PyLith 1.0: A Finite-Element Code for Modeling Quasi-Static and Dynamic Crustal Deformation

Objectives
- Create a fully-featured, computationally efficient software for simulating crustal deformation across spatial scales ranging from meters to hundreds of kilometers, and temporal scales ranging from milliseconds to hundreds of years.
- 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.

Motivation
- Most available modeling codes:
  - rarely solve the problem you want to solve
  - are often poorly documented
  - may not work correctly
- Research demands larger, more complex simulations
- Want to avoid multiple, incompatible versions of the same code.

Software Architecture
- Separates code into modules to encapsulate behavior and facilitate reuse.
- Top-level code written in Python:
  - Expressive, high-level, object-oriented language
  - Dynamic typing allows adding/mixing modules at runtime
  - Convenient scripting
- Low-level code written in C++:
  - Compiled (fast execution), object-oriented language
  - Bridges to glue Python & C++ together
- Pyrex/pyrexembed generate C code for calling C++ from Python.
- FIAT is a library for converting between geographic projections.
- SciPy is a suite of general, parallel data structures for storing and manipulating finite-element meshes.

Current Release: 1.0.1 (July 2, 2007)
- Initial release targets quasi-static modeling.
- Cell types include triangles, quadrilaterals, hexahedra, and tetrahedra.
- Kinematic fault interfaces using cohesive cells.
- Dirichlet (displacement) boundary conditions.
- Unlabeled elastic and Maxwell linear viscoelastic materials.
- Quasi-static and dynamic time-stepping.

Planned releases
- 1.1 (October/November 2007):
  - Improve performance and complete testing of features for ground-motion modeling with kinematic ruptures.
  - Discretizing boundary conditions
  - Neumann (traction) boundary conditions
  - Velocity boundary conditions
  - Support for output of state variables and parallel (I/O using HDF5)
  - Generalized Maxwell viscoelastic model
- 2.0 (December 2007):
  - Add support for spontaneous earthquake rupture.
  - Fault friction interface conditions
  - Include several popular fault constitutive models
- 3.0 (Spring 2008):
  - Add support for efficient computation of Green’s functions.
  - Add support for large deformations and nonlinear material behavior.

Availability
- PyLith is open-source and aims to be a community code.
- Source code: distributed by Google Code at geodynamics.org.
- Binary packages:
  - Linux (2.6.24)
  - MacOS (PowerPC)
- User manual.

Fault Implementation
We modify the topology of the finite-element mesh, inserting cohesive cells on the fault surface.

Fault Slip in 3-D with Dirichlet BC
- Triangular cells
- Quadrilateral cells
- Tetrahedral cells
- Hexagonal cells

Simple Toy Examples
- Simple Shear in 2-D using Dirichlet BC
- Fault Slip in 3-D with Dirichlet BC

Unit and Regression Testing
Automatically run more than 550 tests on multiple platforms whenever code is checked into the source repository.
- Create tests for nearly every function in code during development
  - Remove most bugs during initial implementation
  - Isolate and expose bugs at origin
  - Create new tests to expose reported bugs
  - Prevent new bugs from recurring
- Run tests whenever code is changed
  - Code continually improves (permissive optimization with quality control)
- Binary packages generated automatically upon successful completion of tests.

Running PyLith
- Source code: distributed by Google Code at geodynamics.org.
- Binary packages:
  - Linux (2.6.24)
  - MacOS (PowerPC)
- User manual.

Major external packages
- Pyrex is a science-neutral simulation framework developed at Delft.
- OpenMP is a suite of general, parallel data structures for storing and manipulating finite-element meshes.
- PETSc is a portable, scalable toolkit for scientific computation from the Argonne National Laboratory. It is used to perform operations on matrices and vectors in parallel.
- MPI is a library for converting between geographic projections.
- FIAT generates arbitrary-order instances of Lagrange elements on lines, triangles, and tetrahedra.

Role of the CIG
The CIG is an NSF-funded membership-governed organization that supports Earth science by developing and maintaining software for computational geophysics.
- PyLith is a fully-supported CIG code. CIG provides the source repository, web site for distribution, mailing lists, bug-tracking system, and testing and benchmarking infrastructure.
- CIG provides developer time (Matt Knepley and Leif Strand) and help in writing the documentation (Sue Kientz).
- Development benefits from the expertise the CIG working groups, especially the Short-Term Crustal Dynamics Group.