

# PyLith Modeling Tutorial

## Debugging PyLith Simulations

Brad Aagaard  
Charles Williams  
Matthew Knepley



June 18, 2016

# What parameters are available?

Parameters are specified as a hierarchy of components and properties

- Components (Facilities) are the object building blocks  
**Appendix B of the PyLith manual lists all of the components**
  - Problem `TimeDependent`
  - Boundary conditions `DirichletBC`
  - Faults `FaultCohesiveKin`
  - Materials `MaxwellViscoelastic3D`
  - Output managers `OutputSolnSubset`
  - Readers `MeshIOCubit`
- Properties are the basic types
  - String `mat_viscoelastic.spatialdb`
  - Integer `4`
  - Float `2.3`
  - Dimensioned quantity `2.5*year`
  - Array of Strings, Integers, or Floats `[0, 0, 1]`

# How do I show the values of the current parameters?

Case study: examples/3d/hex8/step01

- All current parameters and their values

```
pylithinfo [--verbose] [-o pylith.parameters.txt] [-h] [PyLith args]  
pylithinfo --verbose step01.cfg
```

- Components and properties for given component `--help`

```
step01.cfg [pylithapp.timedependent.bc.z.neg]  
shell pylith step01.cfg --timedependent.bc.z.neg.help
```

- Current components of a given component `--help-components`

```
step01.cfg [pylithapp.timedependent.bc.z.neg]  
shell pylith step01.cfg --timedependent.bc.z.neg.help-components
```

- Current properties of a given component `--help-properties`

```
step01.cfg [pylithapp.timedependent.bc.z.neg]  
shell pylith step01.cfg --timedependent.bc.z.neg.help-properties
```

# What about a GUI?

Browser-based GUI under development

- Use web browser as GUI to parameters
  - See all parameters with descriptions
  - See possible choices for components and properties
- Basic validation of parameters
- Export parameters to single file
  - Facilitate archiving parameters used in given simulation

Started in Oct 2013 but v2.0 and v3.0 releases have higher priority

# Debugging Examples

See examples/debugging

**Step01** Simple shear using Dirichlet BC in static simulation

**Step02** Prescribed fault slip with Dirichlet BC

- Static simulation
- Fault is embedded within the domain

**Step03** Spontaneous rupture with Dirichlet BC

- Static simulation
- Static friction ( $\mu_f = 0.6$ )
- Slip driven by simple shear

Correct files are provided for reference

# Step01: Error 1

Error found while doing very basic validation of parameters

```
$ pylith step01.cfg
```

## Python stacktrace

```
Traceback (most recent call last):
  File "/Volumes/Tools/unix/pylith-dev/gcc-4.7.3/bin/pylith", line 27, in <module>
    start(applicationClass=PyLithApp)
  File "/Volumes/Tools/unix/cig/gcc-4.7.3/lib/python2.7/site-packages/pythia-0.8.1.15-py2.7.egg-shell.run(**kwds)
  File "/Volumes/Tools/unix/cig/gcc-4.7.3/lib/python2.7/site-packages/pythia-0.8.1.15-py2.7.egg-app.applyConfiguration(context)
  File "/Volumes/Tools/unix/cig/gcc-4.7.3/lib/python2.7/site-packages/pythia-0.8.1.15-py2.7.egg
    raise ValueError("%s\nBacktrace - Component %s" % (err.message, aliases))
```

## Error message

```
ValueError: Error while configuring Dirichlet boundary condition (dirichletbc, x_pos):
Error while configuring boundary condition (dirichletbc, x_pos):
Label for group/nodeset/pset in mesh not specified.
```

## Component hierarchy

```
Backtrace - Component dirichletbc, x_pos
Backtrace - Component bc
Backtrace - Component timedependent, problem
Backtrace - Component pylithapp
```

# Step01: Error 1 Resolution

Error found while doing very basic validation of parameters

## Error message

```
ValueError: Error while configuring Dirichlet boundary condition (dirichletbc , x_pos):  
Error while configuring boundary condition (dirichletbc , x_pos):  
Label for group/nodeset/pset in mesh not specified.
```

## Component hierarchy

```
Backtrace -- Component dirichletbc , x_pos  
Backtrace -- Component bc  
Backtrace -- Component timedependent , problem  
Backtrace -- Component pylithapp
```

# Step01: Error 1 Resolution

Error found while doing very basic validation of parameters

## Error message

```
ValueError: Error while configuring Dirichlet boundary condition (dirichletbc , x_pos):  
Error while configuring boundary condition (dirichletbc , x_pos):  
Label for group/nodeset/pset in mesh not specified.
```

## Component hierarchy

```
Backtrace -- Component dirichletbc , x_pos  
Backtrace -- Component bc  
Backtrace -- Component timedependent , problem  
Backtrace -- Component pylithapp
```

Debug: Examine parameters for pylithapp.problem.bc.x\_pos

# Step01: Error 1 Resolution

Error found while doing very basic validation of parameters

## Error message

```
ValueError: Error while configuring Dirichlet boundary condition (dirichletbc , x_pos):  
Error while configuring boundary condition (dirichletbc , x_pos):  
Label for group/nodeset/pset in mesh not specified.
```

## Component hierarchy

```
Backtrace -- Component dirichletbc , x_pos  
Backtrace -- Component bc  
Backtrace -- Component timedependent , problem  
Backtrace -- Component pylithapp
```

## Debug: Examine parameters for pylithapp.problem.bc.x\_pos Resolution

```
[pylithapp.timedependent.bc.x_pos]
```

# Step01: Error 2

Error found in parsing .cfg file

```
$ pylith step01.cfg
```

.cfg file with line number

```
>> step01.cfg:100:
```

## Error message

```
— pyre.inventory(error)
— pylithapp.timedependent.implicit.output.outputsoln.write.filename <- 'output/step01.vtk'
— unknown component
'pylithapp.timedependent.implicit.output.outputsoln.write'
```

## Usage information

```
usage: pylith [—<property>=<value>] [—<facility>.<property>=<value>] [FILE.cfg] ...
component 'pylithapp'
    properties: help, help-components, help-persistence, help-properties, initialize-only, job,
    facilities: job, launcher, mesh-generator, perf-logger, petsc, problem, scheduler, weaver
For more information:
    —help-properties: prints details about user settable properties
    —help-components: prints details about user settable facilities and components
pylithapp: configuration error(s)
```

