Crustal Deformation Modeling Tutorial

Review of PyLith Capabilities and Features

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COMPUTATIONAL INFRASTRUCTURE for GEODYNAMICS

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Crustal Deformation Modeling

Elasticity problems where geometry does not change significantly

Quasi-static modeling associated with earthquakes

- Strain accumulation associated with interseismic deformation
  - What is the stressing rate on faults X and Y?
  - Where is strain accumulating in the crust?
- Coseismic stress changes and fault slip
  - What was the slip distribution in earthquake A?
  - How did earthquake A change the stresses on faults X and Y?
- Postseismic relaxation of the crust
  - What rheology is consistent with observed postseismic deformation?
  - Can aseismic creep or afterslip explain the deformation?

Crustal Deformation Modeling

Elasticity problems where geometry does not change significantly

Dynamic modeling associated with earthquakes

- Modeling of strong ground motions
  - Forecasting the amplitude and spatial variation in ground motion for scenario earthquakes
- Coseismic stress changes and fault slip
  - How did earthquake A change the stresses on faults X and Y?
- Earthquake rupture behavior
  - What fault constitutive models/parameters are consistent with the observed rupture propagation in earthquake A?

Crustal Deformation Modeling

Elasticity problems where geometry does not change significantly

Volcanic deformation associated with magma chambers and/or dikes

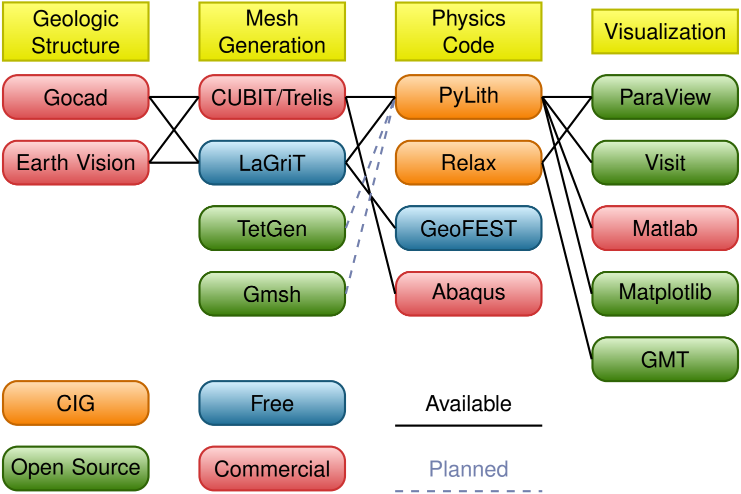
- Inflation
  - What is the geometry of the magma chamber?
  - What is the potential for an eruption?
- Eruption
  - Where is the deformation occurring?
  - What is the ongoing potential for an eruption?
- Dike intrusions
  - What the geometry of the intrusion?

PyLith

- Developers
  - Brad Aagaard (USGS, lead developer))
  - Charles Williams (GNS Science, formerly at RPI)
  - Matthew Knepley (Univ. of Chicago, formerly at ANL)
- Combined dynamic modeling capabilities of EqSim (Aagaard) with the quasi-static modeling capabilities of Tecton (Williams)
- Use modern software engineering (modular design, testing, documentation, distribution) to develop an open-source, community code

Crustal Deformation Modeling

Overview of workflow for typical research problem



Governing Equations

Elasticity equation

$$\sigma_{ij,j} + f_i = \rho \ddot{u} \text{ in } V, \tag{1}$$

$$\sigma_{ij} n_j = T_i \text{ on } S_T, \tag{2}$$

$$u_i = u_i^0 \text{ on } S_u, \text{ and} \tag{3}$$

$$R_{ki}(u_i^+ - u_i^-) = d_k \text{ on } S_f. \tag{4}$$

Multiply by weighting function and integrate over the volume,

$$-\int_V (\sigma_{ij,j} + f_i - \rho \ddot{u}_i)\phi_i \, dV = 0 \tag{5}$$

After some algebra,

$$-\int_V \sigma_{ij}\phi_{i,j} \, dV + \int_{S_T} T_i \phi_i \, dS + \int_V f_i \phi_i \, dV - \int_V \rho \ddot{u}_i \phi_i \, dV = 0 \tag{6}$$

