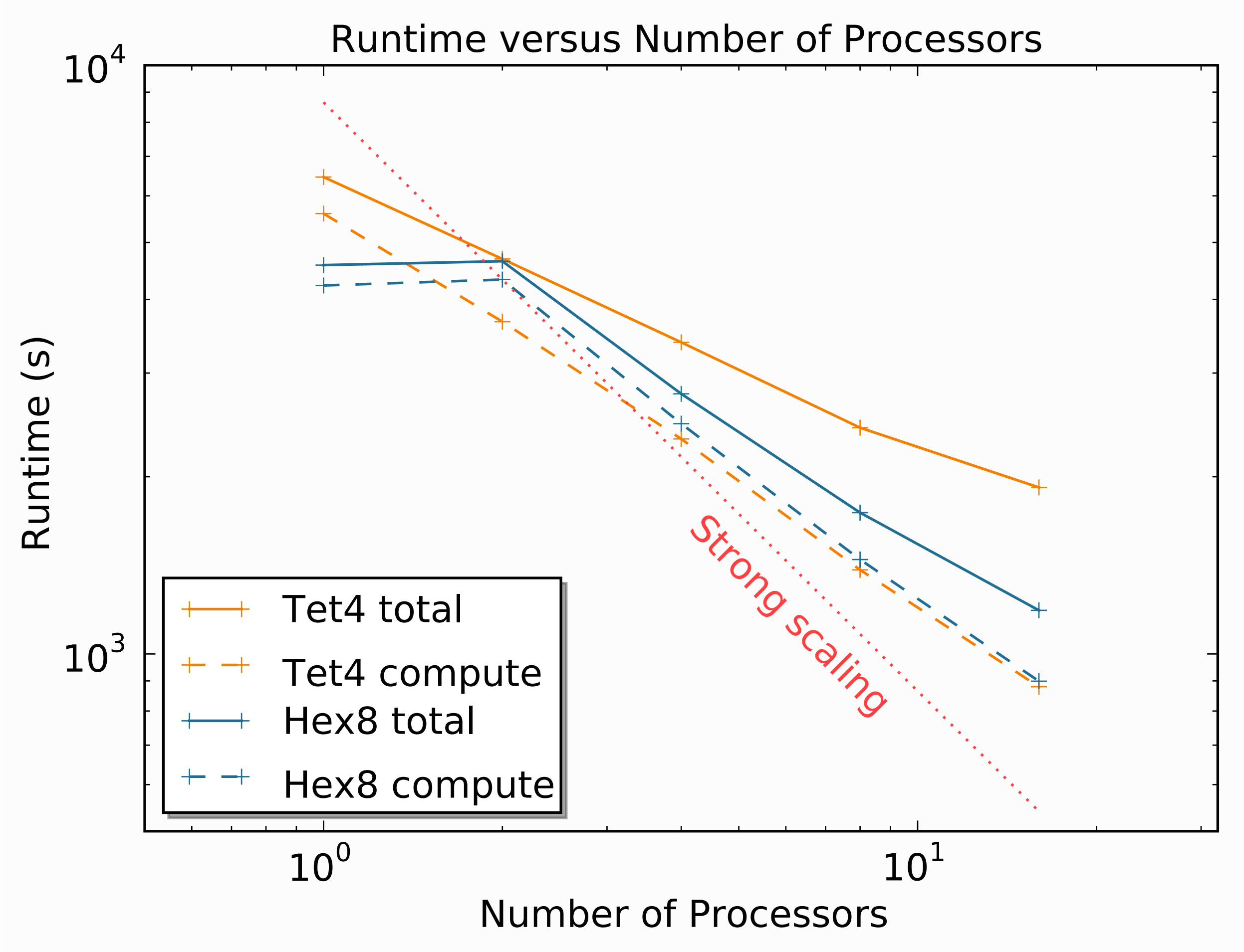
- Automatic and user-controlled time stepping
- Ability to specify initial stress state
- Importing meshes
  - LaGriT: GMV/Pset
  - CUBIT: Exodus II
  - ASCII: PyLith mesh ASCII format (intended for toy problems only)
- Output: VTK files
  - Solution over volume
  - Solution over surface boundary
  - 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



