PyLith

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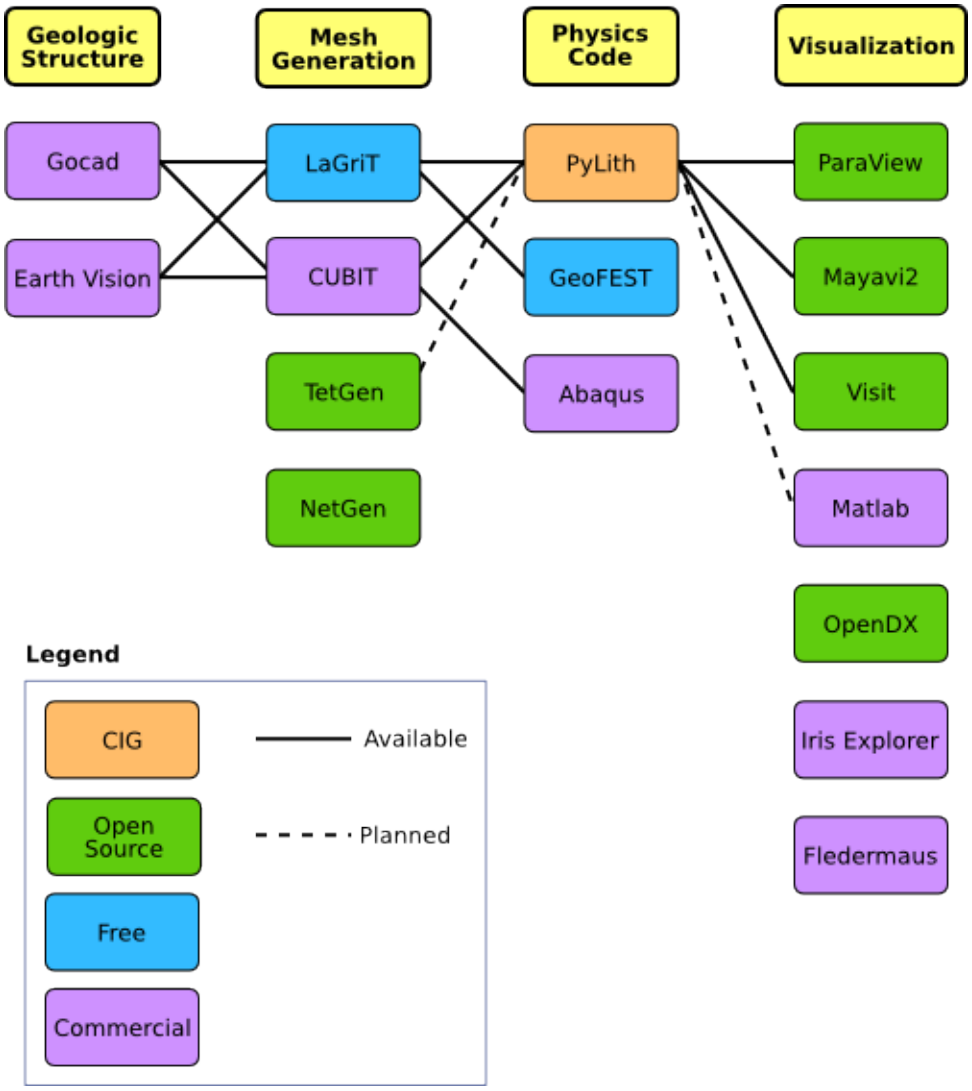
PyLith

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
  - Local/regional ground-motion modeling

Crustal Deformation Modeling

Overview of workflow for typical research problem



Computational Infrastructure for Geodynamics

Features in PyLith 1.3

- Spatial dimensions: 1-D, 2-D, or 3-D
- 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)
- Boundary and interface conditions
  - Dirichlet (prescribed displacement and velocity) boundary conditions
  - Neumann (traction) boundary conditions
  - Absorbing boundary conditions
  - Kinematic (prescribed slip) fault interfaces w/multiple ruptures
  - Gravitational body forces

Features in PyLith 1.3 (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)

