Workflows with HTCondor’s DAGMan

Thursday, July 28
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Goals for this Session

• Why create a workflow?
• Describe workflows as directed acyclic graphs (DAGs)
• Workflow execution via DAGMan (DAG Manager)
• Stopping, resuming, troubleshooting
• Node-level options in a DAG
• Modular organization of DAG components
Automation!

- Objective: Submit jobs in a particular order, automatically.
- Especially if: Need to replicate the same workflow multiple times in the future.
DAG = ”directed acyclic graph”

- topological ordering of vertices (“nodes”) is established by directional connections (“edges”)
- “acyclic” aspect requires a start and end, with no looped repetition
  - can contain cyclic subcomponents, covered in later slides for DAG workflows
DESCRIBING WORKFLOWS WITH DAGMAN
DAGMan Workflows

DAGMan is a HTCondor tool that allows multiple jobs to be organized in workflows, represented as a directed acyclic graph (DAG). A DAGMan workflow automatically submits jobs in a particular order, such that certain jobs need to complete before others start running. This allows the outputs of some jobs to be used as inputs for others, and makes it easy to replicate a workflow multiple times in the future.

Describing Workflows with DAGMan

A DAGMan workflow is described in a DAG input file. The input file specifies the nodes of the DAG as well as the dependencies that order the DAG.

A node within a DAG represents a unit of work. It contains the following:

- **Job**: An HTCondor job, defined in a submit file.
- **PRE script** (optional): A script that runs before the job starts. Typically used to verify that all inputs are valid.
- **POST script** (optional): A script that runs after the job finishes. Typically used to verify outputs and clean up temporary files.
An Example HTC Workflow

- User must communicate the “nodes” and directional “edges” of the DAG

![Diagram of a directed acyclic graph (DAG) with nodes 1, 2, 3, ..., N and labeled edges.]
Simple Example for this Tutorial

- The DAG input file will communicate the “nodes” and directional “edges” of the DAG
Basic DAG input file: **JOB** nodes, **PARENT-CHILD** edges

my.dag

<table>
<thead>
<tr>
<th>JOB</th>
<th>nodes</th>
<th>PARENT</th>
<th>CHILD</th>
</tr>
</thead>
<tbody>
<tr>
<td>A</td>
<td>A.sub</td>
<td>A</td>
<td></td>
</tr>
<tr>
<td>B1</td>
<td>B1.sub</td>
<td>B1</td>
<td></td>
</tr>
<tr>
<td>B2</td>
<td>B2.sub</td>
<td>B2</td>
<td></td>
</tr>
<tr>
<td>B3</td>
<td>B3.sub</td>
<td>B3</td>
<td></td>
</tr>
<tr>
<td>C</td>
<td>C.sub</td>
<td>C</td>
<td></td>
</tr>
</tbody>
</table>

PARENT A CHILD B1 B2 B3
PARENT B1 B2 B3 CHILD C

- Node names will be used by various DAG features to modify their execution by DAGMan.
Basic DAG input file:

**JOB** nodes, **PARENT-CHILD** edges

- Node names and filenames are your choice.
- Node name and submit filename do not have to match.
Endless Workflow Possibilities

Wikimedia Commons

https://confluence.pegasus.isi.edu/display/pegasus/WorkflowGenerator
DAGs are also useful for non-sequential work

‘bag’ of HTC jobs

\[ \text{B1, B2, B3, ... BN} \]

disjointed workflows

\[
\text{A} \rightarrow \text{B} \\
\text{C} \rightarrow \text{D} \rightarrow \text{E} \\
\text{F} \rightarrow \text{G} \rightarrow \text{H} \\
\text{I} \\
\]

\[
\text{A} \rightarrow \text{B} \\
\text{C} \rightarrow \text{D} \rightarrow \text{E} \\
\text{F} \rightarrow \text{G} \rightarrow \text{H} \\
\text{I} \\
\]
Basic DAG input file:

**JOB** nodes, **PARENT-CHILD** edges

```
my.dag

JOB A A.sub
JOB B1 B1.sub
JOB B2 B2.sub
JOB B3 B3.sub
JOB C C.sub
PARENT A CHILD B1 B2 B3
PARENT B1 B2 B3 CHILD C
```
SUBMITTING AND MONITORING A DAGMAN WORKFLOW
Submitting a DAG to the queue