Writing the trial and weighting functions in terms of basis (shape) functions,

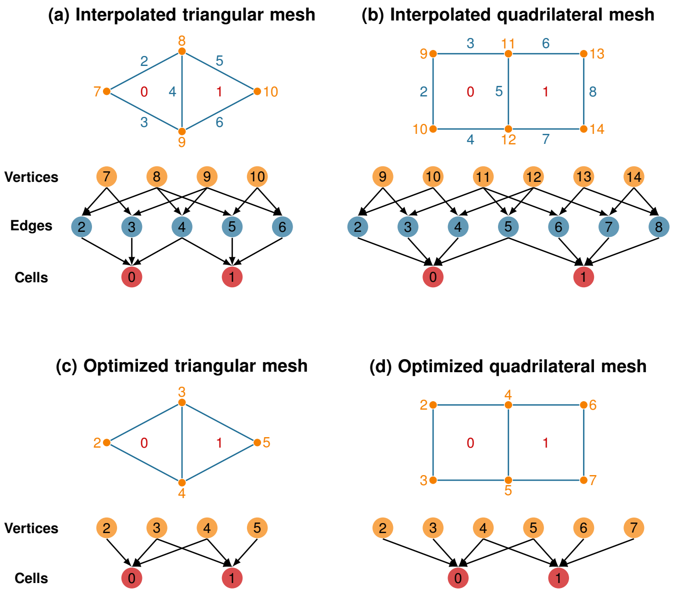
$$u_i(x_i, t) = \sum_m a_i^m(t) N^m(x_i), \tag{7}$$

$$\phi_i(x_i, t) = \sum_n c_i^n(t) N^n(x_i). \tag{8}$$

After some algebra, the equation for degree of freedom *i* of vertex *n* is

$$-\int_V \sigma_{ij} N^n_{,j} \, dV + \int_{S_T} T_i N^n \, dS + \int_V f_i N^n \, dV - \int_V \rho \sum_m \ddot{a}_i^m N^m N^n \, dV = 0 \tag{9}$$

Discretize Domain Using Finite Elements



Governing Equations

Using numerical quadrature we convert the integrals to sums over the cells and quadrature points

$$-\sum_{\text{vol cells}}\sum_{\text{quad pts}} \sigma_{ij} N^n_{,j} w_q |J_{\text{cell}}| + \sum_{\text{surf cells}}\sum_{\text{quad pts}} T_i N^n w_q |J_{\text{cell}}|$$
$$+ \sum_{\text{vol cells}}\sum_{\text{quad pts}} f_i N^n w_q |J_{\text{cell}}|$$
$$- \sum_{\text{vol cells}}\sum_{\text{quad pts}} \rho \sum_m \ddot{a}^m_i N^m N^n w_q |J_{\text{cell}}| = \vec{0} \quad (10)$$