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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

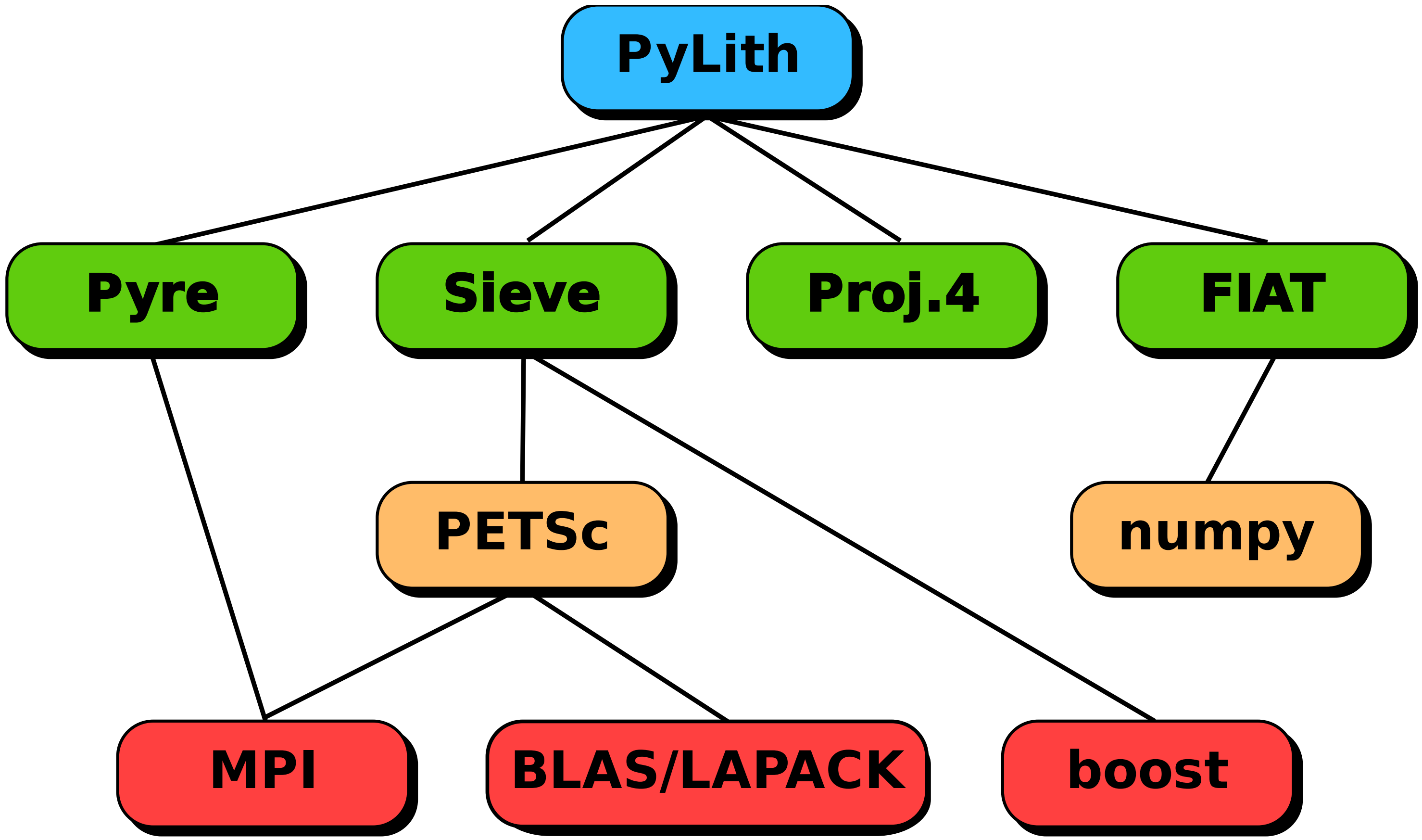
PyLith is a Community Code

