PyLith 1.5 Tutorial

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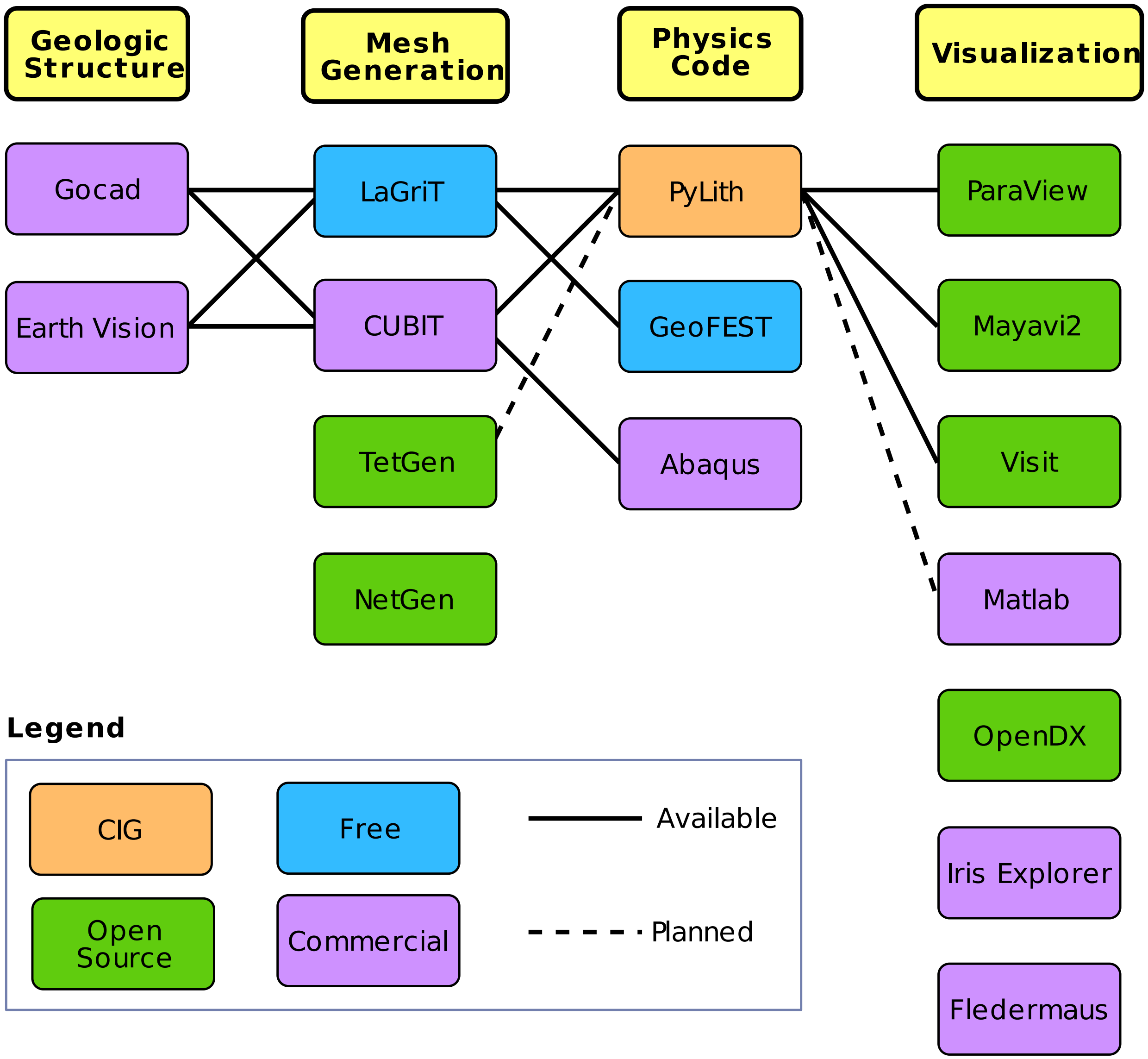
Computational Infrastructure for Geodynamics