Quasi-static Solution

Neglect inertial terms

Form system of algebraic equations

$$\underline{A}(t)\vec{u}(t) = \vec{b}(t) \tag{11}$$

where

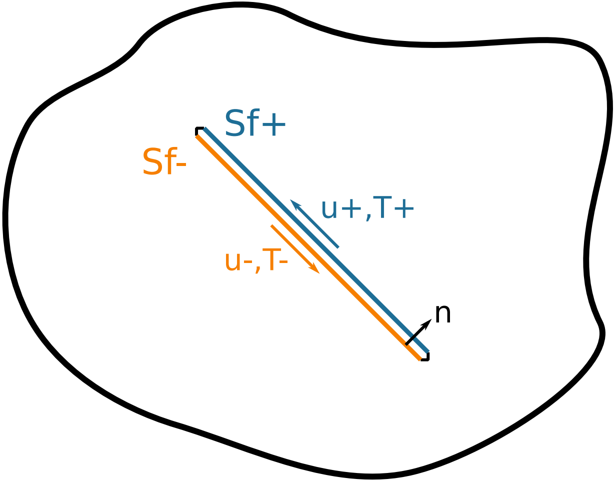
$$A_{ij}^{nm}(t) = \sum_{\text{vol cells}} \sum_{\text{quad pts}} \frac{1}{4} C_{ijkl}(t)(N_{,l}^{m} + N_{,k}^{m})(N_{,j}^{n} + N_{,i}^{n}) w_q |J_{\text{cell}}| \tag{12}$$

$$b_i(t) = \sum_{\text{surf cells}} \sum_{\text{quad pts}} T_i(t) N^n w_q |J_{\text{cell}}| + \sum_{\text{vol cells}} \sum_{\text{quad pts}} f_i(t) N^n w_q |J_{\text{cell}}| \tag{13}$$

and solve for $\vec{u}(t)$.

Fault Interface

Fault tractions couple deformation across interface



Fault Implementation: Governing Equations

Terms in governing equation associated with fault

- Tractions on fault surface are analogous to boundary tractions

$$\ldots + \underbrace{\int_{S_T} \vec{\phi} \cdot \vec{T}\, dS}_{\text{Neumann BC}} - \underbrace{\int_{S_{f+}} \vec{\phi} \cdot \vec{l}\, dS}_{\text{Fault +}} + \underbrace{\int_{S_{f-}} \vec{\phi} \cdot \vec{l}\, dS}_{\text{Fault -}} \ldots = 0$$

- Constraint equation relates slip to relative displacement

$$\int_{S_f} \vec{\phi} \cdot (\underbrace{\vec{d}}_{\text{Slip}} - \underbrace{(\vec{u}_+ - \vec{u}_-)}_{\text{Relative Disp.}}) dS = 0$$

Governing Equations (cont.)

Express weighting function $\vec{\phi}$, displacement field $\vec{u}$, Lagrange multipliers (fault tractions) $\vec{l}$, and fault slip $\vec{d}$ as linear combinations of basis functions,

$$\vec{\phi} = \overline{N}_m \cdot \vec{a}_m \tag{14}$$

$$\vec{u} = \overline{N}_n \cdot \vec{u}_n \tag{15}$$

$$\vec{l} = \overline{N}_p \cdot \vec{l}_p \tag{16}$$

$$\vec{d} = \overline{N}_p \cdot \vec{d}_p \tag{17}$$

Governing Equations (cont.)

- Lagrange multiplier (fault traction) terms:

$$\ldots - \int_{S_{f+}} \overline{N}_m^T \cdot \overline{N}_p \cdot \vec{l}_p \, dS + \int_{S_{f-}} \overline{N}_m^T \cdot \overline{N}_p \cdot \vec{l}_p \, dS = \vec{0} \qquad (18)$$

- Constraint equation

$$\int_{S_f} \overline{N}_p^T \cdot \left(\overline{N}_p \cdot \vec{d}_p - \overline{N}_{n^+} \cdot \vec{u}_{n^+} + \overline{N}_{n^-} \cdot \vec{u}_{n^-} \right) \, dS = \vec{0} \qquad (19)$$

Fault Slip Implementation

Use Lagrange multipliers to specify slip

- System without cohesive cells
  - Conventional finite-element elasticity formulation