• Submission command:

```
condor_submit_dag dag_file
```

```
$ condor_submit_dag my.dag

File for submitting this DAG to HTCondor : mydag.dag.condor.sub
Log of DAGMan debugging messages : mydag.dag.dagman.out
Log of HTCondor library output : mydag.dag.lib.out
Log of HTCondor library error messages : mydag.dag.lib.err
Log of the life of condor_dagman itself : mydag.dag.dagman.log

Submitting job(s).
1 job(s) submitted to cluster 128.
```
A submitted DAG creates a **DAGMan job** in the queue

- **DAGMan runs on the access point, as a job in the queue**
- **At first:**

```
$ condor_q
-- Schedd: submit-3.chtc.wisc.edu : <128.104.100.44:9618?...
 OWNER   BATCH_NAME   SUBMITTED  DONE    RUN    IDLE   TOTAL  JOB_IDS
 alice    my.dag+128  4/30 18:08   _     _     _     _     0.0
 1 jobs; 0 completed, 0 removed, 0 idle, 1 running, 0 held, 0 suspended

$ condor_q -nobatch
-- Schedd: submit-3.chtc.wisc.edu : <128.104.100.44:9618?...
   ID    OWNER     SUBMITTED  RUN_TIME ST PRI SIZE   CMD
 128.0  alice    4/30 18:08  0+00:00:06 R 0 0.3 condor_dagman
 1 jobs; 0 completed, 0 removed, 0 idle, 1 running, 0 held, 0 suspended
```
Jobs are automatically submitted by the DAGMan job

- Seconds later, node A is submitted:

$ condor_q
-- Schedd: submit-3.chtc.wisc.edu : <128.104.100.44:9618>...
OWNER   BATCH_NAME  SUBMITTED  DONE  RUN  IDLE  TOTAL  JOB_IDS
alice    my.dag+128  4/30  18:08  _   _   1     5    129.0
2 jobs; 0 completed, 0 removed, 1 idle, 1 running, 0 held, 0 suspended

$ condor_q -nobatch
-- Schedd: submit-3.chtc.wisc.edu : <128.104.100.44:9618>...
ID  OWNER   SUBMITTED   RUN_TIME ST PRI SIZE CMD
128.0 alice   4/30 18:08  0+00:00:36 R 0 0.3 condor_dagman
129.0 alice   4/30 18:08  0+00:00:00 I 0 0.3 A_split.sh
2 jobs; 0 completed, 0 removed, 1 idle, 1 running, 0 held, 0 suspended
Jobs are automatically submitted by the DAGMan job

- After A completes, B1-3 are submitted

```
$ condor_q
-- Schedd: submit-3.chtc.wisc.edu : <128.104.100.44:9618>?...
OWNER BATCH_NAME SUBMITTED DONE RUN IDLE TOTAL JOB_IDS
alice my.dag+128 4/30 18:08 1 _ 3 5 130.0...132.0
4 jobs; 0 completed, 0 removed, 3 idle, 1 running, 0 held, 0 suspended
```

```
$ condor_q -nobatch
-- Schedd: submit-3.chtc.wisc.edu : <128.104.100.44:9618>?...
ID OWNER SUBMITTED RUN_TIME ST PRI SIZE CMD
128.0 alice 4/30 18:08 0+00:20:36 R 0 0.3 condor_dagman
130.0 alice 4/30 18:18 0+00:00:00 I 0 0.3 B_run.sh
131.0 alice 4/30 18:18 0+00:00:00 I 0 0.3 B_run.sh
132.0 alice 4/30 18:18 0+00:00:00 I 0 0.3 B_run.sh
4 jobs; 0 completed, 0 removed, 3 idle, 1 running, 0 held, 0 suspended
```
Jobs are automatically submitted by the DAGMan job

- **After B1-3 complete, node C is submitted**

```bash
$ condor_q
-- Schedd: submit-3.chtc.wisc.edu : <128.104.100.44:9618>?

OWNER  BATCH_NAME  SUBMITTED  DONE  RUN  IDLE  TOTAL  JOB_IDS
alice  my.dag+128  4/30 18:08  4   __  1   5  133.0

2 jobs; 0 completed, 0 removed, 1 idle, 1 running, 0 held, 0 suspended

$ condor_q -nobatch
-- Schedd: submit-3.chtc.wisc.edu : <128.104.100.44:9618>?

ID  OWNER  SUBMITTED  RUN_TIME ST  PRI  SIZE  CMD
128.0  alice  4/30 18:08  0+00:46:36  R  0  0.3 condor_dagman
133.0  alice  4/30 18:54  0+00:00:00  I  0  0.3 C_combine.sh

2 jobs; 0 completed, 0 removed, 1 idle, 1 running, 0 held, 0 suspended
```
Status files are created at the time of DAG submission