# Step01: Error 2 Resolution

Error found in parsing .cfg file

## Error message

```
— pyre.inventory(error)
— pylithapp.timedependent.implicit.output.outputsoln.write.filename <- 'output/step01.vtk'
— unknown component
'pylithapp.timedependent.implicit.output.outputsoln.write'
```

# Step01: Error 2 Resolution

Error found in parsing .cfg file

## Error message

```
— pyre.inventory(error)
— pylithapp.timedependent.implicit.output.outputsoln.write.filename <- 'output/step01.vtk'
— unknown component
'pylithapp.timedependent.implicit.output.outputsoln.write'
```

Debug: Look up the properties of the OutputSoln object

# Step01: Error 2 Resolution

Error found in parsing .cfg file

## Error message

```
— pyre.inventory(error)
— pylithapp.timedependent.implicit.output.outputsoln.write.filename <- 'output/step01.vtk'
— unknown component
'pylithapp.timedependent.implicit.output.outputsoln.write'
```

Debug: Look up the properties of the OutputSoln object

## Resolution

```
[pylithapp.problem.formulation.output.domain]
writer.filename = output/step01.vtk
```

# Step01: Error 3

Error found when initializing integrators

```
$ pylith step01.cfg
```

## Error message

```
terminate called after throwing an instance of 'std::runtime_error'  
what(): Error occurred while reading spatial database file 'mat_elastic.spatialdb'.  
I/O error while reading SimpleDB data.
```

## Abort message

```
[0]0:Return code = 0, signaled with Abort trap: 6
```

# Step01: Error 3 Resolution

Error found when initializing integrators

## Error message

```
terminate called after throwing an instance of 'std::runtime_error'  
what(): Error occurred while reading spatial database file 'mat_elastic.spatialdb'.  
I/O error while reading SimpleDB data.
```

# Step01: Error 3 Resolution

Error found when initializing integrators

## Error message

```
terminate called after throwing an instance of 'std::runtime_error'  
what(): Error occurred while reading spatial database file 'mat_elastic.spatialdb'.  
I/O error while reading SimpleDB data.
```

Debug: Look at `mat_elastic.spatialdb` for errors in data

# Step01: Error 3 Resolution

Error found when initializing integrators

## Error message

```
terminate called after throwing an instance of 'std::runtime_error'  
what(): Error occurred while reading spatial database file 'mat_elastic.spatialdb'.  
I/O error while reading SimpleDB data.
```

Debug: Look at `mat_elastic.spatialdb` for errors in data

Resolution

```
num_locs = 1 // number of locations
```

# Step01: Error 4

Error found when initializing integrators

```
$ pylith step01.cfg
```

## Error message

```
terminate called after throwing an instance of 'std::runtime_error'  
what(): Error occurred while reading spatial database file 'mat_elastic.spatialdb'.  
Number of dimensions in coordinates of spatial distribution (2) does not match number of dimensions (1)
```

## Abort message

```
[0]0:Return code = 0, signaled with Abort trap: 6
```

# Step01: Error 4 Resolution

Error found when initializing integrators

## Error message

```
terminate called after throwing an instance of 'std::runtime_error'  
what(): Error occurred while reading spatial database file 'mat_elastic.spatialdb'.  
Number of dimensions in coordinates of spatial distribution (2) does not match number of dimensions
```

# Step01: Error 4 Resolution

Error found when initializing integrators

## Error message

```
terminate called after throwing an instance of 'std::runtime_error'  
what(): Error occurred while reading spatial database file 'mat_elastic.spatialdb'.  
Number of dimensions in coordinates of spatial distribution (2) does not match number of dimensions
```

Debug: Look at coordinate system in `mat_elastic.spatialdb` header

# Step01: Error 4 Resolution

Error found when initializing integrators

## Error message

```
terminate called after throwing an instance of 'std::runtime_error'  
what(): Error occurred while reading spatial database file 'mat_elastic.spatialdb'.  
Number of dimensions in coordinates of spatial distribution (2) does not match number of dimensions
```

**Debug: Look at coordinate system in `mat_elastic.spatialdb` header  
Resolution**

`space_dim = 3`

# Step01: Error 5

Error found when setting up solution field

```
$ pylith step01.cfg
```

## Python stacktrace

```
Fatal error. Calling MPI_Abort() to abort PyLith application.  
Traceback (most recent call last):  
  File "/Volumes/Tools/unix/pylith-dev/gcc-4.7.3/lib/python2.7/site-packages/pylith/apps/PetscA  
    self.main(*args, **kwds)  
  File "/Volumes/Tools/unix/pylith-dev/gcc-4.7.3/lib/python2.7/site-packages/pylith/apps/PyLithA  
    self.problem.initialize()  
  File "/Volumes/Tools/unix/pylith-dev/gcc-4.7.3/lib/python2.7/site-packages/pylith/problems/Tir  
    self.formulation.initialize(self.dimension, self.normalizer)  
  File "/Volumes/Tools/unix/pylith-dev/gcc-4.7.3/lib/python2.7/site-packages/pylith/problems/Im  
    self._initialize(dimension, normalizer)  
  File "/Volumes/Tools/unix/pylith-dev/gcc-4.7.3/lib/python2.7/site-packages/pylith/problems/Fo  
    constraint.setConstraintSizes(solution)  
  File "/Volumes/Tools/unix/pylith-dev/gcc-4.7.3/lib/python2.7/site-packages/pylith/bc/bc.py",  
    def setConstraintSizes(self, *args): return _bc.DirichletBC.setConstraintSizes(self, *args)
```

## Error message

```
RuntimeError: Found overly constrained point while setting up constraints for  
DirichletBC boundary condition 'face_zneg'. Number of DOF at point 503 is 3  
and number of attempted constraints is 4.
```

## Abort information

```
application called MPI_Abort(MPI_COMM_WORLD, -1) — process 0  
/Volumes/Tools/unix/cig/gcc-4.7.3/bin/nemesis: mpirun: exit 255  
/Volumes/Tools/unix/pylith-dev/gcc-4.7.3/bin/pylith: /Volumes/Tools/unix/cig/gcc-4.7.3/bin/neme
```

# Step01: Error 5 Resolution

Error found when setting up solution field

## Error message

RuntimeError: Found overly constrained point while setting up constraints for DirichletBC boundary condition 'face\_zneg'. Number of DOF at point 503 is 3 and number of attempted constraints is 4.