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

  - Fault slip associated with relative displacements across fault

$$\underline{C}\vec{u} = \vec{d}$$

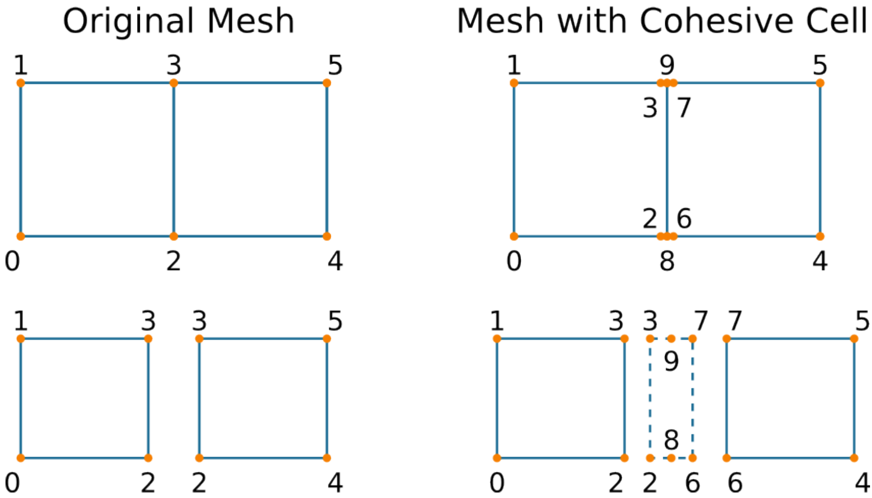
- System with Lagrange multiplier constraints for fault slip

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

- Prescribed (kinematic) slip
  Specify fault slip ($\vec{d}$) and solve for Lagrange multipliers ($\vec{l}$)
- Spontaneous (dynamic) slip
  Adjust fault slip to be compatible with fault constitutive model

Implementation: Fault Interfaces

Use cohesive cells to control fault behavior



Implementing Fault Slip with Lagrange multipliers

- Advantages
  - Fault implementation is local to cohesive cell
  - Solution includes tractions generating slip (Lagrange multipliers)
  - Retains block structure of matrix, including symmetry
  - Offsets in mesh mimic slip on natural faults
- Disadvantages
  - Cohesive cells require adjusting topology of finite-element mesh
  - Scalable preconditioner/solver is more complex

Ingredients for Running PyLith

- 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 or USGS Bay Area Velocity model
  - Simple ASCII files

Spatial Databases

User-specified field/value in space

- Examples
  - Uniform value for Dirichlet (0-D)
  - Piecewise linear variation in tractions for Neumann BC (1-D)
  - SCEC CVM-H seismic velocity model (3-D)
- Generally independent of discretization for problem
- Available spatial databases

UniformDB Optimized for uniform value
SimpleDB Simple ASCII files (0-D, 1-D, 2-D, or 3-D)
SCECCVMH SCEC CVM-H seismic velocity model v5.3
ZeroDispDB Special case of UniformDB

Features in PyLith 1.9

A few small, under-the-hood changes and several parallel processing bug fixes

- Time integration schemes and elasticity formulations
  - Implicit for quasistatic problems (neglect inertial terms)
    - Infinitesimal strains
    - Small strains
  - Explicit for dynamic problems
    - Infinitesimal strains
    - Small strains
    - Numerical damping via viscosity
- Bulk constitutive models
  - Elastic model (1-D, 2-D, and 3-D)
  - Linear Maxwell viscoelastic models (2-D and 3-D)
  - Generalized Maxwell viscoelastic models (2-D and 3-D)
  - Power-law viscoelastic model (2-D and 3-D)
  - Drucker-Prager elastoplastic model (2-D and 3-D)

Features in PyLith 1.9 (cont.)

- 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
  - Linear time-weakening
  - Dieterich-Ruina rate and state friction w/ageing law

Features in PyLith 1.9 (cont.)