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

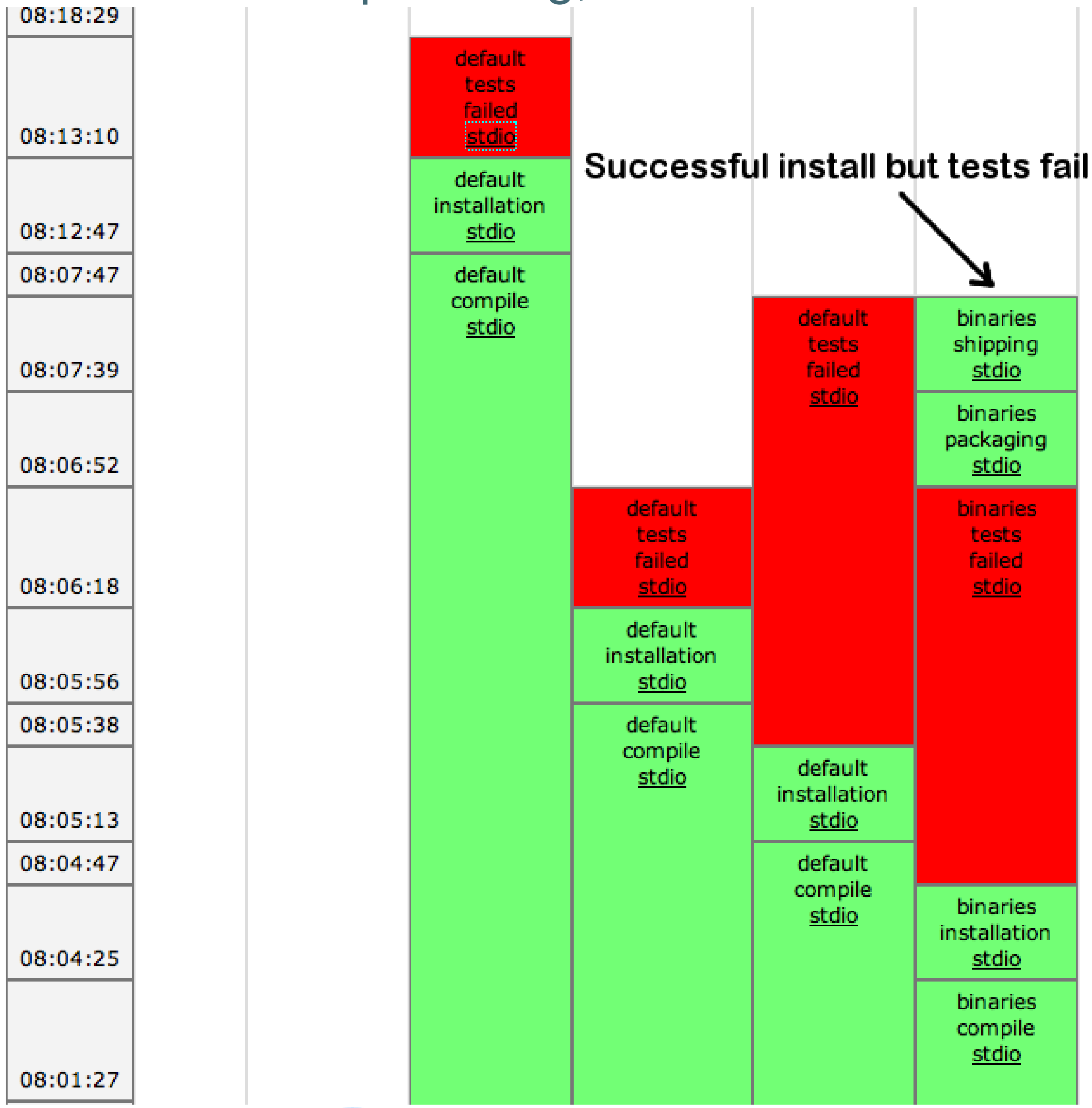
PyLith Design

Tests, tests, and more tests (>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