PyLith 1.x: Planned Releases

Current productivity is about 2 feature releases per year

- PyLith 1.4: June 2009
  - Power-law viscoelastic rheology and PETSc nonlinear solvers
  - Ability to specify initial stress, strain, and state variables
  - Automatic, transparent nondimensionalization
  - Use SWIG for Python/C++ interface
- PyLith 1.5: anticipate release in Fall 2009
  - Fault constitutive behavior with several widely used friction models
- PyLith 1.6: anticipate release in Spring/Summer 2010
  - Time dependent boundary conditions
  - 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

Motivation for Developing PyLith

- Available modeling codes
  - rarely solve the problem **you** want to solve
  - are often poorly documented
  - may not work correctly
- Current research demands larger, more complex simulations
- Want to avoid multiple, incompatible versions of the same code

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

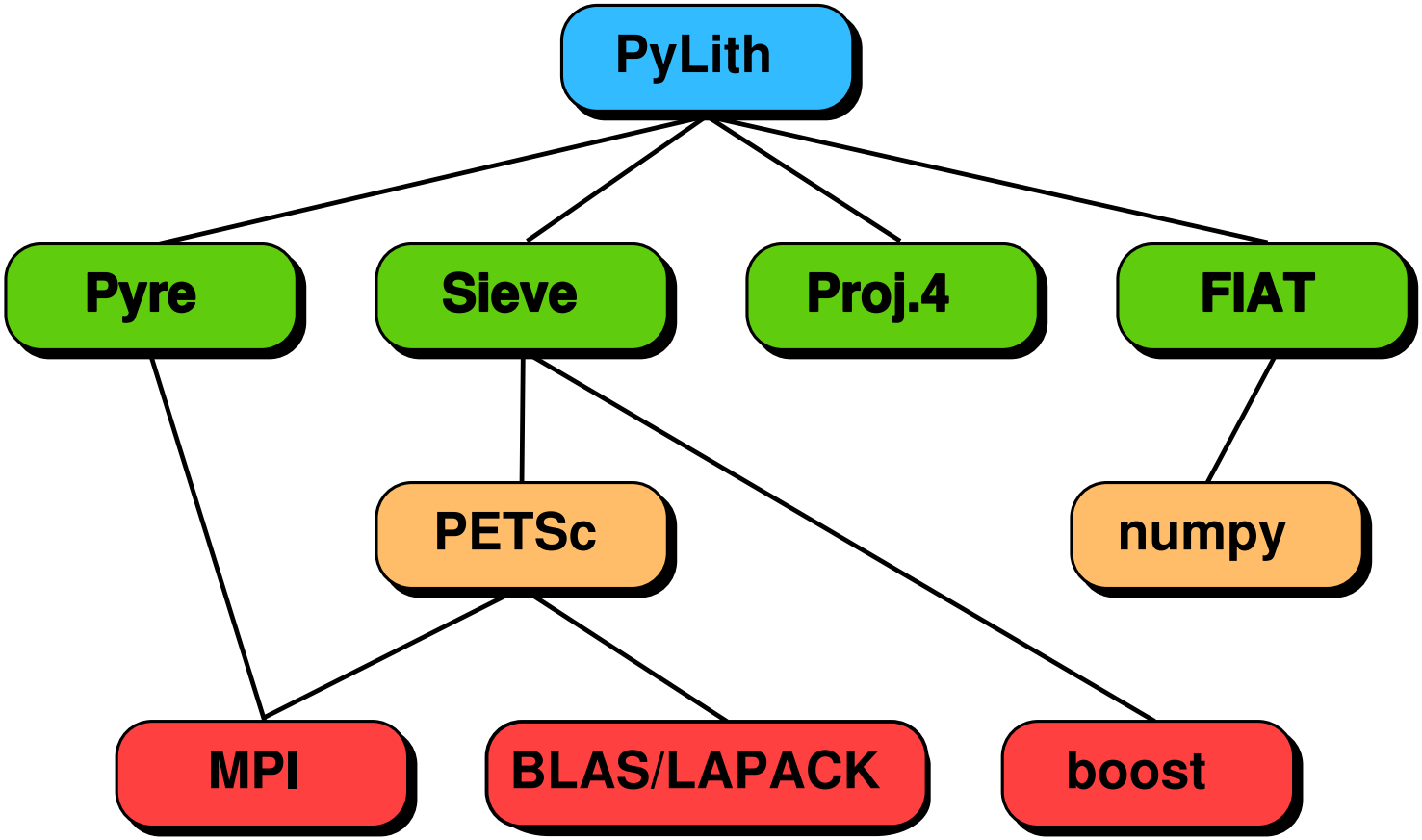
PyLith is a Community Code

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
  - Pyrex/pyrexembed generate C code for calling C++ from Python

