

Crustal Deformation Modeling Workshop

Introduction to PyLith

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June 12, 2014

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

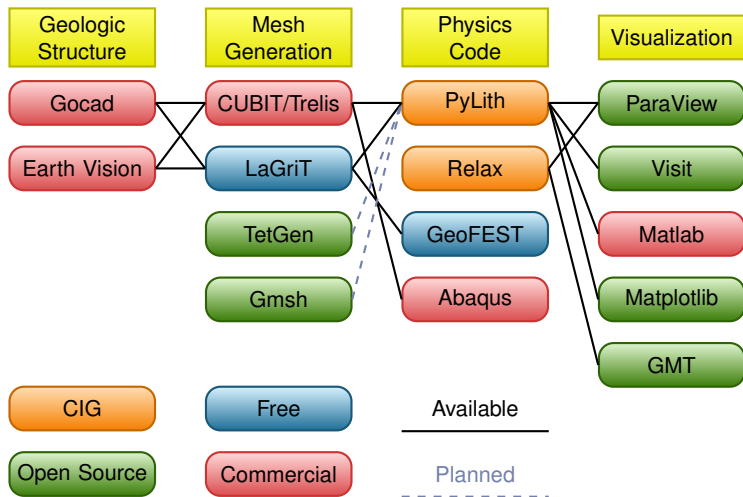
Volcanic deformation associated with magma chambers and/or dikes

- 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 is the geometry of the intrusion?
 - What is the pressure change and/or amount of opening/dilatation?

- 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

$$\sigma_{ij,j} + f_i = \rho \ddot{u}_i \text{ in } V, \quad (1)$$

$$\sigma_{ij} n_j = T_i \text{ on } S_T, \quad (2)$$

$$u_i = u_i^0 \text{ on } S_u, \text{ and} \quad (3)$$

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

Multiply by weighting function and integrate over the volume,

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

After some algebra,

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

Governing Equations

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

$$u_i(x_i, t) = \sum_m a_i^m(t) N^m(x_i), \quad (7)$$

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

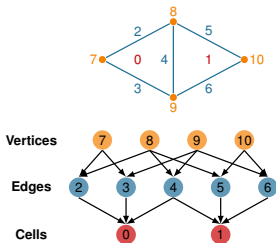
After some algebra, the equation for degree of freedom i of vertex n is

$$-\int_V \sigma_{ij} N_j^n dV + \int_{S_T} T_i N^n dS + \int_V f_i N^n dV - \int_V \rho \sum_m \ddot{a}_i^m N^m N^n dV = 0 \quad (9)$$

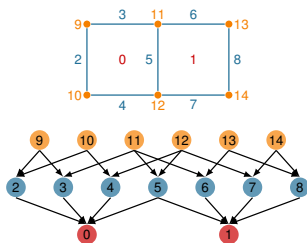
Discretize Domain Using Finite Elements

PyLith v2.0.0 uses interpolated meshes

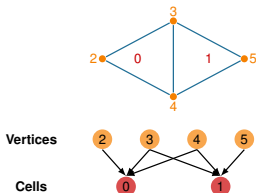
Interpolated triangular mesh



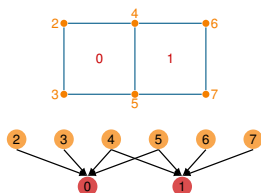
Interpolated quadrilateral mesh



Optimized triangular mesh



Optimized quadrilateral mesh



Governing Equations

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

$$\begin{aligned} - \sum_{\text{vol cells}} \sum_{\text{quad pts}} \sigma_{ij} N_j^n w_q |J_{\text{cell}}| &+ \sum_{\text{surf cells}} \sum_{\text{quad pts}} T_i N^n w_q |J_{\text{cell}}| \\ &+ \sum_{\text{vol cells}} \sum_{\text{quad pts}} f_i N^n w_q |J_{\text{cell}}| \\ - \sum_{\text{vol cells}} \sum_{\text{quad pts}} \rho \sum_m \ddot{a}_i^m N^m N^n w_q |J_{\text{cell}}| &= \vec{0} \quad (10) \end{aligned}$$