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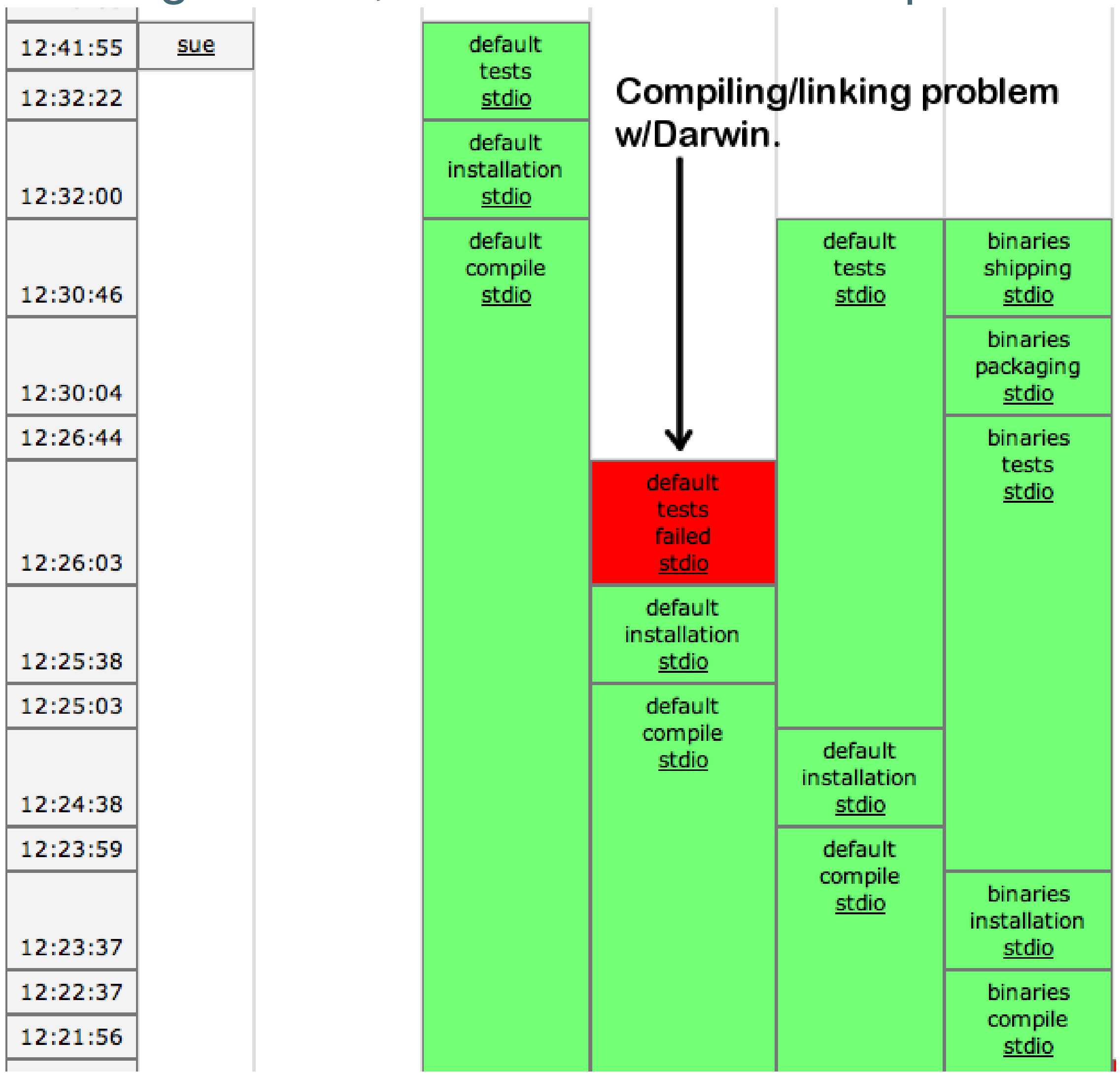
Automated Building and Testing

