Day 13: Scripting Workflows II DAGMan

Turn In Homework

Homework Review

Advanced DAGMan

Retrying Nodes

RETRY *name count* UNLESS-EXIT *value*

- Specifies number of times to retry given node
- Affects entire node, not just its job
- Especially useful if job is sensitive to environment

JOB Analyze1 analysis.sub RETRY Analyze1 3 UNLESS-EXIT 99

Node Directories

JOB name submit-file DIR directory

- Use *directory* for all files for this node
- Submit file, executable, inputs, outputs, everything
- Effectively:

cd *directory* condor_submit *submit-file*

• In submit, reference common files as, e.g., .../foo

JOB Wibble wibble.sub DIR wibble

% ls wibble go-wibble.py input-1.txt wibble.sub

Node Priorities

PRIORITY *name value*

- Sets **DAGMan** priority for the given node
- Determines when DAGMan submits job to queue
- Hence, different than job priority (set in submit file)
- Useful when throttling jobs (-maxjobs, -maxidle)
- Integer (+/–), defaults to 0, higher submits sooner

JOB Analyze1 analysis.sub PRIORITY Analyze1 10

JOB Analyze2 analysis.sub PRIORITY Analyze2 5

Skipping Nodes

PRE_SKIP name exit-status

- If node's Pre-Script exits with the given exit status, skip rest of node
- Node is marked as successful

JOB Foo foo.sub SCRIPT PRE Foo set-up-foo.py PRE_SKIP Foo 1

Node Variables

VARS *name macroname="value"* ...

- Define *macro(s)* (= variable(s)) for submit file
- *macroname* is \w+, cannot start with queue
- Multiple macros for node on same line, or separate
- In value, \$(JOB) expands to node *name*

```
JOB Foo foo.sub
VARS Foo arg1="hello" arg2="42"
VARS Foo arg3="$(JOB)"
```

Using Node Variables

• In submit file, reference macro as \$(macroname)

```
JOB Foo foo.sub
VARS Foo arg1="hello" arg2="42"
VARS Foo arg3="$(JOB)"
```

```
executable = /bin/echo
universe = local
output = test.out
error = test.err
log = test.log
arguments = "A1=$(arg1) A2=$(arg2) ..."
queue
```

Node Variables Can Simplify Submit Files

- Move data from *many* submit files to 1 DAGMan file
- Use VARS, \$(cluster), and/or \$(process)

JOB Analysis1 analysis.sub
VARS Analysis1 jobname="\$(JOB)" arg="ABW"
JOB Analysis2 analysis.sub
VARS Analysis2 jobname="\$(JOB)" arg="ADO"

```
output = analysis.$(jobname).out
error = analysis.$(jobname).err
log = analysis.log
arguments = "$(arg)"
queue
```

Scripting Simple DAGs

Designing DAGs for Scripting

- Mostly, focus on wide, parallel parts
- Consider pros and cons of each choice
- VARS and 1 submit file, or 1 submit file per node?
 - Often easier to script one complex DAG submit file
 - Submit file can specify subdirectories (initialdir)
- Use sub-directories?
 - Same considerations as without DAG
 - More useful with distinct inputs or lots of output files
 - Put common files in .../ or .../common/
- Consider using DAGMan for independent jobs

Scripting DAG Submit Files

```
def psub(text): ... # add text to submit file
psub(dag submit header)
\mathbf{n} = \mathbf{0}
for t in product(parameter_1, parameter_2):
  n += 1
  psub('JOB N%d node.sub DIR node-%d' % (n, n))
  psub('RETRY N%d 3 UNLESS-EXIT 1' % (n))
  if t[0] < 1.0: psub('PRIORITY N%d 10' % (n))
  args = '%d %s' % (n, t[1])
  psub('SCRIPT PRE N%d pre.py %s' % (n, args))
  psub('PARENT Start CHILD N%d' % (n))
  write node dir(sources, n, t)
psub(dag submit footer)
```

Setting Up Node Directories

• Much like before, but need to include submit file

sources: dict from filename to contents

def prepare_node_dir(sources, node, params):
 node_dir = 'node-%d' % (node)
 os.mkdir(node_dir)

write node submit file, incl. job arguments
node_sub = os.path.join(node_dir, 'node.sub')
write_node_submit(node_sub, params)

for filename in sources:
 text = sources[filename]
 target = os.path.join(dirname, filename)
 write_template(text, target, params)

