Workflows with HTCondor's DAGMan

Thursday, August 10

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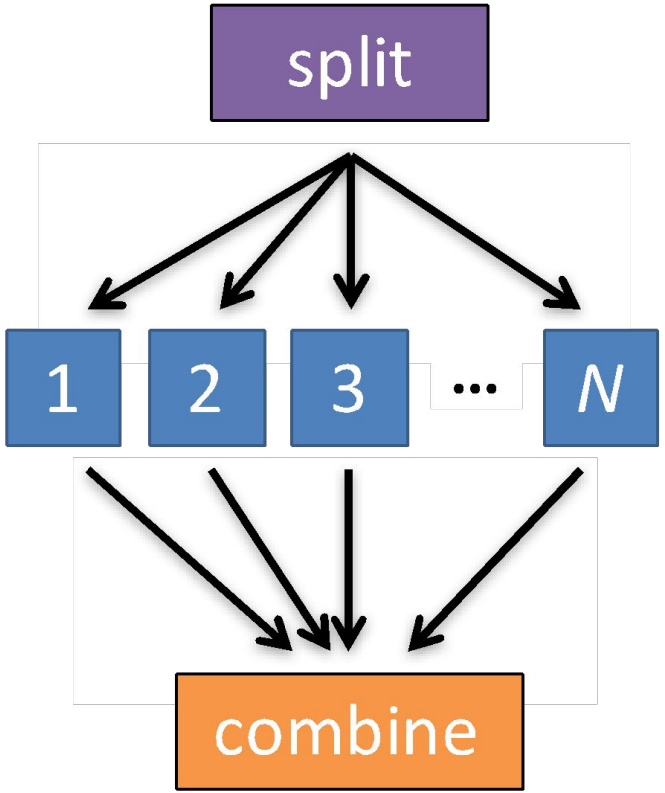
Goals for this Session

- 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

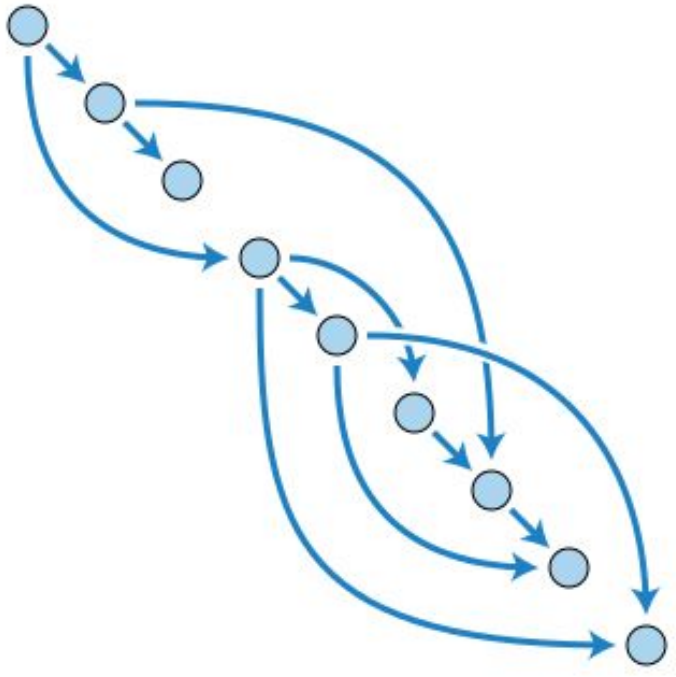
Automation!