Bug is fixed, buildbot shows tests pass



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Implementation: Finite-Element Data Structures

Use Sieve for storage and manipulating mesh information

- PyLith makes only a few MPI calls

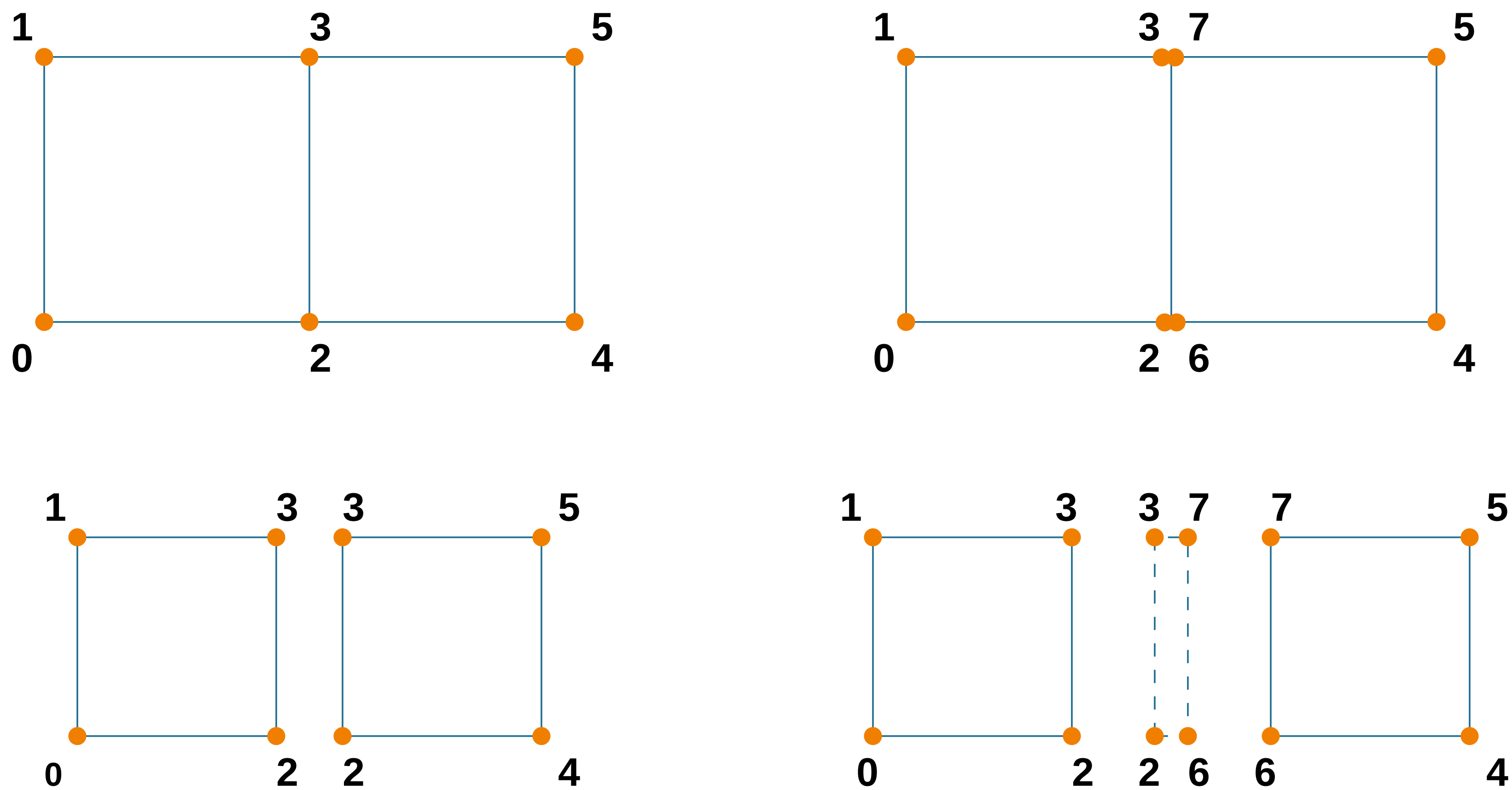
- Data structures are independent of basis functions and reference cells
  - Same code for many cell shapes and types
  - Physics implementation limits code, not data structures