June 14, 2010

Crustal Deformation Modeling

Overview of workflow for typical research problem



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 1.5

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

Time-Dependent Boundary Conditions

Dirichlet, Neumann, and Point Forces

$$f(\vec{x}) =$$

$$\begin{array}{ll} f_0(\vec{x}) + & \texttt{db\_initial} \\ \dot{f}_1(\vec{x})(t - t_1(\vec{x})) + & \texttt{db\_rate} \\ f_2(\vec{x})a(t - t_2(\vec{x})) & \texttt{db\_change} \end{array}$$

db_initial Initial value (constant in time)

db_rate Constant rate of change (spatially variable start time)

db_change Time history (spatially variable amplitude and start time)

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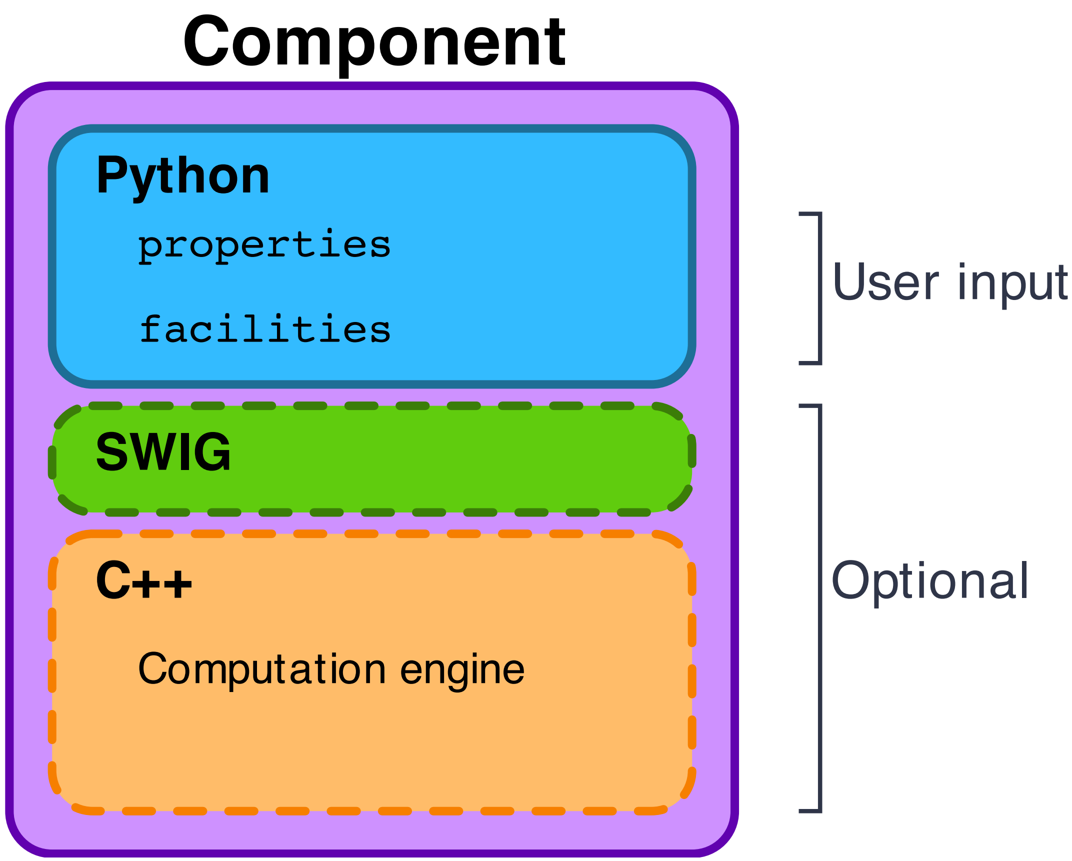
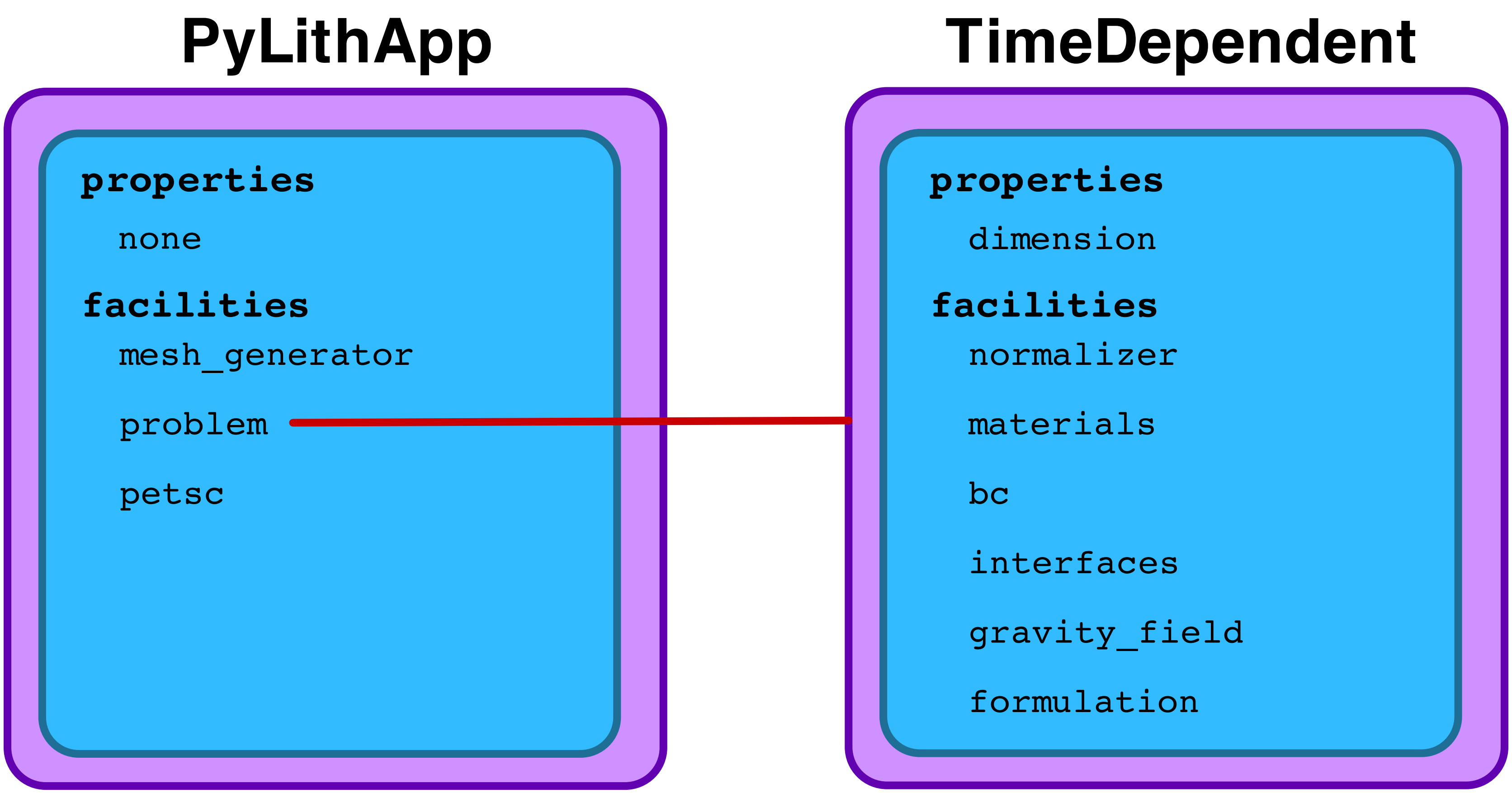
PyLith as a Hierarchy of Components