- Automatic and user-controlled time stepping
- Ability to specify initial stress/strain state
- Importing meshes
  - LaGriT: GMV/Pset
  - CUBIT: Exodus II
  - ASCII: PyLith mesh ASCII format (intended for toy problems only)
- Output: VTK and HDF5 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
- Parallel uniform global refinement
- PETSc linear and nonlinear solvers
  - Custom preconditioner with algebraic multigrid solver

PyLith Development

- Short-term priorities
  - Under-the-hood improvements
    - New finite-element data structures [done]
    - Support higher order basis functions [in progress]
      Provides much higher resolution for a given mesh
    - Prepare for multi-physics [done]
  - Multi-cycle earthquake modeling
    - Resolve interseismic, coseismic, and postseismic deformation
    - Elastic/viscoelastic/plastic rheologies
    - Coseismic slip, afterslip, and creep
- Long-term priorities
  - Multiphysics: Elasticity + Fluid flow + Heat flow
  - Scaling to 1000 processors

PyLith Development

Planned Releases

- v2.0 (Summer 2013)
  - New finite-element data structures
  - Support for higher order basis functions
- v2.1 (Spring 2014)
  - Coupling of quasi-static and dynamic simulations
  - Moment tensor point sources
- v2.2 (Fall 2014)
  - Support for incompressible elasticity
  - Heat and fluid flow coupled to elastic deformation
- v2.x
  - Support for finite-element integrations on GPUs

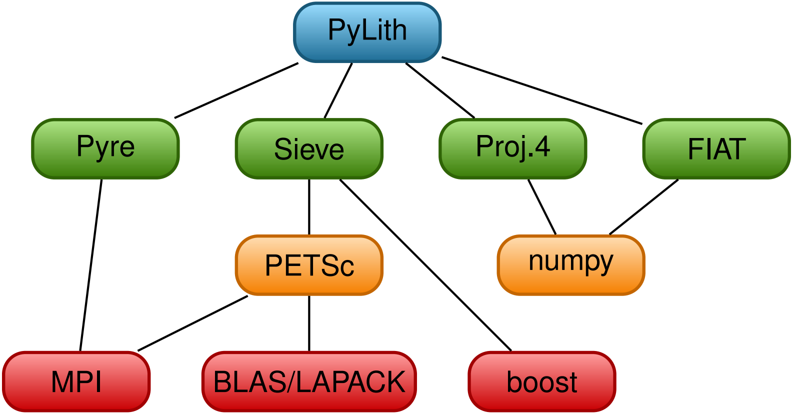
Design Philosophy

Modular, extensible, and smart

- Code should be flexible and modular
- Users should be able to add new features without modifying code, for example:
  - Boundary conditions
  - Bulk constitutive models
  - Fault constitutive models
- Input/output should be user-friendly
- Top-level code written in Python (expressive, dynamic typing)
- Low-level code written in C++ (modular, fast)