- 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

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

- System with cohesive cells

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

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

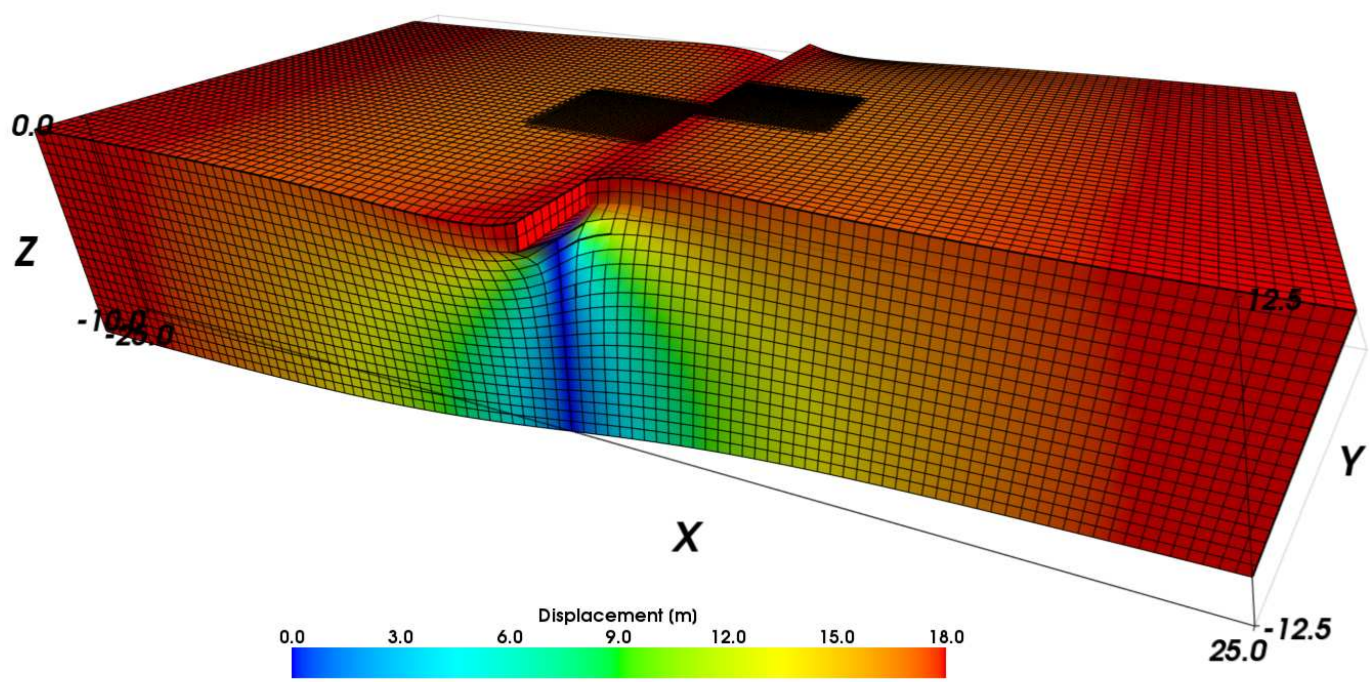
Implementing Fault Slip with Lagrange multipliers