Components are the basic building blocks



PyLith as a Hierarchy of Components

PyLith Application and Time-Dependent Problem



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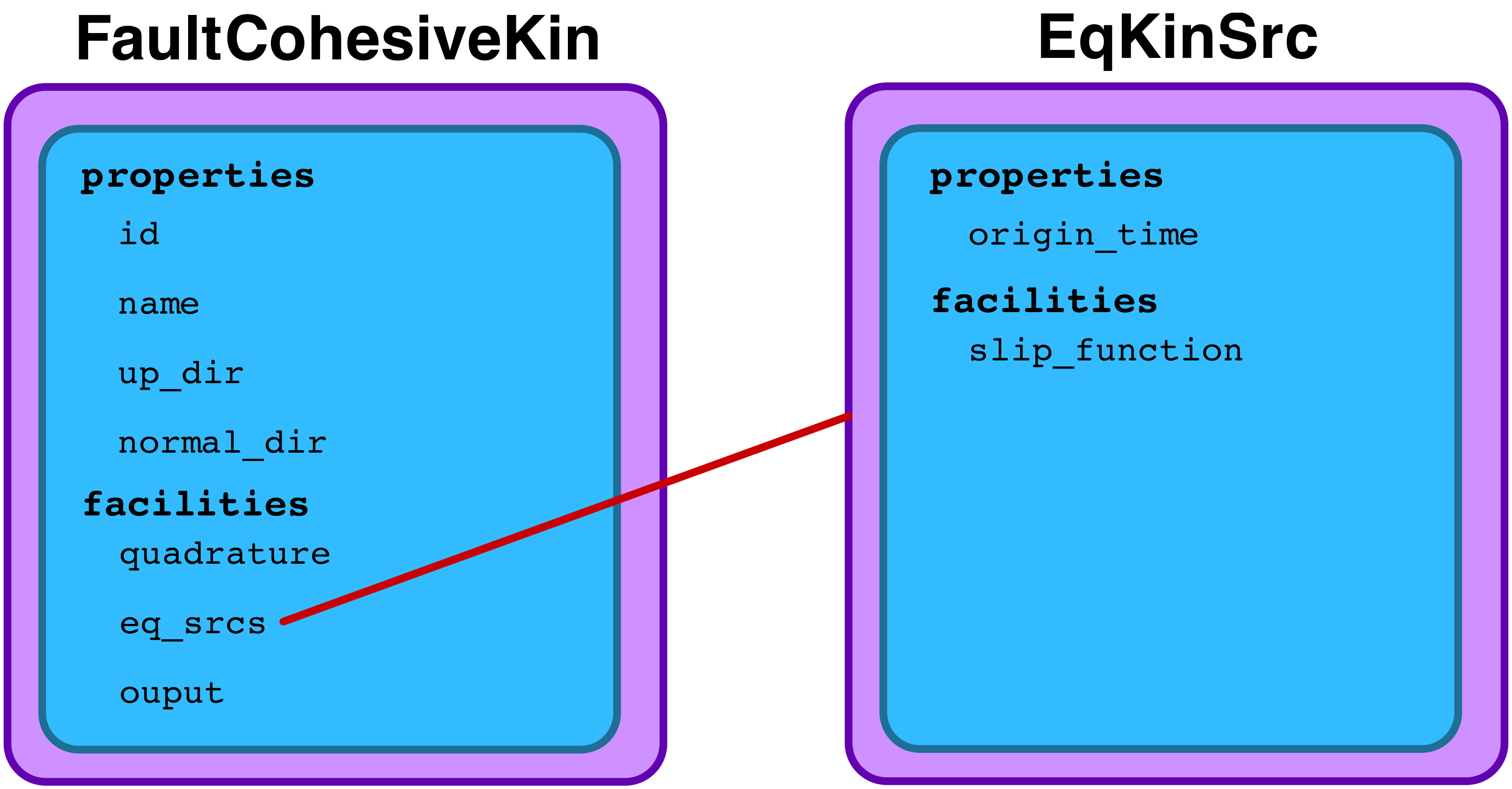
PyLith as a Hierarchy of Components