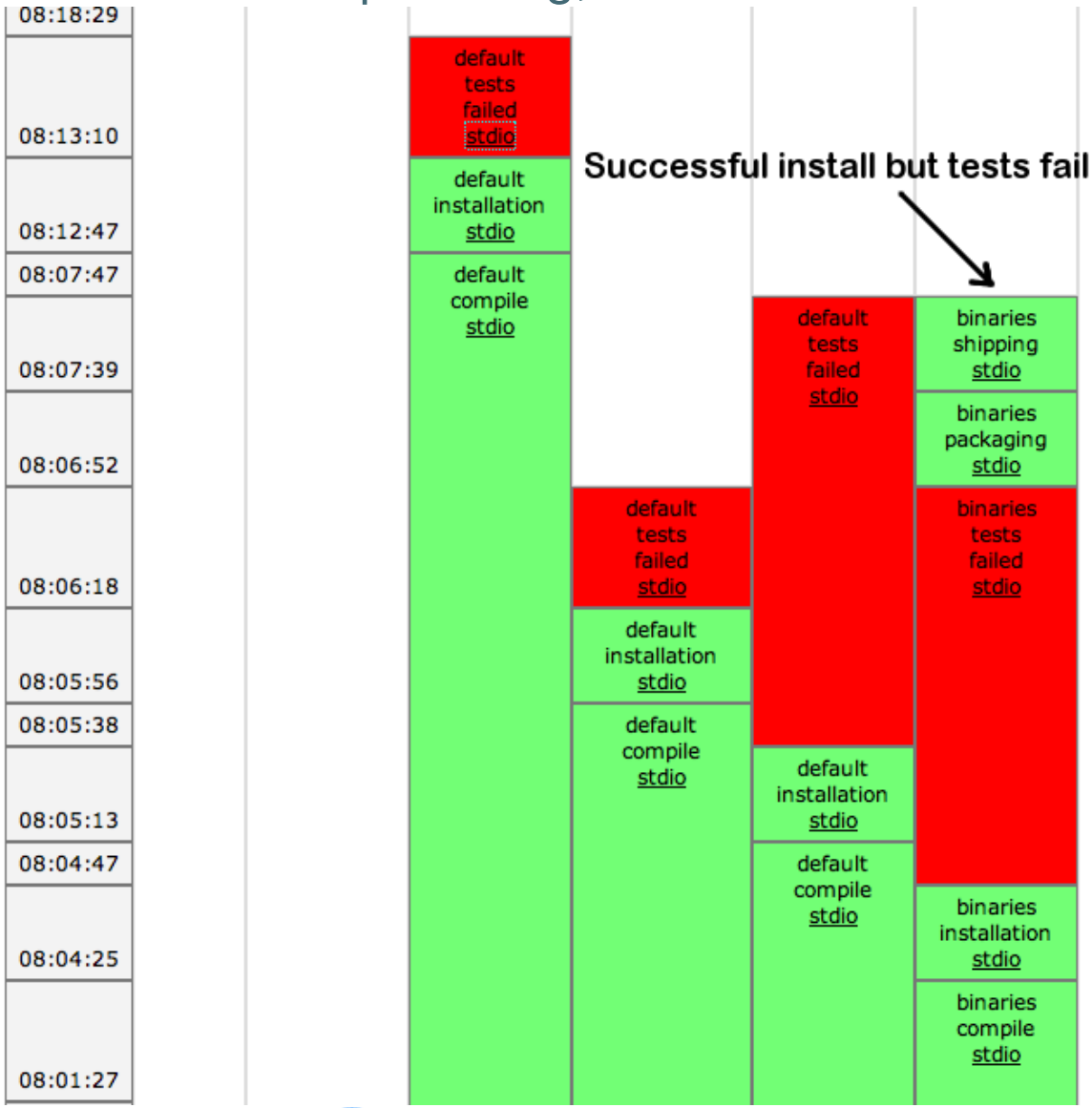
PyLith Design

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