- 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



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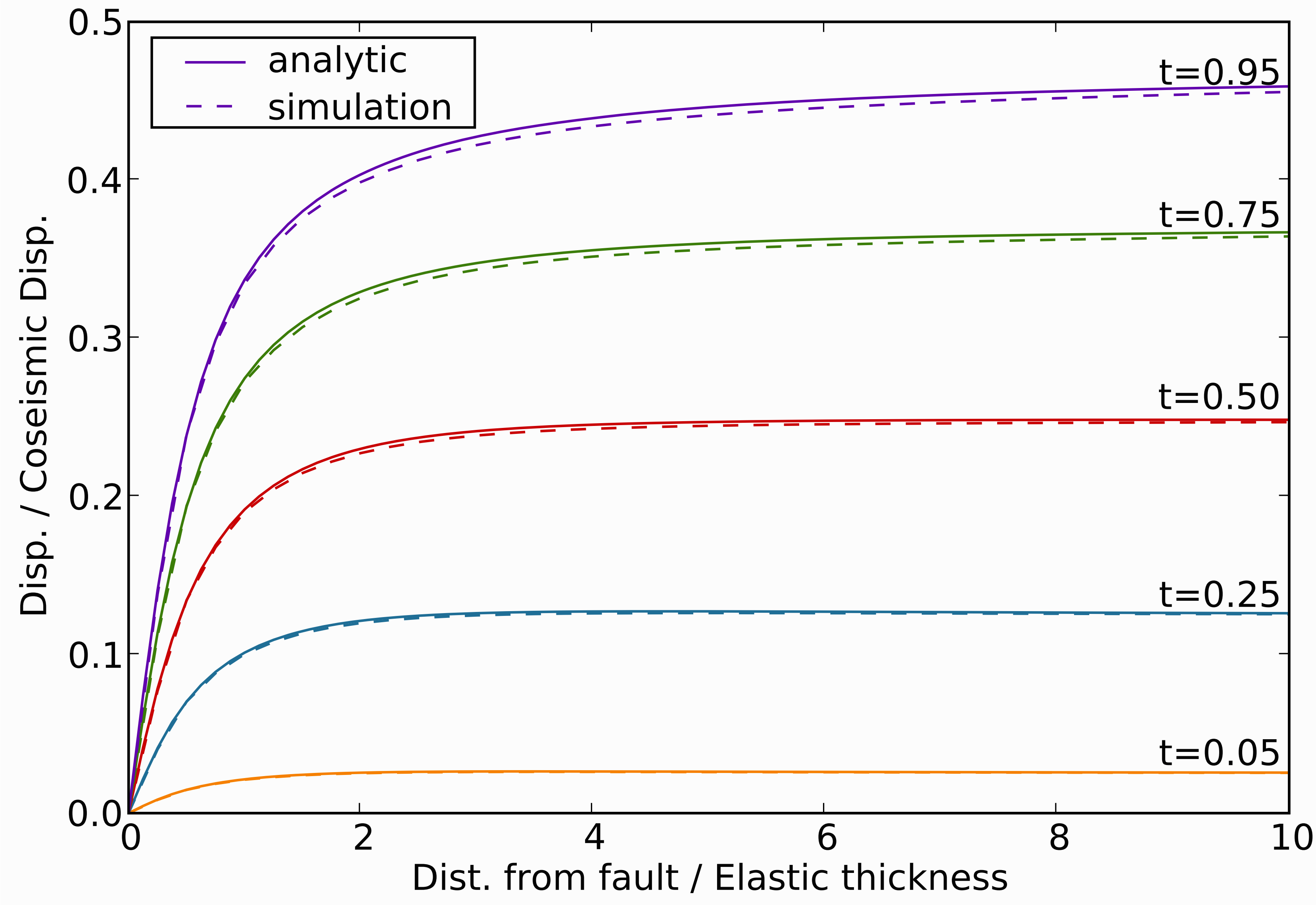
Benchmarking PyLith