# Step01: Error 5 Resolution

Error found when setting up solution field

## Error message

```
RuntimeError: Found overly constrained point while setting up constraints for  
DirichletBC boundary condition 'face_zneg'. Number of DOF at point 503 is 3  
and number of attempted constraints is 4.
```

Debug: Look at overlap of constraints in Dirichlet BC

# Step01: Error 5 Resolution

Error found when setting up solution field

## Error message

RuntimeError: Found overly constrained point while setting up constraints for DirichletBC boundary condition 'face\_zneg'. Number of DOF at point 503 is 3 and number of attempted constraints is 4.

## Debug: Look at overlap of constraints in Dirichlet BC Resolution

```
[pylithapp.timedependent.bc.y-pos]
bc_dof = [0]
...
[pylithapp.timedependent.bc.y-neg]
bc_dof = [0]
```

# Step02: Error 1

Error found in parsing .cfg file

```
$ pylith step02.cfg
```

## Configuration error

```
>> step02.cfg:30:  
— pyre.inventory(error)  
— timedependent.nondimelasticquasistatic.relaxation_time <- '2.0*years'  
— name 'years' is not defined  
pylithapp: configuration error(s)
```

# Step02: Error 1 Resolution

Error found in parsing .cfg file

## Error message

```
>> step02.cfg:30:  
— pyre.inventory(error)  
— timedependent.nondimelasticquasistatic.relaxation_time <- '2.0*years'  
— name 'years' is not defined  
pylithapp: configuration error(s)
```

# Step02: Error 1 Resolution

Error found in parsing .cfg file

## Error message

```
>> step02.cfg:30:  
— pyre.inventory(error)  
— timedependent.nondimelasticquasistatic.relaxation_time <- '2.0*years'  
— name 'years' is not defined  
pylithapp: configuration error(s)
```

Debug: Pyre is poorly documented. Look for example. :(

# Step02: Error 1 Resolution

Error found in parsing .cfg file

## Error message

```
>> step02.cfg:30:  
  pyre.inventory(error)  
  timedependent.nondimelasticquasistatic.relaxation_time <- '2.0*years'  
  name 'years' is not defined  
pylithapp: configuration error(s)
```

Debug: Pyre is poorly documented. Look for example. :(

```
$ python
```

```
>>> from pyre.units.time import *  
>>> dir()  
['__builtins__', '__doc__', '__name__', '__package__', 'day', 'hour', 'micro', 'microsecond',  
'milli', 'millisecond', 'minute', 'ms', 'nano', 'nanosecond', 'ns', 'pico',  
'picosecond', 'ps', 's', 'second', 'us', 'year']
```

## Resolution

```
relaxation_time = 2.0*year
```

# Step02: Error 2

Error doing some basic validation of input

```
$ pylith step02.cfg
```

## Python stacktrace

```
Fatal error. Calling MPI_Abort() to abort PyLith application.  
Traceback (most recent call last):  
  File "/Volumes/Tools/unix/pylith-dev/gcc-4.7.3/lib/python2.7/site-packages/pylith/apps/PetscA  
    self.main(*args, **kwds)  
  File "/Volumes/Tools/unix/pylith-dev/gcc-4.7.3/lib/python2.7/site-packages/pylith/apps/PyLithA  
    self.problem.verifyConfiguration()  
  File "/Volumes/Tools/unix/pylith-dev/gcc-4.7.3/lib/python2.7/site-packages/pylith/problems/Tir  
    self.formulation.verifyConfiguration()  
  File "/Volumes/Tools/unix/pylith-dev/gcc-4.7.3/lib/python2.7/site-packages/pylith/problems/Fo  
    integrator.verifyConfiguration()  
  File "/Volumes/Tools/unix/pylith-dev/gcc-4.7.3/lib/python2.7/site-packages/pylith/faults/Fau  
    ModuleFaultCohesiveKin.verifyConfiguration(self, self.mesh())  
  File "/Volumes/Tools/unix/pylith-dev/gcc-4.7.3/lib/python2.7/site-packages/pylith/faults/fau  
    def verifyConfiguration(self, *args): return  
_faults.FaultCohesiveLagrange.verifyConfiguration(self, *args)
```

## Error message

```
RuntimeError: Number of dofs in reference cell (3) is not compatible  
with number of edges (4) in cohesive cell 256 for fault 'fault_ext'.
```

## Abort info

```
application called MPI_Abort(MPI_COMM_WORLD, -1) — process 0  
/Volumes/Tools/unix/cig/gcc-4.7.3/bin/nemesis: mpirun: exit 255  
/Volumes/Tools/unix/pylith-dev/gcc-4.7.3/bin/pylith: /Volumes/Tools/unix/cig/gcc-4.7.3/bin/neme
```

# Step02: Error 2 Resolution

Error doing some basic validation of input

## Error message

```
RuntimeError: Number of dofs in reference cell (3) is not compatible  
with number of edges (4) in cohesive cell 256 for fault 'fault_ext'.
```

# Step02: Error 2 Resolution

Error doing some basic validation of input

## Error message

RuntimeError: Number of dofs in reference cell (3) is not compatible with number of edges (4) in cohesive cell 256 for fault 'fault\_ext'.

## Debug: Turn on journal for quadrature

```
$ pylith step02.cfg --problem.interfaces.fault.quadrature.help-components
facilities of 'quadrature':
  cell=<component name>: Reference cell with basis fns and quadrature rules.
    current value: 'fiatsimplex', from {default}
    configurable as: fiatsimplex, cell
```

# Step02: Error 2 Resolution

Error doing some basic validation of input

## Error message

```
RuntimeError: Number of dofs in reference cell (3) is not compatible  
with number of edges (4) in cohesive cell 256 for fault 'fault_ext'.
```

## Debug: Turn on journal for quadrature

```
$ pylith step02.cfg --problem.interfaces.fault.quadrature.help-components  
facilities of 'quadrature':  
    cell=<component name>: Reference cell with basis fns and quadrature rules.  
        current value: 'fiatsimplex', from {default}  
        configurable as: fiatsimplex, cell
```

```
[pylithapp.journal.info]  
fiatlagrange = 1  
fiatsimplex = 1
```