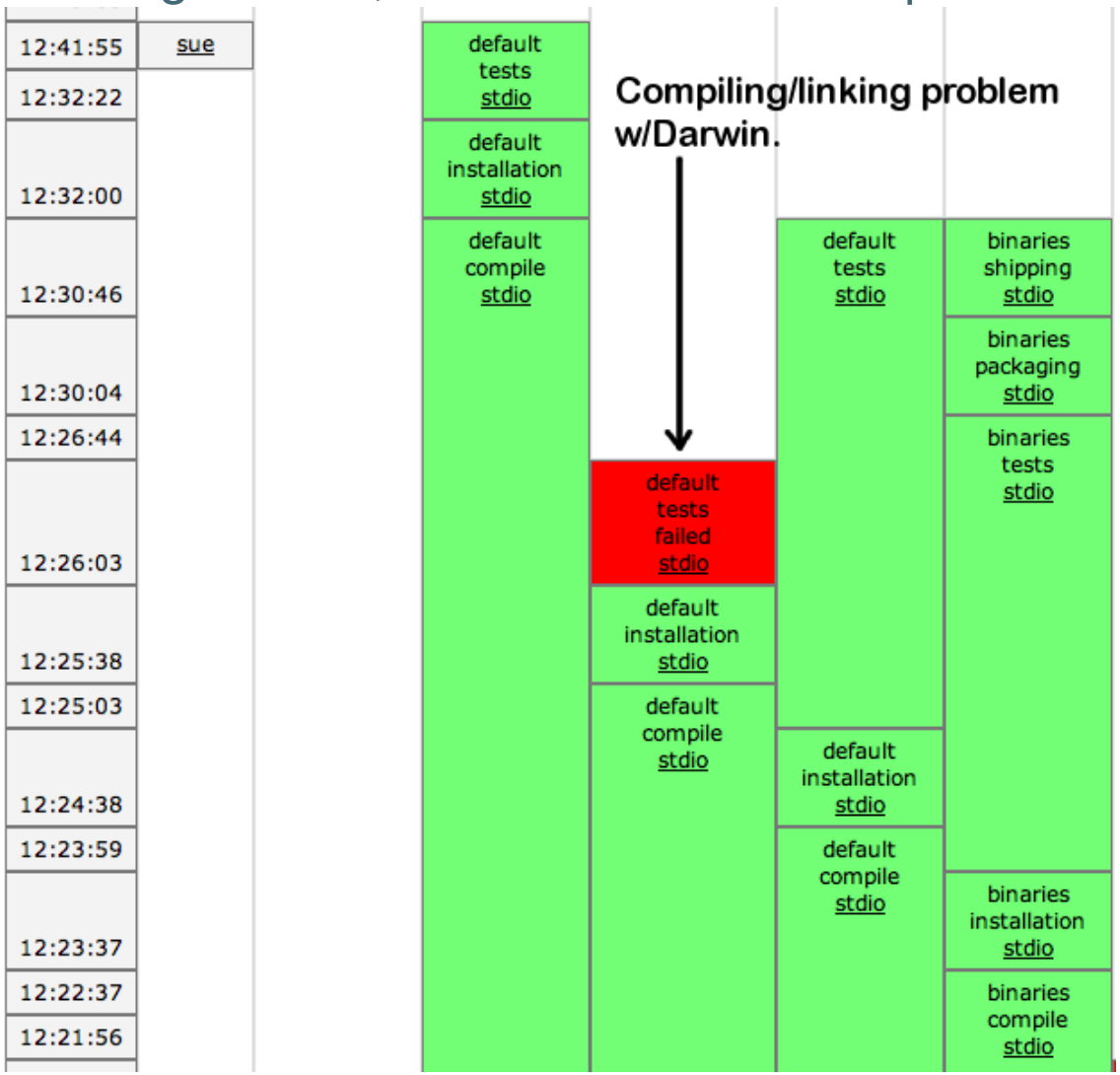
Example of Automated Building and Testing