(dag_dir)/

<table>
<thead>
<tr>
<th>A.sub</th>
<th>B1.sub</th>
<th>B2.sub</th>
</tr>
</thead>
<tbody>
<tr>
<td>B3.sub</td>
<td>C.sub</td>
<td>(other job files)</td>
</tr>
<tr>
<td>my.dag</td>
<td>my.dag.condor.sub</td>
<td>my.dag.dagman.log</td>
</tr>
<tr>
<td>my.dag.dagman.out</td>
<td>my.dag.lib.err</td>
<td>my.dag.lib.out</td>
</tr>
<tr>
<td>my.dag.nodes.log</td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

*.condor.sub and *.dagman.log describe the queued DAGMan job process, as for any other jobs

*.dagman.out has DAGMan-specific logging (look to first for errors)

*.lib.err/out contain std err/out for the DAGMan job process

*.nodes.log is a combined log of all jobs within the DAG
DAG Completion

(dag_dir)/

<table>
<thead>
<tr>
<th>A.sub</th>
<th>B1.sub</th>
<th>B2.sub</th>
</tr>
</thead>
<tbody>
<tr>
<td>B3.sub</td>
<td>C.sub</td>
<td></td>
</tr>
<tr>
<td>my.dag</td>
<td></td>
<td></td>
</tr>
<tr>
<td>my.dag.dagman.out</td>
<td>my.dag.lib.err</td>
<td>my.dag.lib.out</td>
</tr>
<tr>
<td>my.dag.nodes.log</td>
<td>my.dag.dagman.metrics</td>
<td></td>
</tr>
</tbody>
</table>

*.dagman.metrics is a summary of events and outcomes

*.dagman.log will note the completion of the DAGMan job

*.dagman.out has detailed logging (look to first for errors)
STOPPING, RESTARTING, AND TROUBLESHOOTING
Removing a DAG from the queue

• Remove the DAGMan job in order to stop and remove the entire DAG:

\texttt{condor\_rm \ dagman\_jobID}

• Creates a \texttt{rescue file} so that only incomplete or unsuccessful NODES are repeated upon resubmission

```
$ condor\_q
-- Schedd: submit-3.chtc.wisc.edu : <128.104.100.44:9618>...
OWNER BATCH\_NAME SUBMITTED DONE RUN IDLE TOTAL \text{JOB\_IDS}
alice my.dag+128 4/30 8:08 4 _ 1 6 129.0...133.0
2 jobs; 0 completed, 0 removed, 1 idle, 1 running, 0 held, 0 suspended
$ condor\_rm 128
All jobs in cluster 128 have been marked for removal
```
Removal of a DAG creates a rescue file

(dag_dir)/

A.sub  B1.sub  B2.sub  B3.sub  C.sub  (other job files)
my.dag  my.dag.condor.sub  my.dag.dagman.log
my.dag.dagman.out  my.dag.lib.err  my.dag.lib.out
my.dag.metrics  my.dag.nodes.log  my.dag.rescue001

• Named `dag_file.rescue001`
  ▪ increments if more rescue DAG files are created
• Records which NODES have completed successfully
  ▪ does not contain the actual DAG structure
Rescue Files
For Resuming a Failed DAG

• A rescue file is created when:
  – a node fails, and after DAGMan advances through any other possible nodes
  – the DAG is removed from the queue (or aborted, see manual)
  – the DAG is halted and not unhalted (see manual)

• Resubmission uses the rescue file (if it exists) when the original DAG file is resubmitted
  – override: condor_submit_dag dag_file -f
Node Failures
Result in DAG Failure

• If a node JOB fails (non-zero exit code)
  – DAGMan continues to run other JOB nodes until it can no longer make progress

• Example at right:
  – B2 fails
  – Other B* jobs continue
  – DAG fails and exits after B* and before node C
Best Workflow Control Achieved with One Process per JOB Node

- While submit files can ‘queue’ many processes, a **single job process per submit file** is usually best for DAG JOBs
  - Failure of any queued process in a JOB node results in failure of the **entire node** and immediate removal of all other processes in the node.
  - RETRY of a JOB node retries the entire submit file.
Resolving held node jobs