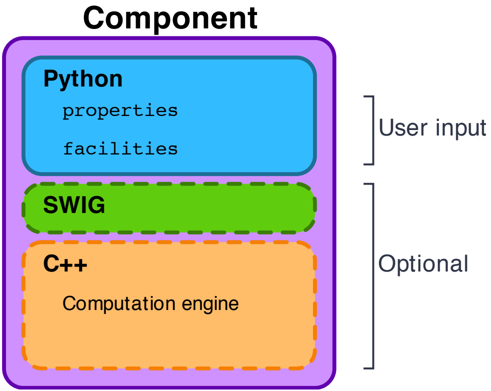
PyLith Design: Focus on Geodynamics

Leverage packages developed by computational scientists



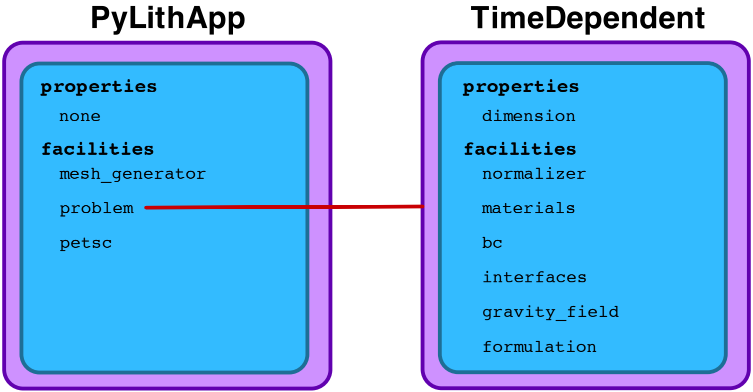
PyLith as a Hierarchy of Components

Components are the basic building blocks



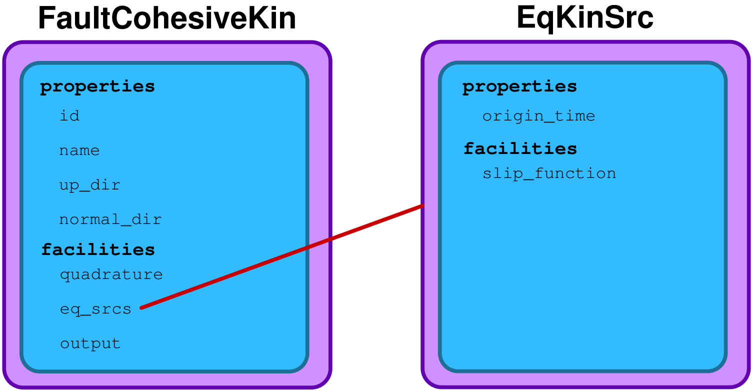
PyLith as a Hierarchy of Components

PyLith Application and Time-Dependent Problem



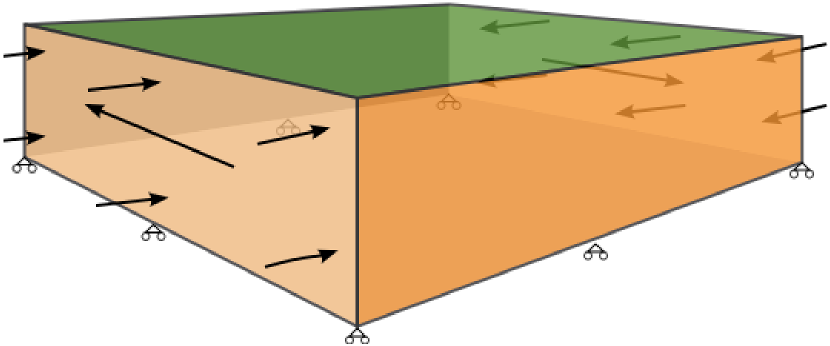
PyLith as a Hierarchy of Components

Fault with kinematic (prescribed slip) earthquake rupture

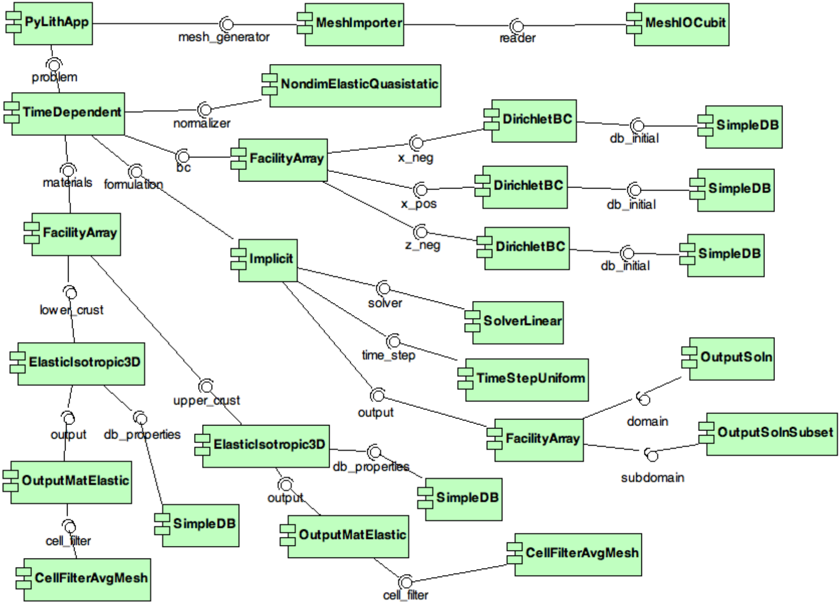


PyLith as a Hierarchy of Components

Diagram of simple toy problem



PyLith as a Hierarchy of Components



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PyLith Application Flow

PyLithApp

```
main()
  mesher.create()
  problem.initialize()
  problem.run()
```