Fault with kinematic (prescribed slip) earthquake rupture



PyLith Application Flow

PyLithApp

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

TimeDependent (Problem)

```
initialize()
  formulation.initialize()

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

Implicit (Formulation)

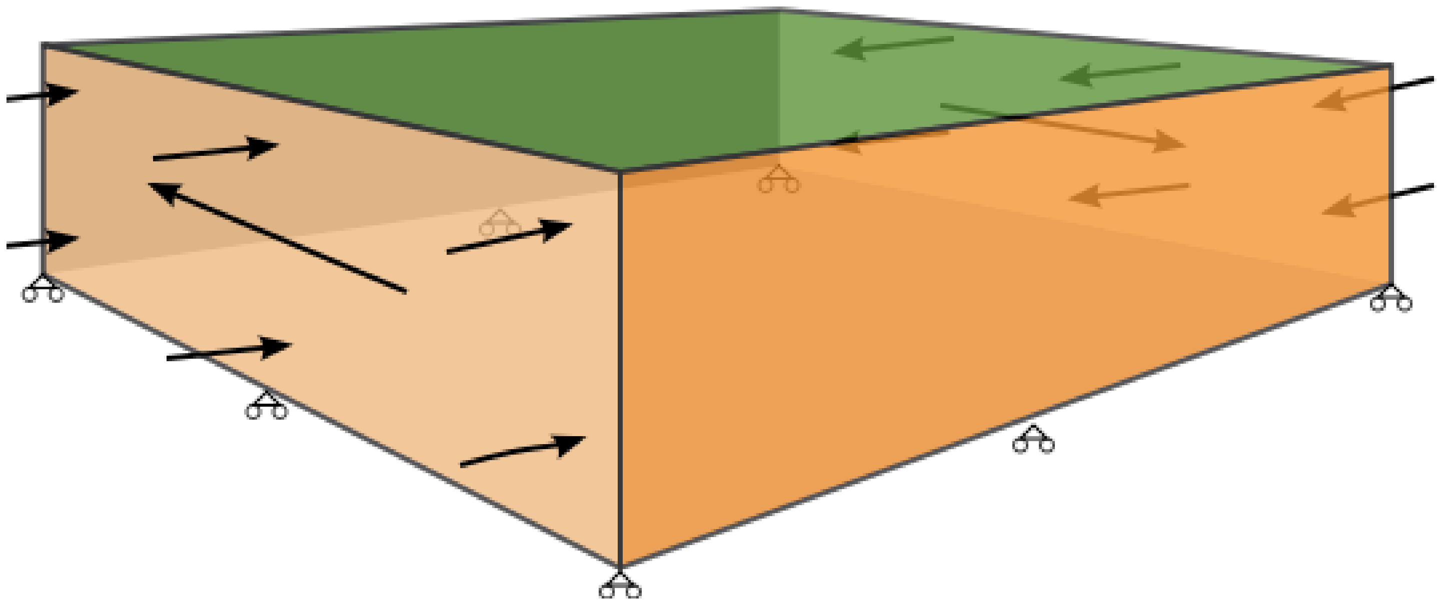
```
initialize()