Splices

Understanding Splices

- Reusable DAG fragment, *inserted into* larger DAG
- Like a function, if you think about it
- Common use: write outer DAG once, replace insides



Splice Syntax

SPLICE name inner-dag-file DIR directory

- Like the JOB statement, except it names a DAG file
- All nodes in splice become part of (outer) DAG
- Can create **PARENT / CHILD** relationships for splice, which affect all of its initial/final nodes

```
JOB Start start.sub
JOB End end.sub
```

SPLICE Diamond1 diamond.dag SPLICE Diamond2 diamond.dag

PARENT Start CHILD Diamond1 Diamond2

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Splice Example



Splice

JOB A a.sub VARS A x="\$(JOB)" JOB B b.sub VARS B x="\$(JOB)" PARENT A CHILD B

```
# Outer
JOB X x.sub
SPLICE Y000 spl.dag
...
SPLICE Y999 spl.dag
JOB Z z.sub
PARENT X CHILD Y000
PARENT Y000 CHILD Z
```

Sub-DAGs

Understanding Sub-DAGs

- Reusable DAG fragment, *submitted by* larger DAG
- Also like a function, if you think about it
- Splices are better in most cases, except for one...



SUBDAG Syntax

SUBDAG EXTERNAL *name inner-dag* DIR *dir*

- Like the JOB statement, except it names a DAG file
- Nodes in sub-DAG *do not* become part of DAG
- DAGman submits **inner-dag** when job is run

JOB Start start.sub JOB End end.sub

SUBDAG EXTERNAL Diamond1 diamond.dag SUBDAG EXTERNAL Diamond2 diamond.dag

PARENT Start CHILD Diamond1 Diamond2 PARENT Diamond1 Diamond2 CHILD End

Running Nested DAGs

- DAGMan does condor_submit_dag on DAG file
 - Hence, another copy of DAGMan is running
 - If there are many copies, submit machine may suffer
- Sub-DAG not processed until needed
 - Allows for some cool tricks...
 - Errors not discovered until run-time!
- Rescue DAGs are complicated, but still work

Dynamic DAGs

The Need for Dynamic DAGs

- Suppose the exact number of parallel jobs depends on some initial (significant) input processing
 - ... or exact number of stages ...
 - ... or exact DAG shape ...
- We *could*:
 - Run one job to process input, then...
 - Manually run script to generate rest of DAG
 - But we want to automate!
- Dynamic DAG build (part of) DAG *during* run

Dynamic DAGs

- How to implement:
 - In DAG, add one or more **SUBDAG EXTERNAL** nodes
 - (Re)Write their DAGMan submit files in earlier node (or, even in the node's pre-script!)
- Again, errors not found until sub-DAG is submitted
- Outer DAG can be very simple and/or generic:

$$\bigcirc \longrightarrow \bigcirc \longrightarrow \bigcirc$$

Dynamic DAG Example

• DAGMan submit file for simple, generic outer DAG:

JOB Start start.sub SUBDAG EXTERNAL Innards dynamic.dag JOB End end.sub SCRIPT PRE Innards generate-dag.py PARENT Start CHILD Innards PARENT Innards CHILD End



Workflow Management Systems

makeflow

- Different way to describe workflow DAG
 - Uses syntax like make
 - Handles data transfers (so does Condor/DAGMan)
 - Highly fault tolerant (so is DAGMan)
- Works with several distributed computing systems
 - Condor
 - Sun Grid Engine (SGE)
 - Work Queue (also from CCL)
- From Doug Thain's Cooperative Computing Lab http://nd.edu/~ccl/software/makeflow/

Pegasus WMS

- Supports higher-level workflow abstractions
- Compiles down to DAG
- Works with Condor, OSG, Amazon EC2, TeraGrid, ...
- Used on a wide variety of complex science projects
- Lots of cool example applications online
- From Information Sciences Institute, USC http://pegasus.isi.edu/

SOAR

- System Of Automated Runs
- Automatically scans directories for jobs to run
- Each "job" can be a complete DAG in itself
- Puts jobs into DAG and manages workflow
- Also handles R and MATLAB jobs well
- Provides extra tracking and reporting tools
- From Bill Taylor, CHTC Team http://submit.chtc.wisc.edu/SOAR/

Homework

Homework

- Script a workflow!
- Using the Mandelbrot generator again, but adding the stitching step at the end
- Note: Use a different universe (scheduler) for the montage node (only)!
- If you have an alternate workflow that you would like to work on instead, talk to me