Quasi-static Solution

Neglect inertial terms

Form system of algebraic equations

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

where

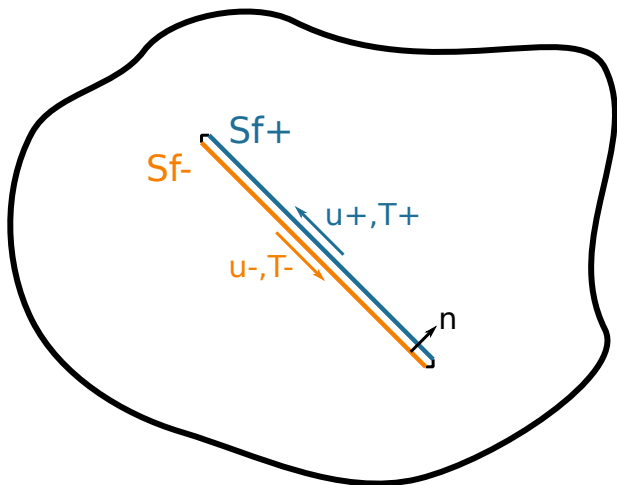
$$A_{ij}^{nm}(t) = \sum_{\text{vol cells}} \sum_{\text{quad pts}} \frac{1}{4} C_{ijkl}(t) (N_{,l}^m + N_{,k}^m) (N_{,j}^n + N_{,i}^n) w_q |J_{\text{cell}}| \quad (12)$$

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

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

- Traction on fault surface are analogous to boundary tractions

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

- Constraint equation relates slip to relative displacement

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

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,

$$\vec{\phi} = \bar{N}_m \cdot \vec{a}_m \quad (14)$$

$$\vec{u} = \bar{N}_n \cdot \vec{u}_n \quad (15)$$

$$\vec{l} = \bar{N}_p \cdot \vec{l}_p \quad (16)$$

$$\vec{d} = \bar{N}_p \cdot \vec{d}_p \quad (17)$$

Governing Equations (cont.)

- Lagrange multiplier (fault traction) terms:

$$\dots - \int_{S_{f+}} \bar{\mathbf{N}}_m^T \cdot \bar{\mathbf{N}}_p \cdot \vec{l}_p dS + \int_{S_{f-}} \bar{\mathbf{N}}_m^T \cdot \bar{\mathbf{N}}_p \cdot \vec{l}_p dS = \vec{0} \quad (18)$$

- Constraint equation

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

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

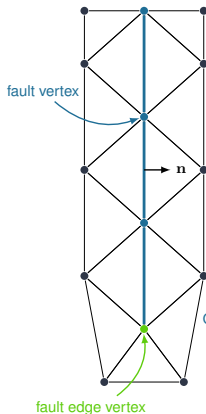
$$\begin{pmatrix} \underline{A} & \underline{C}^T \\ \underline{C} & 0 \end{pmatrix} \begin{pmatrix} \vec{u} \\ \vec{l} \end{pmatrix} = \begin{pmatrix} \vec{b} \\ \vec{d} \end{pmatrix}$$

- 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

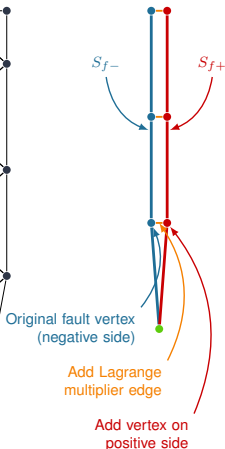
Implementation: Fault Interfaces

Use cohesive cells to control fault behavior

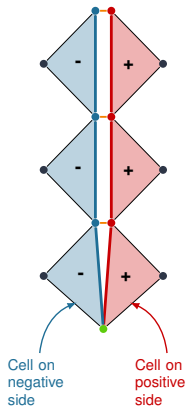
(a) Original mesh



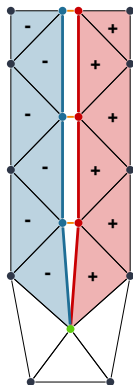
(b) Add collocated vertices



(c) Update cells with fault faces



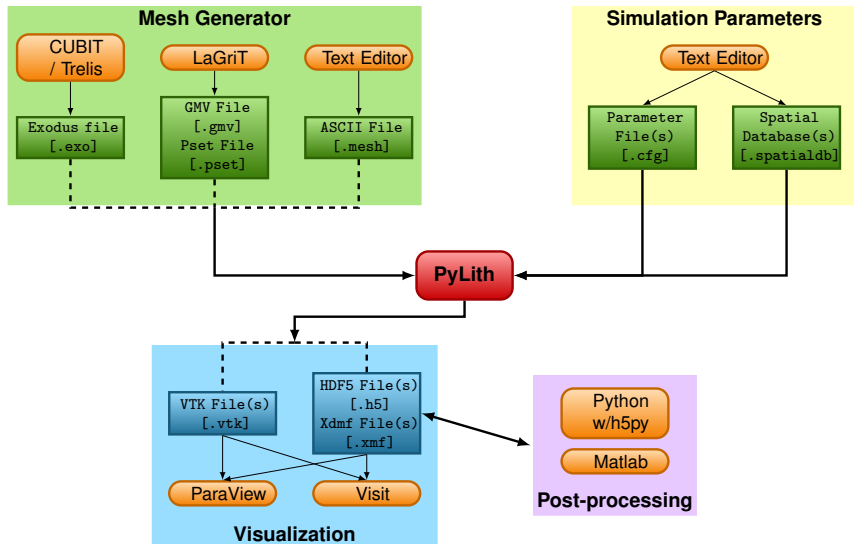
(d) Classify cells and update remaining cells