Test written to expose bug, buildbot shows tests fail



Automated Building and Testing

Bug is fixed, buildbot shows tests pass



Implementation: Finite-Element Data Structures

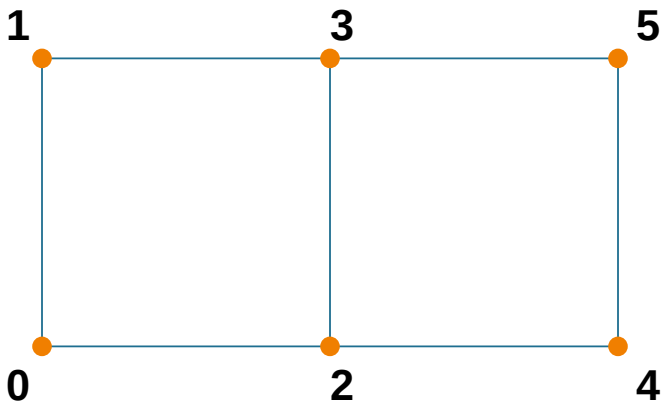
Use Sieve for storage and manipulating mesh information

- 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

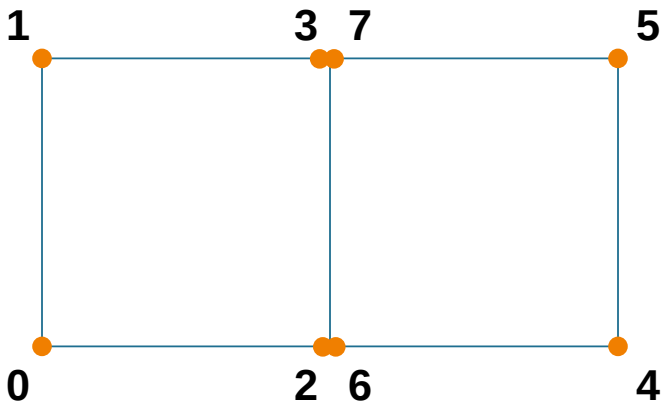
Implementation: Fault Interfaces

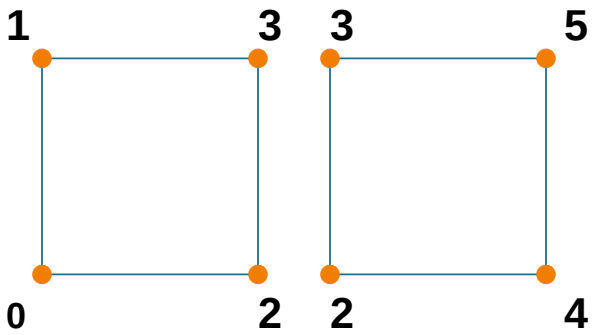
Use cohesive cells to control fault behavior