- Look at the hold reason (in the job log, or with ‘condor_q -hold’)
- Fix the issue and release the jobs (condor_release)
  - OR- remove the entire DAG, resolve, then resubmit the DAG (remember the automatic rescue DAG file!)

```bash
$ condor_q -nobatch
-- Schedd: submit-3.chtc.wisc.edu : <128.104.100.44:9618?...  
<table>
<thead>
<tr>
<th>ID</th>
<th>OWNER</th>
<th>SUBMITTED</th>
<th>RUN_TIME</th>
<th>ST</th>
<th>PRI</th>
<th>SIZE</th>
<th>CMD</th>
</tr>
</thead>
<tbody>
<tr>
<td>128.0</td>
<td>alice</td>
<td>4/30 18:08</td>
<td>0+00:20:36</td>
<td>R</td>
<td>0</td>
<td>0.3</td>
<td>condor_dagman</td>
</tr>
<tr>
<td>130.0</td>
<td>alice</td>
<td>4/30 18:18</td>
<td>0+00:00:00</td>
<td>H</td>
<td>0</td>
<td>0.3</td>
<td>B_run.sh</td>
</tr>
<tr>
<td>131.0</td>
<td>alice</td>
<td>4/30 18:18</td>
<td>0+00:00:00</td>
<td>H</td>
<td>0</td>
<td>0.3</td>
<td>B_run.sh</td>
</tr>
<tr>
<td>132.0</td>
<td>alice</td>
<td>4/30 18:18</td>
<td>0+00:00:00</td>
<td>H</td>
<td>0</td>
<td>0.3</td>
<td>B_run.sh</td>
</tr>
</tbody>
</table>
4 jobs; 0 completed, 0 removed, 0 idle, 1 running, 3 held, 0 suspended
```
BEYOND THE BASIC DAG: NODE-LEVEL MODIFIERS
Default File Organization

- What if you want to organize files into other directories?

```
my.dag

<table>
<thead>
<tr>
<th>JOB</th>
<th>SUB</th>
</tr>
</thead>
<tbody>
<tr>
<td>A</td>
<td>A.sub</td>
</tr>
<tr>
<td>B1</td>
<td>B1.sub</td>
</tr>
<tr>
<td>B2</td>
<td>B2.sub</td>
</tr>
<tr>
<td>B3</td>
<td>B3.sub</td>
</tr>
<tr>
<td>C</td>
<td>C.sub</td>
</tr>
</tbody>
</table>

PARENT A CHILD B1 B2 B3
PARENT B1 B2 B3 CHILD C

(dag_dir)/

<p>| | |</p>
<table>
<thead>
<tr>
<th></th>
<th></th>
</tr>
</thead>
<tbody>
<tr>
<td>A.</td>
<td>sub</td>
</tr>
<tr>
<td>B1</td>
<td>.sub</td>
</tr>
<tr>
<td>B2</td>
<td>.sub</td>
</tr>
<tr>
<td>B3</td>
<td>.sub</td>
</tr>
<tr>
<td>C.</td>
<td>sub</td>
</tr>
</tbody>
</table>

(my.dag)

(other job files)
```
Node-specific File Organization with **DIR**

- **DIR** sets the submission directory of the node

```
my.dag

<table>
<thead>
<tr>
<th>JOB</th>
<th>Submission Directory</th>
</tr>
</thead>
<tbody>
<tr>
<td>A</td>
<td>A.sub</td>
</tr>
<tr>
<td>B1</td>
<td>B1.sub</td>
</tr>
<tr>
<td>B2</td>
<td>B2.sub</td>
</tr>
<tr>
<td>B3</td>
<td>B3.sub</td>
</tr>
<tr>
<td>C</td>
<td>C.sub</td>
</tr>
</tbody>
</table>

PARENT A CHILD B1 B2 B3
PARENT B1 B2 B3 CHILD C
```

```
(dag_dir)/

<table>
<thead>
<tr>
<th>JOB</th>
<th>Submission Directory</th>
</tr>
</thead>
<tbody>
<tr>
<td>A</td>
<td>A.sub (A job files)</td>
</tr>
<tr>
<td>B</td>
<td>B1.sub B2.sub</td>
</tr>
<tr>
<td>B1</td>
<td>B1.sub B2.sub</td>
</tr>
<tr>
<td>B2</td>
<td>B3.sub (B job files)</td>
</tr>
<tr>
<td>B3</td>
<td></td>
</tr>
<tr>
<td>C</td>
<td>C.sub (C job files)</td>
</tr>
</tbody>
</table>

my.dag
```

```
**PRE and POST scripts run on the access point, as part of the node**

my.dag