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

Workflow for Running PyLith



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 2.0

Complete rewrite of finite-element data structures

- 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 (2-D, and 3-D)
 - Elastic model
 - Linear Maxwell viscoelastic models
 - Generalized Maxwell viscoelastic models
 - Power-law viscoelastic model
 - Drucker-Prager elastoplastic model

Features in PyLith 2.0 (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
- Green's functions for slip impulses

Features in PyLith 2.0 (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
 - Solution interpolated to user-specified points
 - 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

See PyLith User Resources for detailed development plan

- Immediate priorities [\[in progress\]](#)
 - New fault implementation for spontaneous rupture
Much faster convergence for quasi-static simulations
 - Improved handling of fault intersections
- Short-term priorities
 - Under-the-hood improvements
 - Support higher order basis functions [\[in progress\]](#)
Provides much higher resolution for a given mesh
 - Multigrid nonlinear solver [\[in progress\]](#)
 - Prepare for multi-physics
 - Multi-cycle earthquake modeling
Resolve interseismic, coseismic, and postseismic deformation
 - Coupling solvers for quasistatic and dynamic deformation
 - Adaptive time stepping
 - Multiphysics: Elasticity + Fluid flow + Heat flow
 - Scaling to 1000 cores

- v2.1 (Summer 2014)
 - New fault implementation for spontaneous rupture
 - Improved handling of fault intersections
- v3.0 (Early 2015)
 - Support for higher order basis functions
 - Adaptive time stepping
- v3.1 (Mid-Late 2015)
 - Support for incompressible elasticity
 - Heat and fluid flow coupled to elastic deformation

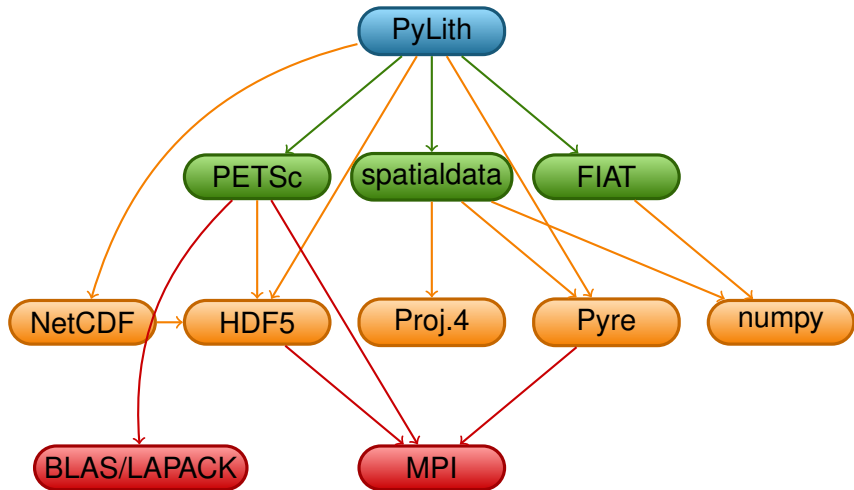
Design Philosophy

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)