Simulation closely matches analytical solution during 10th eq cycle



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Benchmarking PyLith

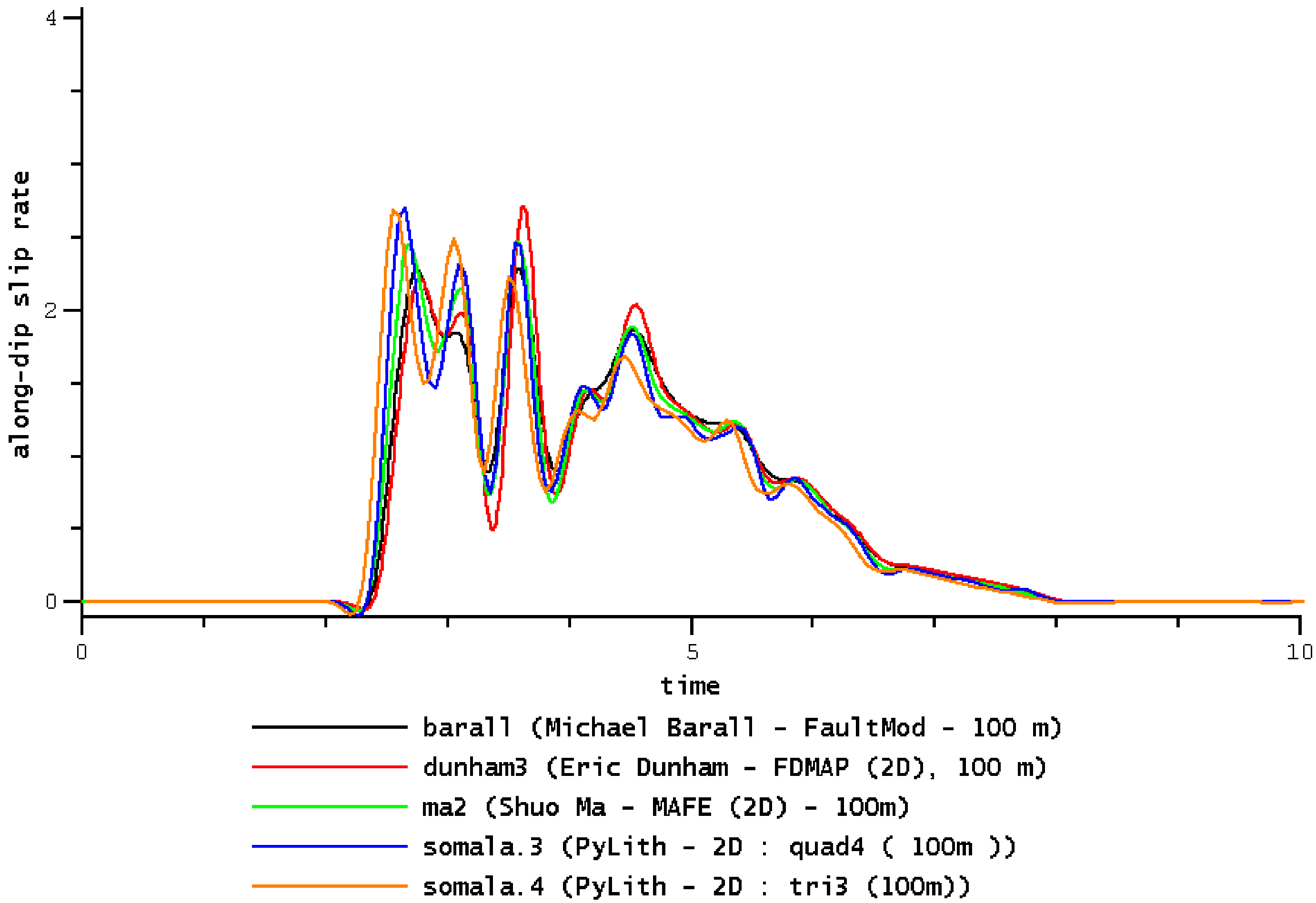
SCEC Dynamic Rupture Verification Benchmarks

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

ADD FIGURE HERE

Benchmarking PyLith

Close agreement with other dynamic rupture codes



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