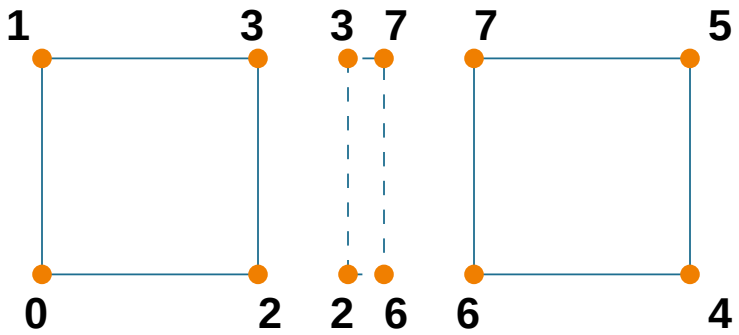
Original Mesh



Mesh with Cohesive Cell







Exploded view of meshes

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

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

- System with cohesive cells & conditioning

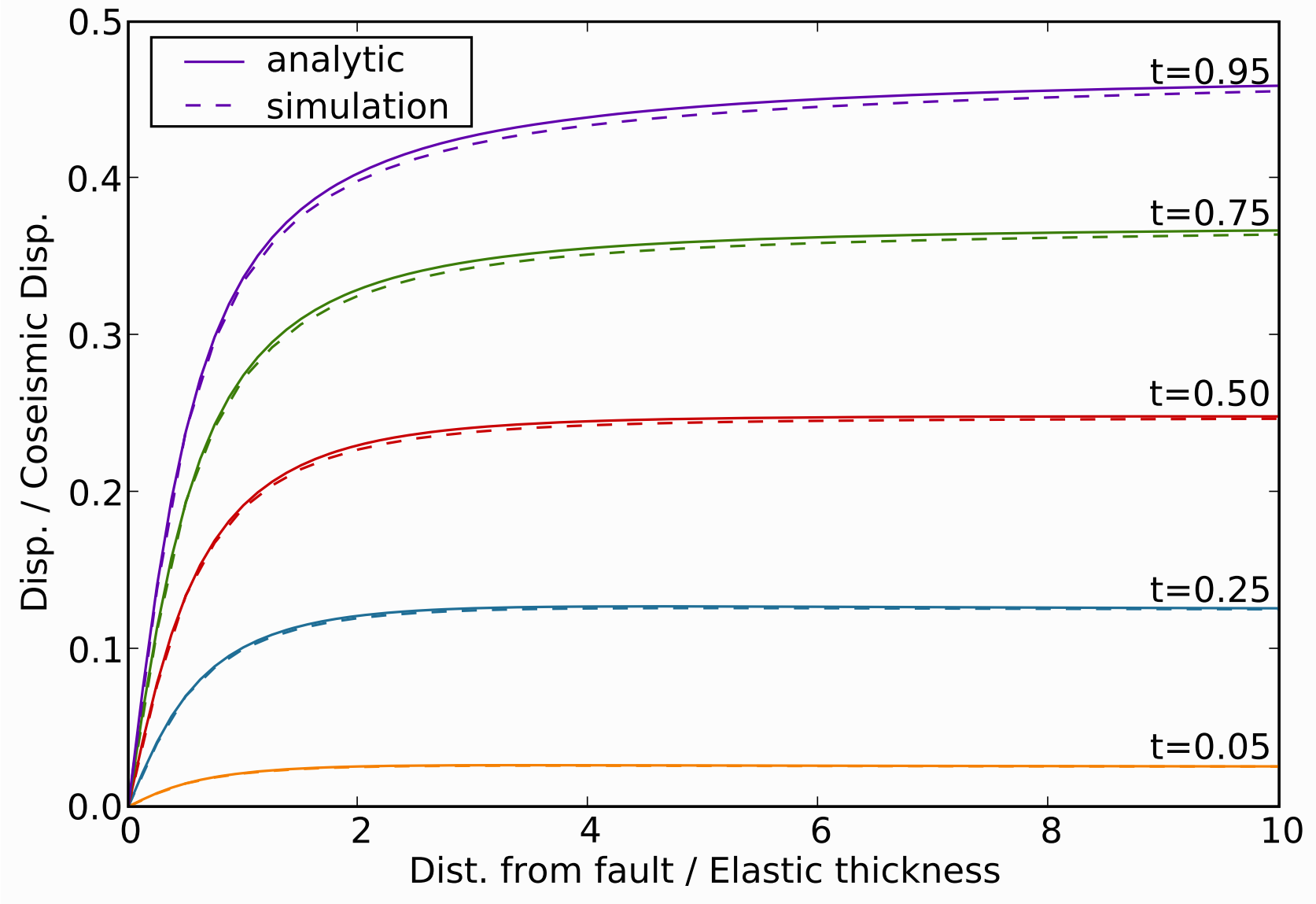
$$\begin{pmatrix} \underline{\mathsf{A}} & a\underline{\mathsf{C}}^T \\ \underline{\mathsf{C}} & 0 \end{pmatrix} \begin{pmatrix} \vec{u} \\ \frac{1}{a}\vec{L} \end{pmatrix} = \begin{pmatrix} \vec{b} \\ \vec{D} \end{pmatrix}$$

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
  - Conditioned matrix is non-symmetric
  - Mixes displacements and forces in solution

Benchmarking PyLith

Simulation closely matches analytical solution during 10th eq cycle



Running PyLith

Ingredients

- Simulation parameters
- Finite-element mesh
  - Mesh exported from LaGriT
  - Mesh exported from CUBIT
  - Mesh constructed by hand (PyLith mesh ASCII format)
- Spatial databases for physical properties, boundary conditions, and rupture parameters
  - SCEC CVM-H, USGS Bay Area Velocity model, or simple ASCII files
  - Independent of discretization scheme and size