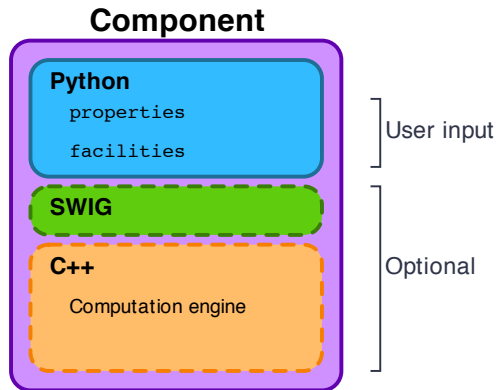
PyLith Design: Focus on Geodynamics

Leverage packages developed by computational scientists



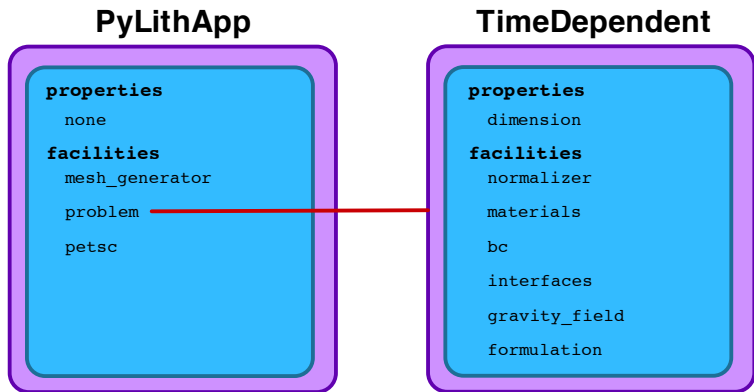
PyLith as a Hierarchy of Components

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

FaultCohesiveKin

properties

id
name
up_dir
normal_dir

facilities

quadrature
eq_srcs
output

EqKinSrc

properties

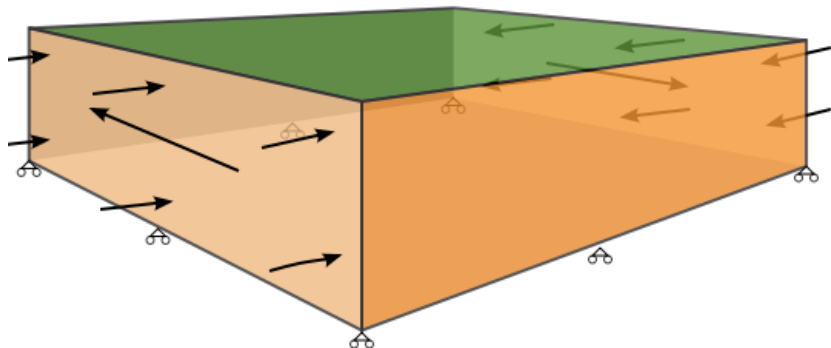
origin_time

facilities

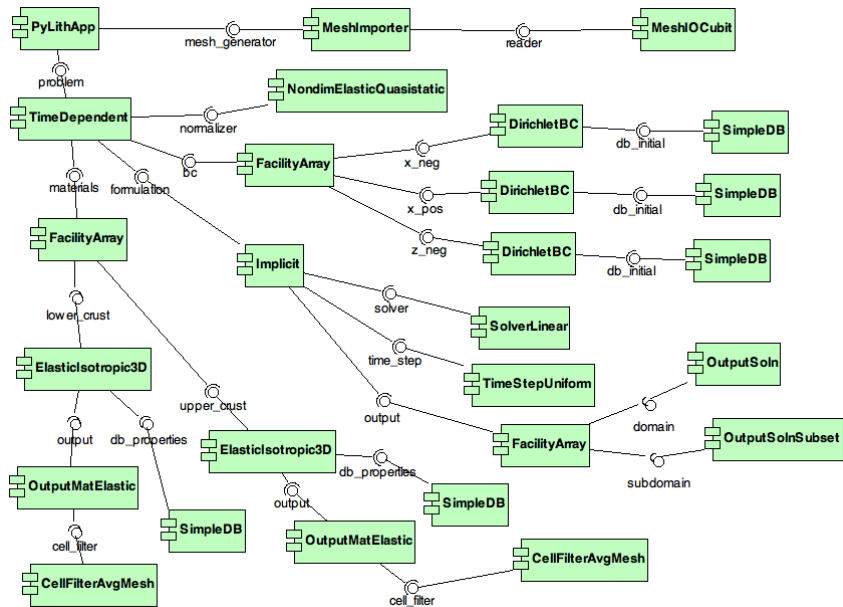
slip_function

PyLith as a Hierarchy of Components

Diagram of simple toy problem



PyLith as a Hierarchy of Components



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 parallel regression 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
 - Start with an exact solver
 - 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
 - Start with an exact solver
 - 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

- 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://wiki.geodynamics.org/software:pylith:start>

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-2.0.0/examples`
 - Input files are provided with the PyLith source tarball
`src/examples`
- Modify an example to look like a problem of interest

Installing PyLith, CUBIT/Trelis, and ParaView

- PyLith - geodynamics.org/cig/software/pylith/
- CUBIT/Trelis
 - Non-US gov't institutions: Trelis - www.csimsoft.com
(30-day free trial available)
 - US gov't agencies: CUBIT - cubit.sandia.gov
(minimal cost)
- ParaView - www.paraview.org/download/

Example: `examples/3d/hex8/step03`

- 1 Download and install CUBIT or Trelis, PyLith, and ParaView
- 2 Create the finite-element mesh using Trelis
- 3 Setup PyLith `.cfg` parameter files
- 4 Setup spatial database files input files
- 5 Run PyLith
- 6 Visualize results via ParaView