## Resolution

```
[pylithapp.timedependent.interfaces.fault]  
quadrature.cell = pylith.feassemble.FIATLagrange
```

# Step02: Error 3

Error found when initializing integrators

```
$ pylith step02.cfg
```

## Python stacktrace

```
Fatal error. Calling MPI_Abort() to abort PyLith application.  
Traceback (most recent call last):  
  File "/Volumes/Tools/unix/pylith-dev/gcc-4.7.3/lib/python2.7/site-packages/pylith/apps/PetscA  
    self.main(*args, **kwds)  
  File "/Volumes/Tools/unix/pylith-dev/gcc-4.7.3/lib/python2.7/site-packages/pylith/apps/PyLithA  
    self.problem.initialize()  
  File "/Volumes/Tools/unix/pylith-dev/gcc-4.7.3/lib/python2.7/site-packages/pylith/problems/Ti  
    self.formulation.initialize(self.dimension, self.normalizer)  
  File "/Volumes/Tools/unix/pylith-dev/gcc-4.7.3/lib/python2.7/site-packages/pylith/problems/Im  
    self._initialize(dimension, normalizer)  
  File "/Volumes/Tools/unix/pylith-dev/gcc-4.7.3/lib/python2.7/site-packages/pylith/problems/Fo  
    integrator.initialize(totalTime, numTimeSteps, normalizer)  
  File "/Volumes/Tools/unix/pylith-dev/gcc-4.7.3/lib/python2.7/site-packages/pylith/fesassemble/  
    ModuleElasticityImplicit.initialize(self, self.mesh())  
  File "/Volumes/Tools/unix/pylith-dev/gcc-4.7.3/lib/python2.7/site-packages/pylith/fesassemble/  
    def initialize(self, *args): return _fesassemble.IntegratorElasticity_initialize(self, *args)
```

## Error message

RuntimeError: Determinant of Jacobian ( $1.25e-07$ ) for cell 0 is smaller than minimum permissible value ( $1e-06$ )! The two most likely causes of this are highly distorted cells and nondimensionalization with a length scale that is much larger than the dimensions of the cells.

## Abort info

# Step02: Error 3 Resolution

Error found when initializing integrators

## Error message

RuntimeError: Determinant of Jacobian (1.25e-07) for cell 0 is smaller than minimum permissible value (1e-06)! The two most likely causes of this are highly distorted cells and nondimensionalization with a length scale that is much larger than the dimensions of the cells.

# Step02: Error 3 Resolution

Error found when initializing integrators

## Error message

RuntimeError: Determinant of Jacobian (1.25e-07) for cell 0 is smaller than minimum permissible value (1e-06)! The two most likely causes of this are highly distorted cells and nondimensionalization with a length scale that is much larger than the dimensions of the cells.

Debug: Look at nondimensional scales relative to the parameters

```
$ pylith step02.cfg --problem.normalizer.help-properties
properties of 'nondimelasticquasistatic':
    length_scale=<dimensional>: Value to nondimensionalize length scale.
        default value: 1000*m
        current value: 1e+06*m, from {file='step02.cfg', line=28, column=-1}
        validator: (greater than 0*m)
    relaxation_time=<dimensional>: Relaxatim time to nondimensionalize time.
        default value: 3.15576e+07*s
        current value: 6.31152e+07*s, from {file='step02.cfg', line=30, column=-1}
        validator: (greater than 0*s)
    shear_modulus=<dimensional>: Shear modulus to nondimensionalize pressure.
        default value: 3e+10*m**-1*kg*s**-2
        current value: 3e+10*m**-1*kg*s**-2, from {file='step02.cfg', line=29, column=-1}
        validator: (greater than 0*m**-1*kg*s**-2)
```

# Step02: Error 3 Resolution

Error found when initializing integrators

## Error message

RuntimeError: Determinant of Jacobian (1.25e-07) for cell 0 is smaller than minimum permissible value (1e-06)! The two most likely causes of this are highly distorted cells and nondimensionalization with a length scale that is much larger than the dimensions of the cells.

Debug: Look at nondimensional scales relative to the parameters

```
$ pylith step02.cfg --problem.normalizer.help-properties
properties of 'nondimelasticquasistatic':
    length_scale=<dimensional>: Value to nondimensionalize length scale.
        default value: 1000*m
        current value: 1e+06*m, from {file='step02.cfg', line=28, column=-1}
        validator: (greater than 0*m)
    relaxation_time=<dimensional>: Relaxatim time to nondimensionalize time.
        default value: 3.15576e+07*s
        current value: 6.31152e+07*s, from {file='step02.cfg', line=30, column=-1}
        validator: (greater than 0*s)
    shear_modulus=<dimensional>: Shear modulus to nondimensionalize pressure.
        default value: 3e+10*m**-1*kg*s**-2
        current value: 3e+10*m**-1*kg*s**-2, from {file='step02.cfg', line=29, column=-1}
        validator: (greater than 0*m**-1*kg*s**-2)
```

## Resolution

```
[pylithapp.problem.normalizer]
length_scale = 1.0*km
```

# Step02: Error 4

Error found when initializing fault

```
$ pylith step02.cfg
```

## Error message

```
terminate called after throwing an instance of 'std::runtime_error'  
what(): Could not find value left-lateral-slip in spatial database  
Final slip. Available values are:  
    lateral-slip  
    reverse-slip  
    fault-opening
```

## Abort message

```
[0]0:Return code = 0, signaled with Abort trap: 6
```

# Step02: Error 4 Resolution

Error found when initializing fault

## Error message

```
terminate called after throwing an instance of 'std::runtime_error'  
what(): Could not find value left-lateral-slip in spatial database  
Final slip. Available values are:  
lateral-slip  
reverse-slip  
fault-opening
```

# Step02: Error 4 Resolution

Error found when initializing fault

## Error message

```
terminate called after throwing an instance of 'std::runtime_error'  
what(): Could not find value left-lateral-slip in spatial database  
Final slip. Available values are:  
    lateral-slip  
    reverse-slip  
    fault-opening
```