Useful Tips/Tricks

- Command line arguments
  - `--help`
  - `--help-components`
  - `--help-properties`
  - `--petsc.start_in_debugger` (run in xterm)
  - `--nodes=N` (to run on N processors on local machine)
- PyLith User Manual
- CIG Short-Term Tectonics mailing list
  - `cig-short@geodynamics.org`
- CIG bug tracking system
  - `http://www.geodynamics.org/roundup`

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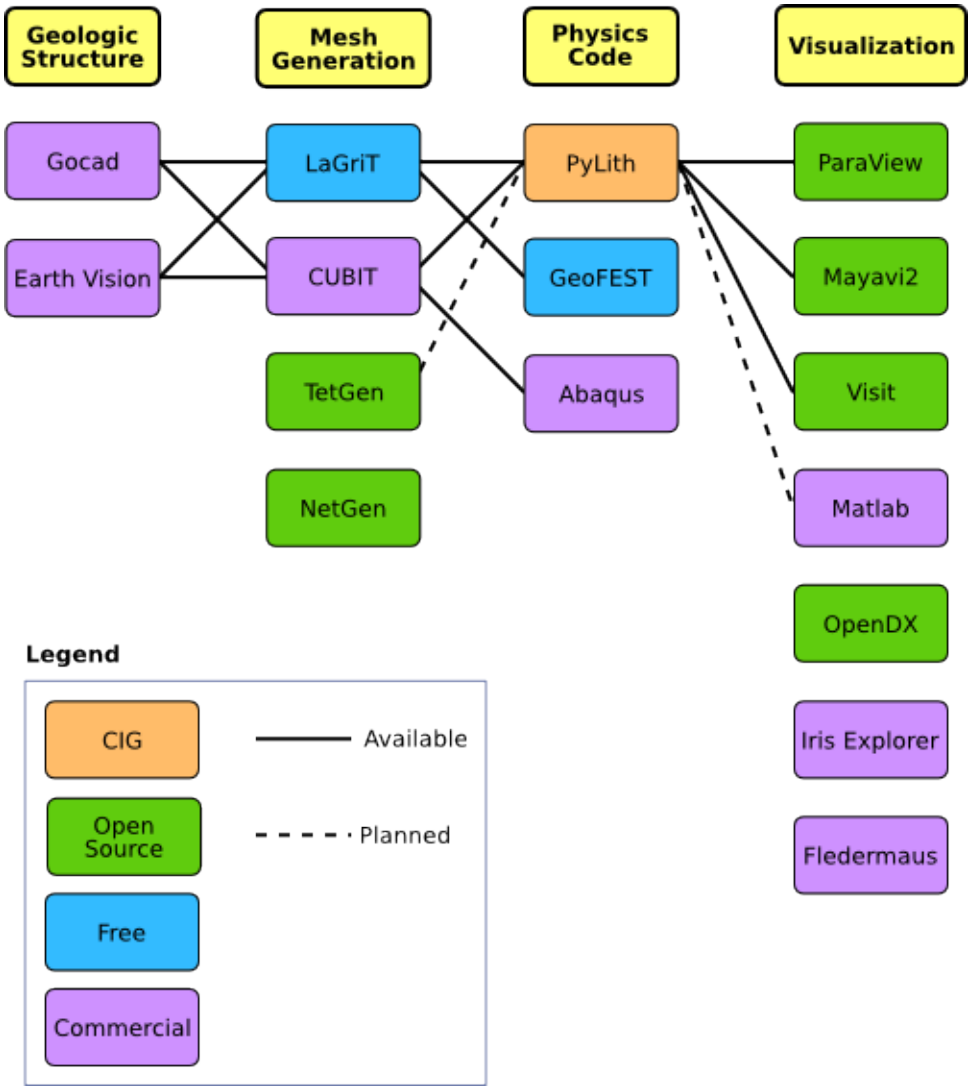

Computational Infrastructure for Geodynamics

Installing PyLith

Download from `geodynamics.org` of copy from CDROM

Recommend copying PyLith and ParaView from CDROM with INSTALL files.

Examples are in src/pylith/examples.