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 is better

```
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)

n = 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

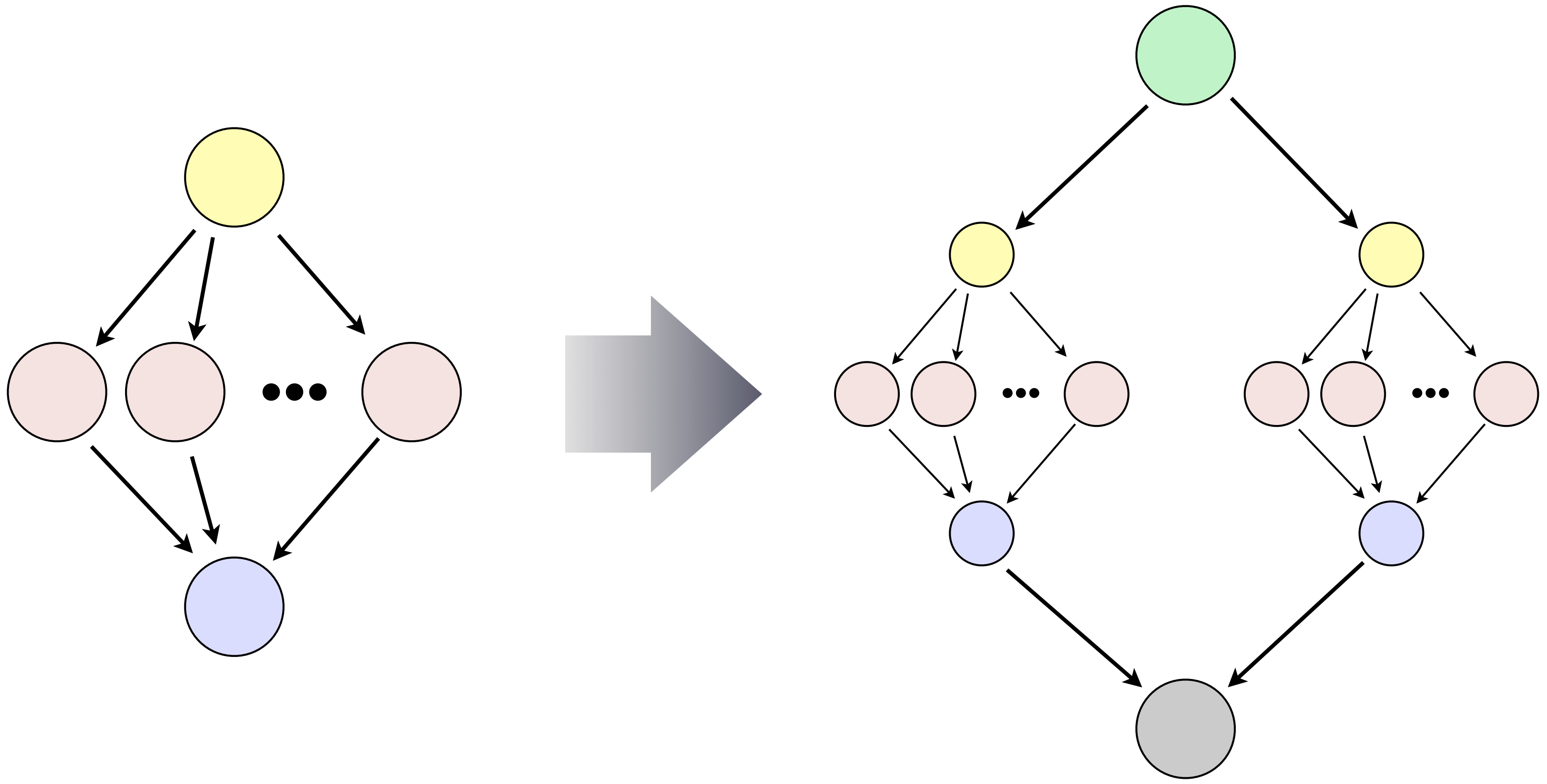
- Much like before, but need to include submit file

```
# 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



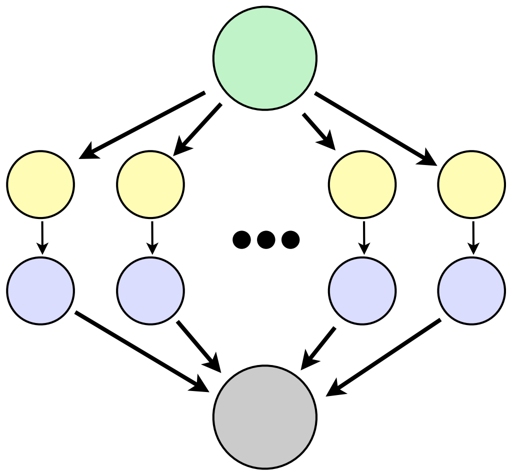
Splice Syntax

```
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
```