## Resolution

```
slip.values = [left-lateral-slip, reverse-slip, fault-opening]
```

# Step02: Error 5

Error found when setting up solution field

```
$ pylith step02.cfg
```

## Python stacktrace

```
Fatal error. Calling MPI_Abort() to abort PyLith application.  
Traceback (most recent call last):  
  File "/Volumes/Tools/unix/pylith-dev/gcc-4.7.3/lib/python2.7/site-packages/pylith/apps/PetscA  
    self.main(*args, **kwds)  
  File "/Volumes/Tools/unix/pylith-dev/gcc-4.7.3/lib/python2.7/site-packages/pylith/apps/PyLithA  
    self.problem.initialize()  
  File "/Volumes/Tools/unix/pylith-dev/gcc-4.7.3/lib/python2.7/site-packages/pylith/problems/Ti  
    self.formulation.initialize(self.dimension, self.normalizer)  
  File "/Volumes/Tools/unix/pylith-dev/gcc-4.7.3/lib/python2.7/site-packages/pylith/problems/Im  
    self._initialize(dimension, normalizer)  
  File "/Volumes/Tools/unix/pylith-dev/gcc-4.7.3/lib/python2.7/site-packages/pylith/problems/Fo  
    integrator.checkConstraints(solution)  
  File "/Volumes/Tools/unix/pylith-dev/gcc-4.7.3/lib/python2.7/site-packages/pylith/faults/faul  
    def checkConstraints(self, *args): return _faults.FaultCohesiveLagrange_checkConstraints(se
```

## Error message

```
RuntimeError: Vertex with label '396' on negative side of fault 'fault_ext' is constrained.  
Fault vertices cannot be constrained.
```

## Abort info

```
application called MPI_Abort(MPI_COMM_WORLD, -1) — process 0  
/Volumes/Tools/unix/cig/gcc-4.7.3/bin/nemesis: mpirun: exit 255  
/Volumes/Tools/unix/pylith-dev/gcc-4.7.3/bin/pylith: /Volumes/Tools/unix/cig/gcc-4.7.3/bin/neme
```

# Step02: Error 5 Resolution

Error found when setting up solution field

## Error message

```
RuntimeError: Vertex with label '396' on negative side of fault 'fault_ext' is constrained.  
Fault vertices cannot be constrained.
```

# Step02: Error 5 Resolution

Error found when setting up solution field

## Error message

```
RuntimeError: Vertex with label '396' on negative side of fault 'fault_ext' is constrained.  
Fault vertices cannot be constrained.
```

Debug: Oops. Didn't mean to use through-going fault!

# Step02: Error 5 Resolution

Error found when setting up solution field

## Error message

```
RuntimeError: Vertex with label '396' on negative side of fault 'fault_ext' is constrained.  
Fault vertices cannot be constrained.
```

Debug: Oops. Didn't mean to use through-going fault!

## Resolution

```
[pylithapp.timedependent.interfaces.fault]  
label = fault
```

# Step02: Error 6

Error when initializing fault

```
$ pylith step02.cfg
```

## Python stacktrace

```
Fatal error. Calling MPI_Abort() to abort PyLith application.  
Traceback (most recent call last):  
  File "/Volumes/Tools/unix/pylith-dev/gcc-4.7.3/lib/python2.7/site-packages/pylith/apps/PetscA  
    self.main(*args, **kwds)  
  File "/Volumes/Tools/unix/pylith-dev/gcc-4.7.3/lib/python2.7/site-packages/pylith/apps/PyLithA  
    self.problem.initialize()  
  File "/Volumes/Tools/unix/pylith-dev/gcc-4.7.3/lib/python2.7/site-packages/pylith/problems/Ti  
    self.formulation.initialize(self.dimension, self.normalizer)  
  File "/Volumes/Tools/unix/pylith-dev/gcc-4.7.3/lib/python2.7/site-packages/pylith/problems/Im  
    self._initialize(dimension, normalizer)  
  File "/Volumes/Tools/unix/pylith-dev/gcc-4.7.3/lib/python2.7/site-packages/pylith/problems/Fo  
    integrator.initialize(totalTime, numTimeSteps, normalizer)  
  File "/Volumes/Tools/unix/pylith-dev/gcc-4.7.3/lib/python2.7/site-packages/pylith/faults/Fau  
    FaultCohesive.initialize(self, totalTime, numTimeSteps, normalizer)  
  File "/Volumes/Tools/unix/pylith-dev/gcc-4.7.3/lib/python2.7/site-packages/pylith/faults/Fau  
    ModuleFault.initialize(self, self.mesh(), self.upDir)  
  File "/Volumes/Tools/unix/pylith-dev/gcc-4.7.3/lib/python2.7/site-packages/pylith/faults/fau  
    def initialize(self, *args): return _faults.Fault_initialize(self, *args)
```

## Error message

```
RuntimeError: Error computing orientation of cell face.  
Up direction (0, 0, 1) cannot be parallel to the face normal (0, 0, 1).  
If the face is horizontal, adjust the up-dir parameter.
```

## Abort info

Error Messages

Step02

-1) — process 0

# Step02: Error 6 Resolution

Error found when initializing fault

## Error message

```
RuntimeError: Error computing orientation of cell face.  
Up direction (0, 0, 1) cannot be parallel to the face normal (0, 0, 1).  
If the face is horizontal, adjust the up_dir parameter.
```

# Step02: Error 6 Resolution

Error found when initializing fault

## Error message

```
RuntimeError: Error computing orientation of cell face.  
Up direction (0, 0, 1) cannot be parallel to the face normal (0, 0, 1).  
If the face is horizontal, adjust the up_dir parameter.
```

## Debug: Change up-dir

```
up_dir = [1,0,1]
```

# Step02: Error 6 Resolution

Error found when initializing fault

## Error message

```
RuntimeError: Error computing orientation of cell face.  
Up direction (0, 0, 1) cannot be parallel to the face normal (0, 0, 1).  
If the face is horizontal, adjust the up_dir parameter.
```

## Debug: Change up-dir

```
up_dir = [1,0,1]
```

## Debug: Look at fault surface

# Step02: Error 6 Resolution

Error found when initializing fault

## Error message

```
RuntimeError: Error computing orientation of cell face.  
Up direction (0, 0, 1) cannot be parallel to the face normal (0, 0, 1).  
If the face is horizontal, adjust the up_dir parameter.
```

## Debug: Change up-dir

```
up_dir = [1,0,1]
```

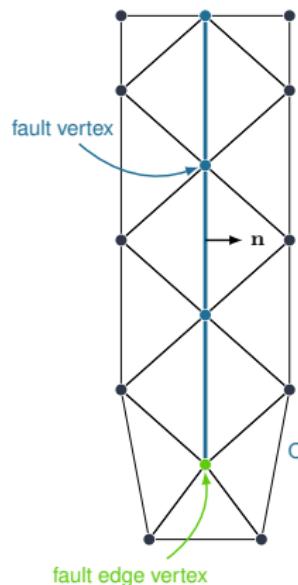
## Debug: Look at fault surface

## Resolution: Mark buried edges

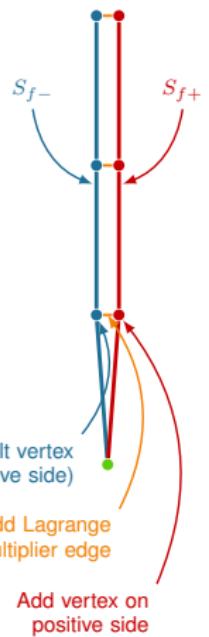
```
[pylithapp.timedependent.interfaces.fault]  
label = fault  
edge = fault_edge  
up_dir = [0,0,1]
```