prestep()
  set constraints

step()
  calculate residual
  solve for displacement increment

poststep()
  update displacement field
  write output
```

Ingredients for Running PyLith

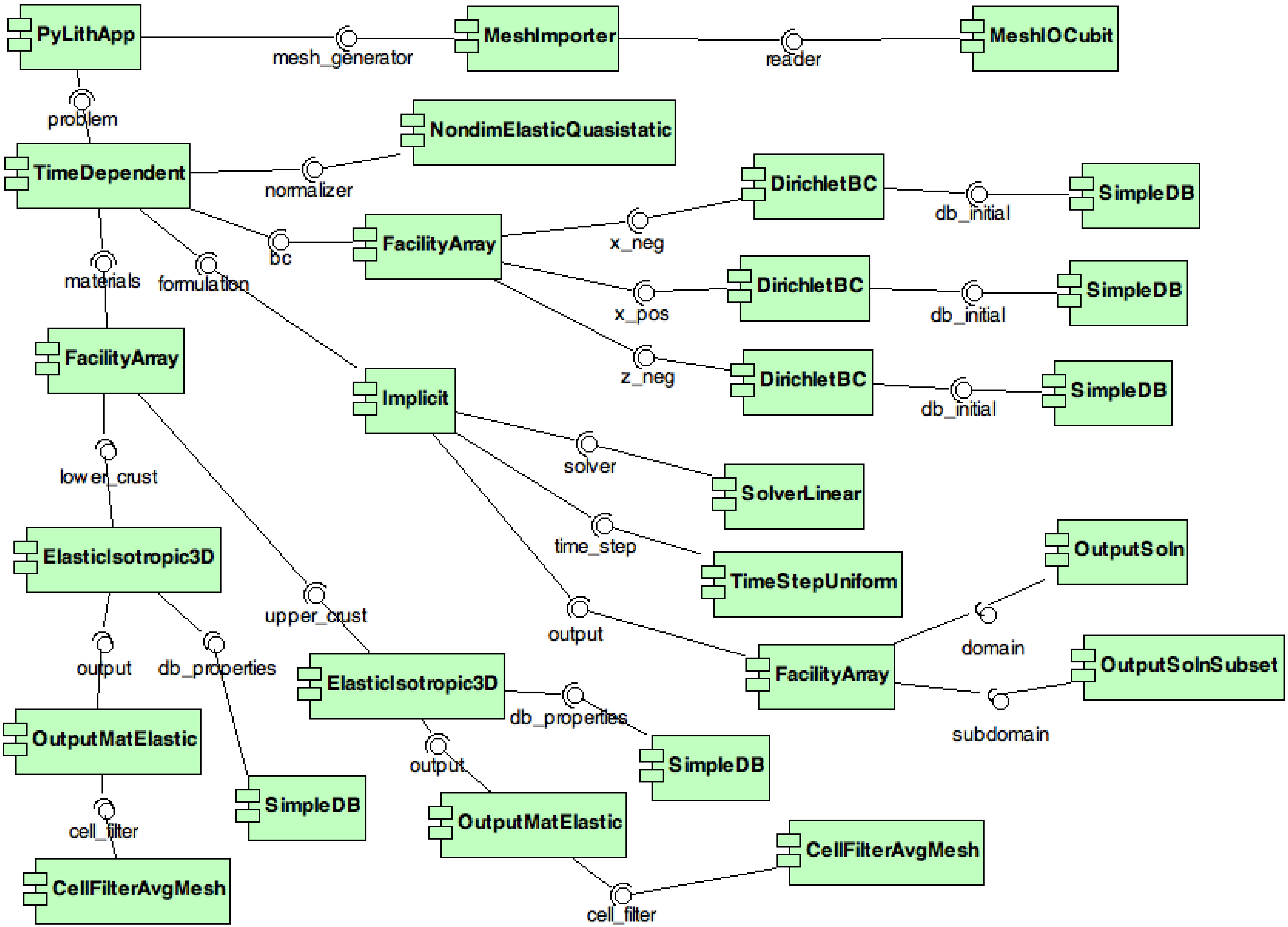
- Simulation parameters
  - `.cfg` ASCII files
  - `pylithapp.cfg` always read if it exists
  - Command line arguments
- Finite-element mesh
  - Mesh exported from LaGriT
  - Mesh exported from CUBIT
  - Mesh constructed by hand (PyLith mesh ASCII format)
- Spatial databases for physical properties, boundary conditions, and rupture parameters

Example: `3d/hex8 step01.cfg`

Compression and shear via prescribed displacements



Example: `3d/hex8 step01.cfg`



Example: `3d/hex8 step01.cfg`

Input