Splice Example



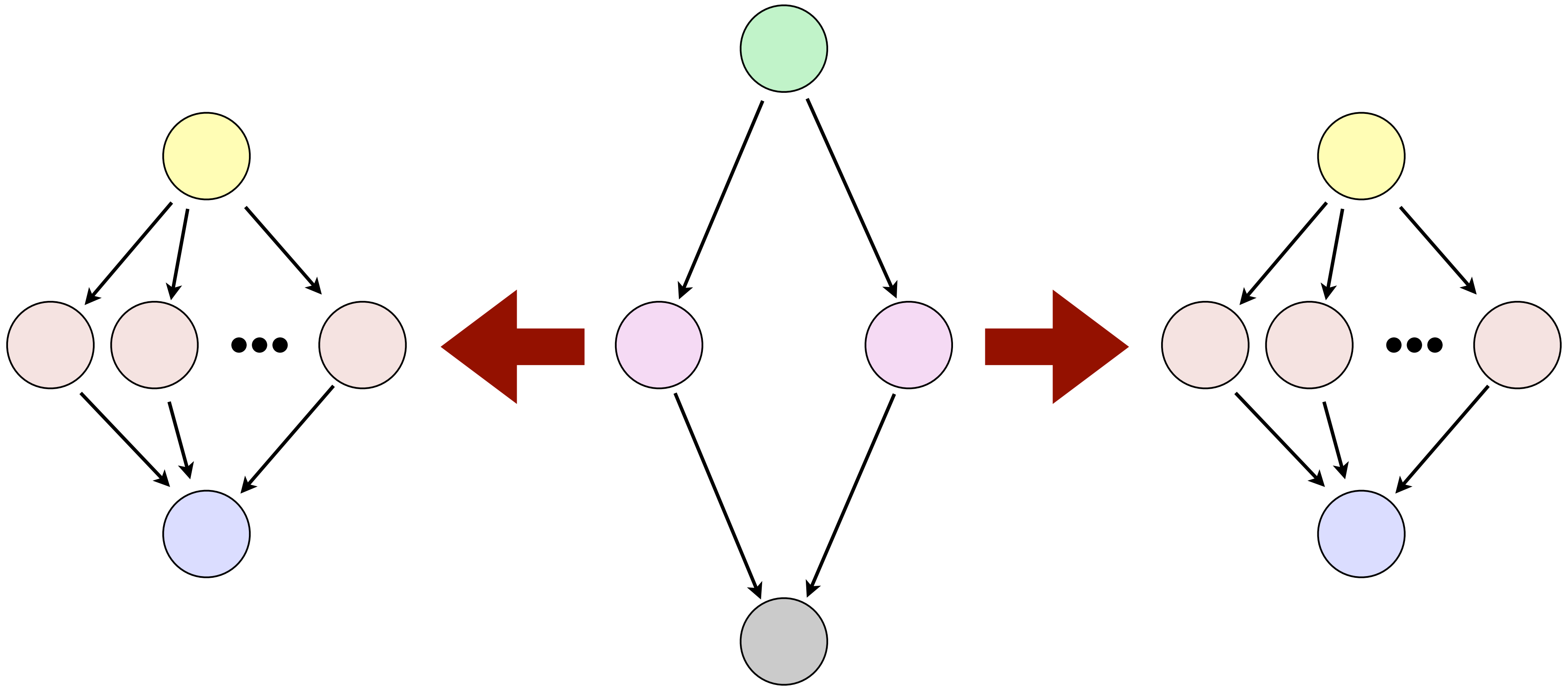
```
# Splice

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 …

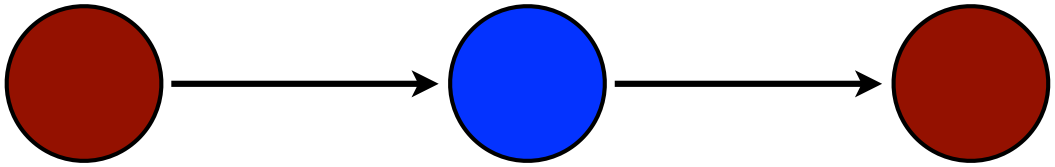
  … or exact DAG shape …

- 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

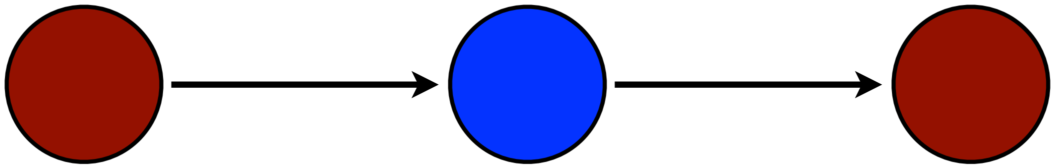
- How to implement:
  - In DAG, add one or more **`SUBDAG EXTERNAL`** nodes
  - (Re)Write their DAGMan submit files in earlier node (or, even in the node's pre-script!)
- Again, errors not found until sub-DAG is submitted
- Outer DAG can be very simple and/or generic:



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