# Insertion of Cohesive Cells

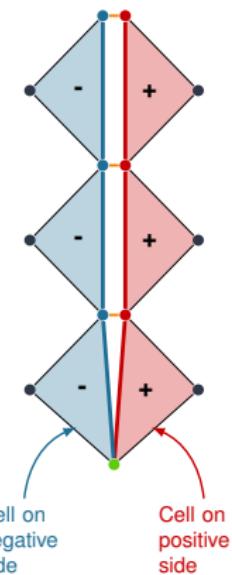
(a) Original mesh



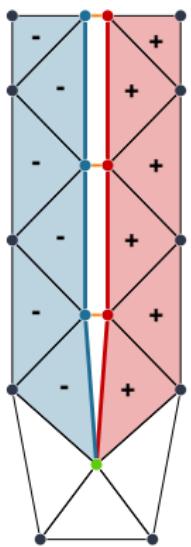
(b) Add colocated vertices



(c) Update cells with fault faces



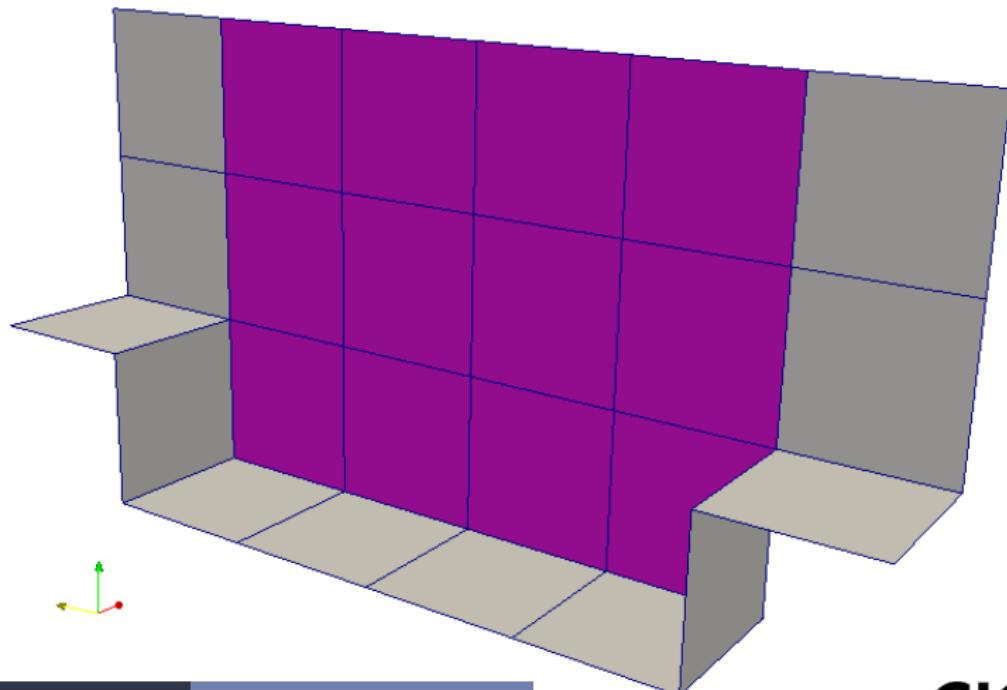
(d) Classify cells and update remaining cells



# Forgetting to Mark Buried Edges

PyLith will extend the fault one cell in an arbitrary fashion

Purple region shows intended fault surface.



# Step03: Error 1

Error doing basic validation on parameters

```
$ pylith step02.cfg
```

## Python stacktrace

```
Fatal error. Calling MPI_Abort() to abort PyLith application.  
Traceback (most recent call last):  
  File "/Volumes/Tools/unix/pylith-dev/gcc-4.7.3/lib/python2.7/site-packages/pylith/apps/PetscA  
    self.main(*args, **kwds)  
...  
  File "/Volumes/Tools/unix/pylith-dev/gcc-4.7.3/lib/python2.7/site-packages/pylith/faults/  
    FaultCohesive.verifyConfiguration(self)  
  File "/Volumes/Tools/unix/pylith-dev/gcc-4.7.3/lib/python2.7/site-packages/pylith/faults/  
    self.output.verifyConfiguration(self.mesh())  
  File "/Volumes/Tools/unix/pylith-dev/gcc-4.7.3/lib/python2.7/site-packages/pylith/meshio/Outp  
    self._verifyFields(self.dataProvider().availableFields)  
  File "/Volumes/Tools/unix/pylith-dev/gcc-4.7.3/lib/python2.7/site-packages/pylith/meshio/Outp  
    raise ValueError(msg)
```

## Error message

```
ValueError: Requested fields not available for output.  
Data provider: 'faultcohesivedyn'  
Field type: 'vertex'  
Data type: 'data'  
Available fields: 'slip' 'slip_rate' 'traction'  
Fields not available: 'initial_traction'
```

## Abort info

```
application called MPI_Abort(MPI_COMM_WORLD, -1) — process 0  
                                     : mpirun: exit 255
```

# Step03: Error 1 Resolution

Error doing basic validation on parameters

## Error message

```
ValueError: Requested fields not available for output.  
Data provider: 'faultcohesivedyn'  
Field type: 'vertex'  
Data type: 'data'  
Available fields: 'slip' 'slip_rate' 'traction'  
Fields not available: 'initial_traction'
```

# Step03: Error 1 Resolution

Error doing basic validation on parameters

## Error message

```
ValueError: Requested fields not available for output.  
Data provider: 'faultcohesivedyn'  
Field type: 'vertex'  
Data type: 'data'  
Available fields: 'slip' 'slip_rate' 'traction'  
Fields not available: 'initial_traction'
```