TimeDependent (Problem)

```
initialize()
  formulation.initialize()

run()
  while (t < tEnd)
    dt = formulation.dt()
    formulation.prestep(dt)
    formulation.step(dt)
    formulation.poststep(dt)
```

Implicit (Formulation)

```
initialize()

prestep()
  set values of constraints

step()
  compute residual
  solve for disp. incr.

poststep()
   update disp. field
   write output
```

Unit and Regression Testing

Automatically run more than 1800 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 bugs from reoccurring
- Rerun tests whenever code is changed
  - Code continually improves (permits optimization with quality control)
- Binary packages generated automatically upon successful completion of tests
- Additional full-scale tests are run before releases

General Numerical Modeling Tips

Start simple and progressively add complexity and increase resolution

- Start in 2-D, if possible, and then go to 3-D
  - Much smaller problems $\Rightarrow$ much faster turnaround
  - Experiment with meshing, boundary conditions, solvers, etc
  - Keep in mind how physics differs from 3-D
- Start with coarse resolution and then increase resolution
  - Much smaller problems $\Rightarrow$ much faster turnaround
  - Experiment with meshing, boundary conditions, solvers, etc.
  - Increase resolution until solution resolves features of interest
    - Resolution will depend on spatial scales in BC, initial conditions, deformation, and geologic structure
    - Is geometry of domain important? At what resolution?
    - Displacement field is integral of strains/stresses
    - Resolving stresses/strains requires fine resolution simulations
- Use your intuition and analogous solutions to check your results!

Mesh Generation Tips

There is no silver bullet in finite-element mesh generation

- Hex/Quad versus Tet/Tri
  - Hex/Quad are slightly more accurate and faster
  - Tet/Tri easily handle complex geometry
  - Easy to vary discretization size with Tet, Tri, and Quad cells
  - There is no easy answer

    For a given accuracy, a finer resolution Tet mesh that varies the discretization size in a more optimal way *might* run faster than a Hex mesh
- Check and double-check your mesh
  - Were there any errors when running the mesher?
  - Do all of the nodesets and blocks look correct?
  - Check mesh quality (aspect ratio should be close to 1)
- CUBIT
  - Name objects and use APREPRO or Python for robust scripts
  - Number of points in spline curves/surfaces has huge affect on mesh generation runtime

PyLith Tips

- Read the PyLith User Manual
- Do not ignore error messages and warnings!
- Use an example/benchmark as a starting point
- Quasi-static simulations
  - Start with a static simulation and then add time dependence
  - Check that the solution converges at every time step
- Dynamic simulations
  - Start with a static simulation
  - Shortest wavelength seismic waves control cell size
- CIG Short-Term Crustal Dynamics mailing list
  cig-short@geodynamics.org
- PyLith User Resources
  http://www.geodynamics.org/cig/software/pylith/user_resources

PyLith Debugging Tools

- `pylithinfo [--verbose] [PyLith args]`
  Dumps all parameters with their current values to text file
- 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)
- Journal info flags turn on writing progress

```
[pylithapp.journal.info]
timedependent = 1
```

  - Turns on/off info for each type of component independently
  - Examples turn on writing lots of info to stdout using journal flags

Getting Started

- Read the PyLith User Manual
- Work through the examples
  - Chapter 7 of the PyLith manual
  - Input files are provided with the PyLith binary
    `src/pylith/examples`
  - Input files are provided with the PyLith source tarball
    `src/examples`
- Modify an example to look like a problem of interest