Concepts Covered in this Session

- Running PyLith in parallel
  - Desktop or laptop with multiple processors and/or cores
  - Cluster with multiple compute nodes
- Optimizing PyLith performance
- Building PyLith from source
- Using PyLith with a queue system
- PyLith parallel performance
Running PyLith in Parallel

- **Laptop/Desktop**
  - Reduce runtime (distribute floating point operations)
  - Available with binary `--nodes=NUMCORES`
- **Cluster**
  - Reduce runtime (distribute floating point operations)
  - Run larger problems (distribute memory usage)
  - Must build from source for proper configuration
  - Requires additional parameters for batch submission
How PyLith Runs in Parallel
Single Program, Multiple Data (SPMD) Parallel Processing

1. Process 0
   1. Read in mesh
   2. Add cohesive cells by adjusting the mesh topology
   3. Partition mesh and determine vertices shared by multiple processes
   4. Distribute relevant portion of mesh to each process

2. All processes
   1. OPTIONAL Each processor refines its part of the mesh
   2. Each processor solves equations on its portion of the mesh, exchanging information as necessary with its neighbors
Optimizing PyLith Performance

Efficiency depends on choice of parameters and hardware

- **Output**
  - **VTK**  Inefficient: each process sends its data to process 0 for writing
  - **HDF5** Efficient: each process writes its own data in binary

- **Solver performance**
  - **Quasi-static** Field split with algebraic multigrid generally scales better than Additive Schwarz
  - **Dynamic** Trivial solve scales extremely well

- **Overall performance**
  - Speed of memory and connection b/t memory and CPU is more important than CPU speed
  - Marginal speed improvement if you compile source for your hardware
Running PyLith in Parallel on a Desktop
Reduce runtime using multiple processors and/or cores

Add number of processes (usually number of cores) as argument:
pylith --nodes=NUMCORES

- **PyLith binary**
  - Allows interprocess communication only within a single computer
  - Works with laptops, desktops, and a single compute node
- **Building PyLith from source**
  - Permits optimizing code for your hardware; may provide modest performance gains
Running PyLith on a Cluster
For large quasi-static and 3-D dynamic simulations

- Differences from usage on a desktop machine
  - Usually requires additional parameters for batch queue system
  - **Strongly** recommend using DataWriterHDF5Ext* for output
    - Parallel output via shared or parallel file system
    - More failsafe than regular HDF5 output (DataWriterHDF5*)
  - Stdout and stderr are written to a log file or files

- Consult your system administrator on MPI parameters
- Read getting started guides provided by computing centers
  - What compiler suites and MPI versions are available?
  - What filesystems are available? Which support parallel I/O?
Hints for Running PyLith on a Cluster
How many compute nodes and cores should I use?

- **General**
  - If you have N compute nodes and want to run J jobs, use N/J compute nodes
  - Use the maximum number allowable by the queue with the shortest wait
  - Don’t overload a compute node (memory use exceeds that available)
  - Don’t overload fileservers

- **Quasi-static problems**
  - Memory use and runtime depends on the solver parameters
  - Memory use is often dominated by the sparse matrix
  - Different bulk rheologies use different amounts of memory

- **Dynamic problems**
  - Don’t overload compute nodes
  - Spontaneous rupture uses more memory than prescribed slip
PyLith Parallel Performance Test
Static solution of prescribed slip on multiple faults
# PyLith Parallel Performance Test

Field split and AMG with custom fault preconditioner performs best

## Number of Iterations in Linear Solve

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<thead>
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<th>Preconditioner</th>
<th>Cell</th>
<th>Problem Size</th>
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PyLith Parallel Performance Test
Weak scaling of field split w/AMG and custom fault preconditioner
Dissecting PETSc Log Summary I
Where are the bottlenecks?

Quasi-Static Simulation
Savage-Prescott Benchmark

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<tr>
<th>Summary of Stages:</th>
<th>Time</th>
<th>Avg</th>
<th>%Total</th>
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<td>5: Solve:</td>
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<td>6: Prestep:</td>
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<td>7: Step:</td>
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Dynamic Simulation
SCEC Dynamic Rupture Benchmark TPV102

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Dissecting PETSc Log Summary II
Identify memory bandwidth saturation and communication bottlenecks

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PyLith v1.9 versus v2.0
Under-the-hood improvements fix some parallel scaling issues

- PyLith v1.9
  - Reading in mesh by single process limits size of calculation
  - Dynamic problems with $>50M$ cells (hex or tet)
  - Memory imbalance of up to 10x for large problems with faults

- PyLith v2.0
  - Reading in mesh by single process limits size of calculation
  - Improved mesh data structures reduce memory use
  - Expect memory balancing to be very good
  - Expect to be able to run problems with $O(10^8)$ cells
Building PyLith from Source
Required for PyLith to use multiple compute nodes on a cluster

Use the PyLith installer utility!!!
pylith-installer-1.9.0-0.tgz

- Downloads, configures, and builds PyLith and dependencies
- User selects which dependencies are needed and installer will do some minimal checks
- Insures versions, configuration, and builds are consistent PyLith requirements
- See INSTALL file in installer tarball for instructions
Submitting Jobs to PBS Queue System

PBS is one of the most common batch queue systems

- PyLith uses Pyre to submit jobs directly to PBS
  1. Perform minimal validation of the simulation parameters
  2. Create a shell script to submit job
  3. Submit job

- Assumes you have already setup running jobs on the cluster
Submitting Jobs to PBS Queue System

Put parameters common to all jobs in
$HOME/.pyre/pylithapp/pylithapp.cfg

[pylithapp]
scheduler = pbs

[pylithapp.pbs]
# Shell used for job script submitted to batch system
shell = /bin/bash
# Command line arguments in qsub command
# -V = Use current environment variables in batch job
# -m bea = Send email when job begins, ends, or aborts
qsub-options = -V -m bea -M johndoe@university.edu

[pylithapp.launcher]
command = mpirun -np ${nodes} -machinefile ${PBS_NODEFILE}
Pass job specific parameters via the command line

```
--nodes=NPROCS  Total number of processes
--scheduler.ppn=PPN  Number of processes per compute node
--job.name=NAME  Name of job
--job.stdout=LOG_FILE  File where stdout is written
```

\[
NPROCS = NCOMPUTENODES \times PPN
\]
Debug Launching Parallel Jobs on Queue System

Use command line help features to see commands being processed

- See default and set parameters
  - `--COMPONENT.help-properties` See properties and their values
  - `--COMPONENT.help-components` See subcomponents
  - `pylithinfo PYLITH_ARGS` Dumps all parameters to `pylith_parameters.txt`

- Submitting to the queue (scheduler)
  - `--scheduler.help` See list of properties/components available
  - `--scheduler.dry` Dump script for batch submission to stdout

- Launching job on compute nodes (launcher)
  - `--launcher.help` Total number of processes
  - `--launcher.dry` Dump launching command to stdout