## Resolution

```
vertex_data_fields = [slip, slip_rate, traction]
```

# Step03: Error 2

## Error creating solution field

```
$ pylith step03.cfg
```

### Python stacktrace

```
Fatal error. Calling MPI_Abort() to abort PyLith application.  
Traceback (most recent call last):  
  File "/Volumes/Tools/unix/pylith-dev/gcc-4.7.3/lib/python2.7/site-packages/pylith/apps/PetscA  
    self.main(*args, **kwds)  
  File "/Volumes/Tools/unix/pylith-dev/gcc-4.7.3/lib/python2.7/site-packages/pylith/apps/PyLithA  
    self.problem.initialize()  
  File "/Volumes/Tools/unix/pylith-dev/gcc-4.7.3/lib/python2.7/site-packages/pylith/problems/Ti  
    self.formulation.initialize(self.dimension, self.normalizer)  
  File "/Volumes/Tools/unix/pylith-dev/gcc-4.7.3/lib/python2.7/site-packages/pylith/problems/Im  
    self._initialize(dimension, normalizer)  
  File "/Volumes/Tools/unix/pylith-dev/gcc-4.7.3/lib/python2.7/site-packages/pylith/problems/Fo  
    constraint.setConstraintSizes(solution)  
  File "/Volumes/Tools/unix/pylith-dev/gcc-4.7.3/lib/python2.7/site-packages/pylith/bc/bc.py",  
    def setConstraintSizes(self, *args): return _bc.DirichletBC.setConstraintSizes(self, *args)
```

### Error message

```
RuntimeError: Found overly constrained point while setting up constraints for DirichletBC  
boundary condition 'face_zneg'. Number of DOF at point 535 is 3 and number of attempted  
constraints is 4.
```

### Abort info

```
application called MPI_Abort(MPI_COMM_WORLD, -1) — process 0  
/Volumes/Tools/unix/cig/gcc-4.7.3/bin/nemesis: mpirun: exit 255  
/Volumes/Tools/unix/pylith-dev/gcc-4.7.3/bin/pylith:  
                                     : exit 1
```

# Step03: Error 2 Resolution

## Error creating solution field

### Error message

```
RuntimeError: Found overly constrained point while setting up constraints for DirichletBC  
boundary condition 'face_zneg'. Number of DOF at point 535 is 3 and number of attempted  
constraints is 4.
```

# Step03: Error 2 Resolution

## Error creating solution field

### Error message

```
RuntimeError: Found overly constrained point while setting up constraints for DirichletBC  
boundary condition 'face_zneg'. Number of DOF at point 535 is 3 and number of attempted  
constraints is 4.
```

Debug: Look for overlap of constraints in Dirichlet BC

# Step03: Error 2 Resolution

## Error creating solution field

### Error message

```
RuntimeError: Found overly constrained point while setting up constraints for DirichletBC
boundary condition 'face_zneg'. Number of DOF at point 535 is 3 and number of attempted
constraints is 4.
```

**Debug:** Look for overlap of constraints in Dirichlet BC  
**Resolution**

```
[ pylithapp.timedependent.bc.x_pos ]
bc_dof = [0, 1]
...
[ pylithapp.timedependent.bc.x_neg ]
bc_dof = [0, 1]
```

# Step03: Error 3

## Error creating solution field

```
$ pylith step03.cfg
```

### Python stacktrace

```
Fatal error. Calling MPI_Abort() to abort PyLith application.  
Traceback (most recent call last):  
  File "/Volumes/Tools/unix/pylith-dev/gcc-4.7.3/lib/python2.7/site-packages/pylith/apps/PetscA  
    self.main(*args, **kwds)  
  File "/Volumes/Tools/unix/pylith-dev/gcc-4.7.3/lib/python2.7/site-packages/pylith/apps/PyLithA  
    self.problem.initialize()  
  File "/Volumes/Tools/unix/pylith-dev/gcc-4.7.3/lib/python2.7/site-packages/pylith/problems/Ti  
    self.formulation.initialize(self.dimension, self.normalizer)  
  File "/Volumes/Tools/unix/pylith-dev/gcc-4.7.3/lib/python2.7/site-packages/pylith/problems/Im  
    self._initialize(dimension, normalizer)  
  File "/Volumes/Tools/unix/pylith-dev/gcc-4.7.3/lib/python2.7/site-packages/pylith/problems/Fo  
    integrator.checkConstraints(solution)  
  File "/Volumes/Tools/unix/pylith-dev/gcc-4.7.3/lib/python2.7/site-packages/pylith/faults/faul  
    def checkConstraints(self, *args): return _faults.FaultCohesiveLagrange_checkConstraints(se
```

### Error message

```
RuntimeError: Vertex with label '605' on negative side of fault 'fault_ext' is constrained.  
Fault vertices cannot be constrained.
```

### Abort info

```
application called MPI_Abort(MPI_COMM_WORLD, -1) — process 0  
/Volumes/Tools/unix/cig/gcc-4.7.3/bin/nemesis: mpirun: exit 255  
/Volumes/Tools/unix/pylith-dev/gcc-4.7.3/bin/pylith:  
/Volumes/Tools/unix/cig/gcc-4.7.3/bin/nemesis: exit 1
```

# Step03: Error 3 Resolution

## Error creating solution field

### Error message

```
RuntimeError: Vertex with label '605' on negative side of fault 'fault_ext' is constrained.  
Fault vertices cannot be constrained.
```

# Step03: Error 3 Resolution

## Error creating solution field

### Error message

```
RuntimeError: Vertex with label '605' on negative side of fault 'fault_ext' is constrained.  
Fault vertices cannot be constrained.
```

Debug: Look for overlap in fault and BC nodesets

# Step03: Error 3 Resolution

Error creating solution field

## Error message

```
RuntimeError: Vertex with label '605' on negative side of fault 'fault_ext' is constrained.  
Fault vertices cannot be constrained.
```

**Debug:** Look for overlap in fault and BC nodesets  
**Resolution**

```
[pylithapp.timedependent.bc.z_neg]  
...  
label = face_zneg.nofault
```

# Step03: Error 4

No error but funky results

## Step03: Error 4 Resolution

No error but funky results

Debug: Did the solver converge?

# Step03: Error 4 Resolution

No error but funky results

Debug: Did the solver converge?