```plaintext
JOB A A.sub
SCRIPT POST A sort.sh
JOB B1 B1.sub
JOB B2 B2.sub
JOB B3 B3.sub
JOB C C.sub
SCRIPT PRE C tar_it.sh
PARENT A CHILD B1 B2 B3
PARENT B1 B2 B3 CHILD C
```

- Use sparingly for lightweight work; otherwise include work in node jobs
RETRY failed nodes to overcome transient errors

- Retry a node up to $N$ times if the exit code is non-zero:
  \[
  \text{RETRY node\_name } N
  \]

Example:
- JOB A A.sub
- \text{RETRY A 5}
- JOB B B.sub
- PARENT A CHILD B

- **Note:** Unnecessary for nodes (jobs) that can use \texttt{max\_retries} in the submit file
- See also: retry except for a particular exit code (\texttt{UNLESS-EXIT}), or retry scripts (\texttt{DEFER})
RETRY applies to whole node, including PRE/POST scripts

- PRE and POST scripts are included in retries
- RETRY of a node with a POST script uses the exit code from the POST script (not from the job)
  - POST script can do more to determine node success, perhaps by examining JOB output
- Achieve repetitive iterations!

Example:

```
JOB A A.sub
SCRIPT POST A checkA.sh
RETRY A 5
```
MODULAR ORGANIZATION OF DAG COMPONENTS
Submit File Templates via VARS

- **VARS** line defines node-specific values that are passed into submit file variables
  
  VARS node_name var1=“value” [var2=“value”]

- Allows a single submit file shared by all B jobs, rather than one submit file for each JOB.

```
my.dag

JOB B1 B.sub
VARS B1 data=“B1” opt=“10”

JOB B2 B.sub
VARS B2 data=“B2” opt=“12”

JOB B3 B.sub
VARS B3 data=“B3” opt=“14”
```

```
B.sub

... InitialDir = $(data) arguments = $(data).csv $(opt)
... queue
```
**SPLICE** subsets of a DAG to simplify lengthy DAG files

```
my.dag
JOB A A.sub
SPLICE B B.spl
JOB C C.sub
PARENT A CHILD B
PARENT B CHILD C

B.spl
JOB B1 B1.sub
JOB B2 B2.sub
...
JOB BN BN.sub
```
Use nested SPLICEs with DIR to achieve templating

my.dag

```
JOB A A.sub DIR A
SPLICE B B.spl DIR B
JOB C C.sub DIR C
PARENT A CHILD B
PARENT B CHILD C
```

B.spl

```
SPLICE B1 ../inner.spl DIR B1
SPLICE B2 ../inner.spl DIR B2
...
SPLICE BN ../inner.spl DIR BN
```

inner.spl

```
JOB 1 ../1.sub
JOB 2 ../2.sub
PARENT 1 CHILD 2
```
Use nested SPLICEs with DIR to achieve templating

my.dag

JOB A A.sub DIR A
SPLICE B B.spl DIR B
JOB C C.sub DIR C
PARENT A CHILD B
PARENT B CHILD C

B.spl

SPLICE B1 ../inner.spl DIR B1
SPLICE B2 ../inner.spl DIR B2
...
SPLICE BN ../inner.spl DIR BN

inner.spl

JOB 1 ../1.sub
JOB 2 ../2.sub
PARENT 1 CHILD 2

(dag_dir)/

my.dag

A/ A.sub (A job files)
B/ B.spl inner.spl
  1.sub 2.sub
  B1/ (1–2 job files)
  B2/ (1–2 job files)
  ...
  BN/ (1–2 job files)
C/ C.sub (C job files)
Repeating DAG Components!!

https://confluence.pegasus.isi.edu/display/pegasus/LIGO+IHOPE
What if some DAG components can’t be known at submit time?

If $N$ can only be determined as part of the work of $A$ …
**A SUBDAG within a DAG**

**my.dag**
- JOB A A.sub
- **SUBDAG EXTERNAL B B.dag**
- JOB C C.sub
- PARENT A CHILD B
- PARENT B CHILD C

**B.dag** (written by A)
- JOB B1 B1.sub
- JOB B2 B2.sub
- ...
- JOB BN BN.sub

![Diagram of a DAG with nodes A, B, and C, and a SUBDAG B within A]
Use a **SUBDAG** to achieve a Cyclic Component within a DAG

- POST script determines whether another iteration is necessary; if so, exits non-zero
- RETRY applies to entire SUBDAG, which may include multiple, sequential nodes

```
my.dag
JOB A A.sub
SUBDAG EXTERNAL B B.dag
SCRIPT POST B iterateB.sh
RETRY B 1000
JOB C C.sub
PARENT A CHILD B
PARENT B CHILD C
```
More in the **HTCondor Manual!!!**
DAGMan Exercises!

- Essential: Exercises 1-4
- Ask questions! ‘See you in Slack!’