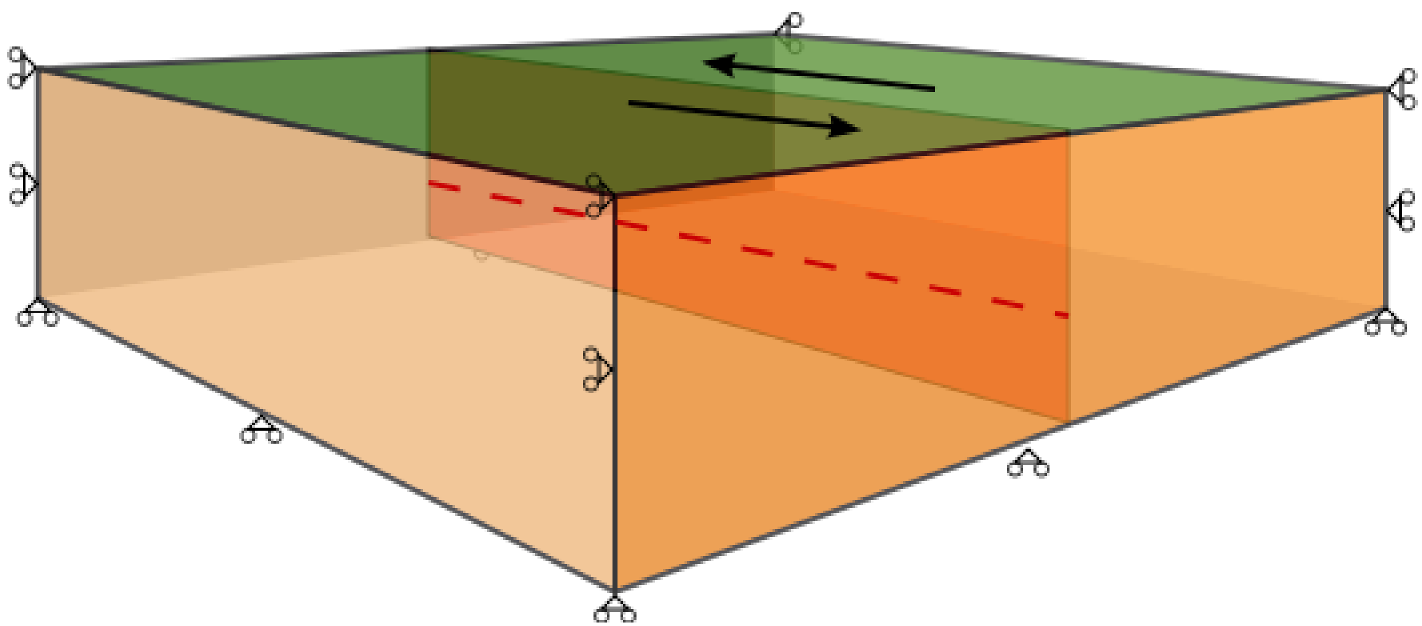
- Simulation parameters
  - `pylithapp.cfg`
  - `step01.cfg`
- CUBIT Mesh: `mesh_hex8_1000m.mesh`
- Spatial databases
  - `mat_elastic.spatialdb`
  - `axialdisp.spatialdb`

Output

- Displacement field
  - `step01_t000000.vtk`
  - `step01-groundsurf_t000000.vtk`
- State variables
  - Upper crust (elastic)
    - `step01-statevars_info.vtk` (physical properties)
    - `step01-statevars_t000000.vtk` (stress and strain)
  - Lower crust (elastic)
    - `step01-statevars_info.vtk` (physical properties)
    - `step01-statevars_t000000.vtk` (stress and strain)

Example: `3d/hex8 step06.cfg`

Creep and repeated rupture on a strike-slip fault



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