Resolution

```
[pylithapp.petsc]
ksp_monitor = true
ksp_converged_reason = true
ksp_error_if_not_converged = true

snes_converged_reason = true
snes_error_if_not_converged = true
snes_monitor = true
```

# Step03: Error 5

Nonlinear solver diverges

## PETSc error message

```
[0]PETSC ERROR: _____ Error Message  
[0]PETSC ERROR: SNESolve has not converged  
[0]PETSC ERROR: See http://www.mcs.anl.gov/petsc/documentation/faq.html for trouble shooting.  
[0]PETSC ERROR: Petsc Development GIT revision: v3.4.4-4559-g852d360 GIT Date: 2014-05-19 15:00  
...  
[0]PETSC ERROR: #1 SNESolve() line 3765 in /Volumes/Tools/unix/petsc-dev/src/snes/interface/sn  
[0]PETSC ERROR: #2 SNESLogConvergenceHistory() line 150 in /Users/baagaard/src/cig/pylith/libsrc
```

## Debugging

### Examine KSP and SNES residuals

Fatal error. Calling MPI\_Abort() to abort PyLith application.

Traceback (most recent call last):

```
File "/Volumes/Tools/unix/pylith-dev/gcc-4.7.3/lib/python2.7/site-packages/pylith/apps/PetscA  
self.main(*args, **kwds)  
File "/Volumes/Tools/unix/pylith-dev/gcc-4.7.3/lib/python2.7/site-packages/pylith/apps/PyLithA  
self.problem.run(self)  
File "/Volumes/Tools/unix/pylith-dev/gcc-4.7.3/lib/python2.7/site-packages/pylith/problems/Tir  
self.formulation.step(t, dt)  
File "/Volumes/Tools/unix/pylith-dev/gcc-4.7.3/lib/python2.7/site-packages/pylith/problems/Im  
self.solver.solve(displncr, self.jacobian, residual)  
File "/Volumes/Tools/unix/pylith-dev/gcc-4.7.3/lib/python2.7/site-packages/pylith/problems/pr  
def solve(self, *args): return _problems.SolverNonlinear_solve(self, *args)
```

## Abort info

RuntimeError: Error detected while in PETSc function.

Error Messages

Step03

-1) — process 0

: mpirun: exit 255



COMPUTATIONAL  
INFRASTRUCTURE  
for  
GEODYNAMICS

# Step03: Error 5 Resolution

Nonlinear solver diverges

## PETSc error message

```
[0]PETSC ERROR: _____ Error Message _____  
[0]PETSC ERROR: SNESolve has not converged  
[0]PETSC ERROR: See http://www.mcs.anl.gov/petsc/documentation/faq.html for trouble shooting.  
[0]PETSC ERROR: Petsc Development GIT revision: v3.4.4-4559-g852d360 GIT Date: 2014-05-19 15:00:00  
...  
[0]PETSC ERROR: #1 SNESolve() line 3765 in /Volumes/Tools/unix/petsc-dev/src/snes/interface/sn...  
[0]PETSC ERROR: #2 SNESLogConvergenceHistory() line 150 in /Users/baagaard/src/cig/pylith/libsrc...
```

# Step03: Error 5 Resolution

Nonlinear solver diverges

## PETSc error message

```
[0]PETSC ERROR: _____ Error Message _____  
[0]PETSC ERROR: SNESolve has not converged  
[0]PETSC ERROR: See http://www.mcs.anl.gov/petsc/documentation/faq.html for trouble shooting.  
[0]PETSC ERROR: Petsc Development GIT revision: v3.4.4-4559-g852d360 GIT Date: 2014-05-19 15:00:00  
...  
[0]PETSC ERROR: #1 SNESolve() line 3765 in /Volumes/Tools/unix/petsc-dev/src/snes/interface/sn...  
[0]PETSC ERROR: #2 SNESLogConvergenceHistory() line 150 in /Users/baagaard/src/cig/pylith/libsrc...
```

Debug: Examine KSP and SNES residuals using log file

```
$ pylith step03.cfg >& step03.log  
  
$ grep " norm" step03.log
```

# Step03: Error 5 Resolution

Nonlinear solver diverges

## PETSc error message

```
[0]PETSC ERROR: _____ Error Message _____  
[0]PETSC ERROR: SNESolve has not converged  
[0]PETSC ERROR: See http://www.mcs.anl.gov/petsc/documentation/faq.html for trouble shooting.  
[0]PETSC ERROR: Petsc Development GIT revision: v3.4.4-4559-g852d360 GIT Date: 2014-05-19 15:00:00  
...  
[0]PETSC ERROR: #1 SNESolve() line 3765 in /Volumes/Tools/unix/petsc-dev/src/snes/interface/snem.c  
[0]PETSC ERROR: #2 SNESLogConvergenceHistory() line 150 in /Users/baagaard/src/cig/pylith/libsrc/pylith/
```

Debug: Examine KSP and SNES residuals using log file

```
$ pylith step03.cfg >& step03.log  
  
$ grep " norm" step03.log
```

## Resolution

```
[pylithapp.timedependent.interfaces.fault]  
zero_tolerance = 1.0e-10  
  
[pylithapp.petsc]  
ksp_rtol = 1.0e-20  
ksp_atol = 1.0e-12  
  
snes_rtol = 1.0e-20  
snes_atol = 1.0e-8
```

# Step03: Error 6

Intended shear to drive fault slip

Debug: Check fault tractions

# Step03: Error 6

Intended shear to drive fault slip

Debug: Check fault tractions

Compare  $T_{shear}/T_{normal}$  against  $\mu_f$

# Step03: Error 6

Intended shear to drive fault slip

Debug: Check fault tractions

Compare  $T_{shear}/T_{normal}$  against  $\mu_f$

Resolution

```
[ pylithapp.timedependent.bc.x_pos ]  
...  
db_initial.data = [-1.0*m, 3.0*m, 0.0*m]  
  
[ pylithapp.timedependent.bc.x_neg ]  
...  
db_initial.data = [1.0*m, -3.0*m, 0.0*m]
```

# Asking For Help

Send email to [cig-short@geodynamics.org](mailto:cig-short@geodynamics.org)

- Try to debug on your own first
- Describe what you are trying to do
  - Overview of problem, BC (**diagrams/sketches are very helpful**)
  - 2-D or 3-D
  - Cell type (tri, quad, hex, tet)
  - Prescribed slip or spontaneous rupture
- Specify which version you are using AND your operating system (**PyLith v2.1.2 binary on Linux x86\_64**)
- Send the **entire** error message, not just what you think is important (**entire log of output is best**)