- 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

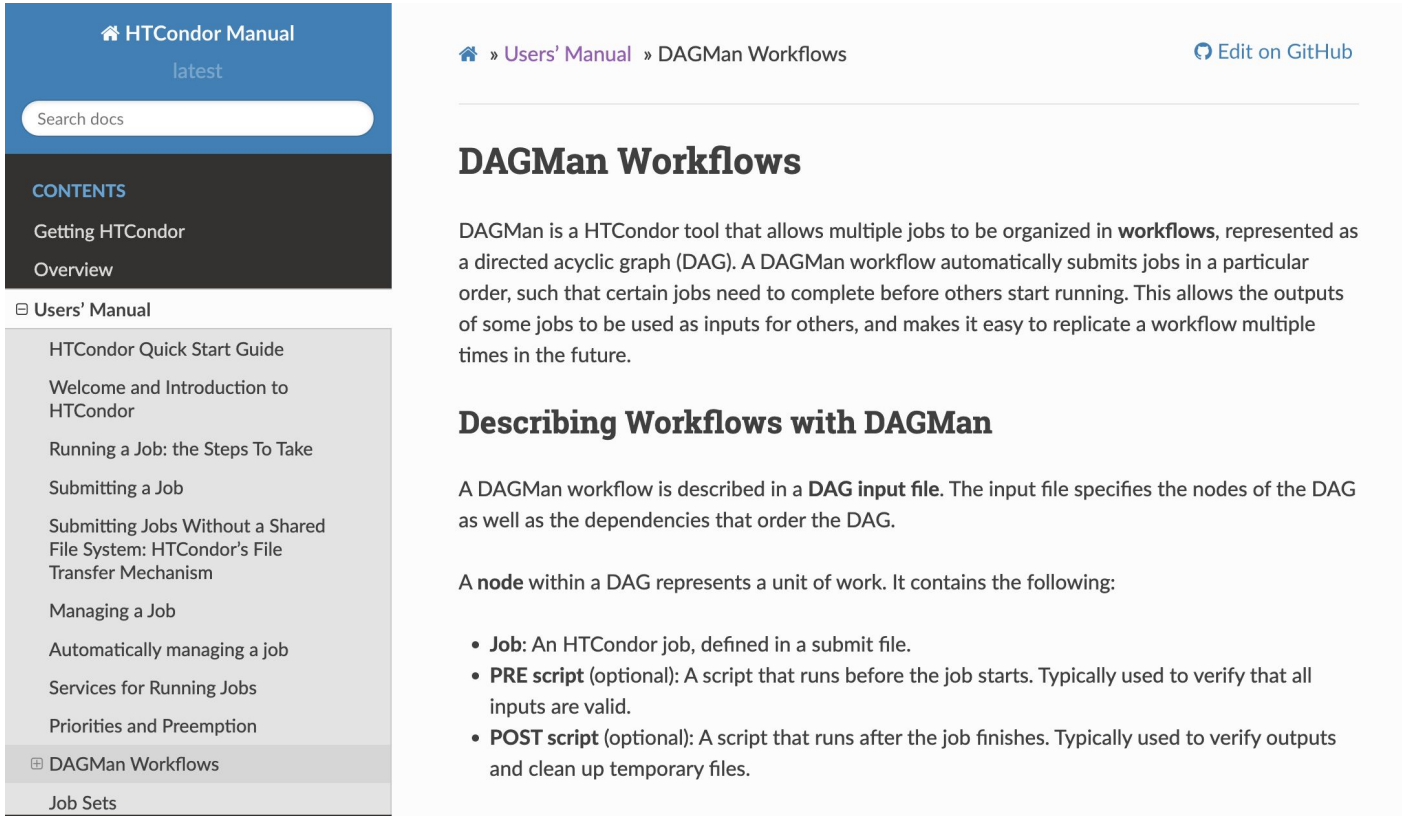


Wikimedia Commons

wikipedia.org/wiki/Directed_acyclic_graph

DESCRIBING WORKFLOWS WITH DAGMAN

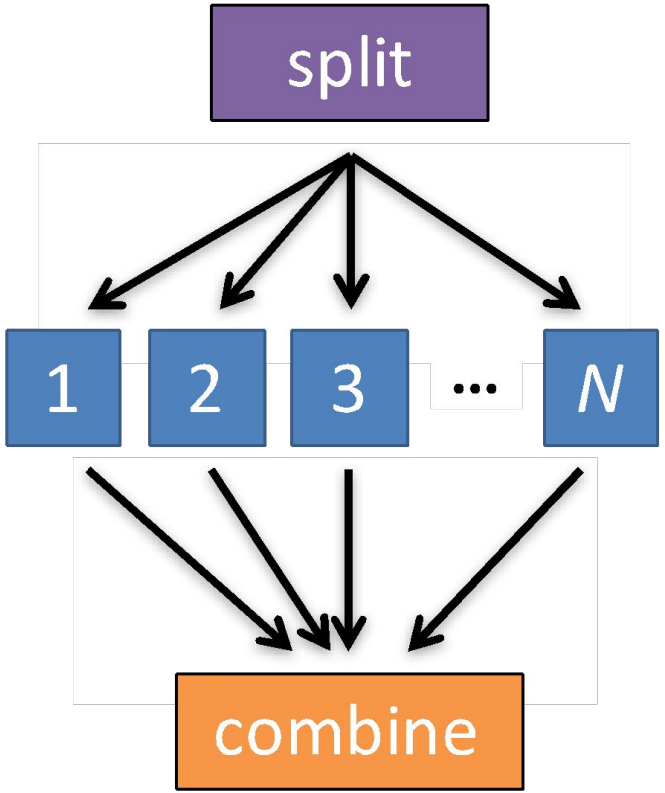
DAGMan in the HTCondor Manual



https://htcondor.readthedocs.io/en/latest/automated-workflows/index.html

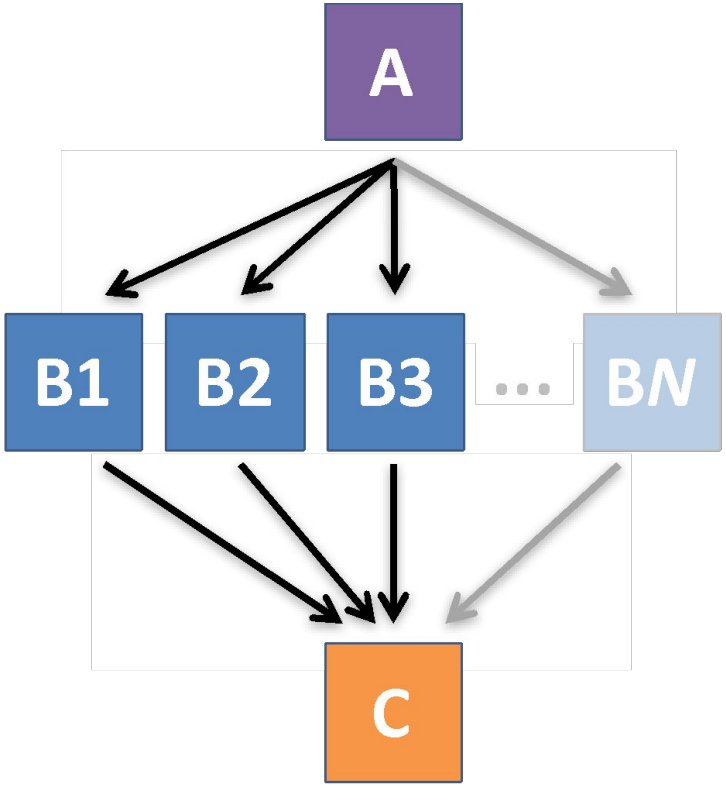
An Example HTC Workflow

- User must communicate the "nodes" and directional "edges" of the DAG



Simple Example for this Tutorial

- **The DAG input file will** communicate the "nodes" and directional "edges" of the DAG

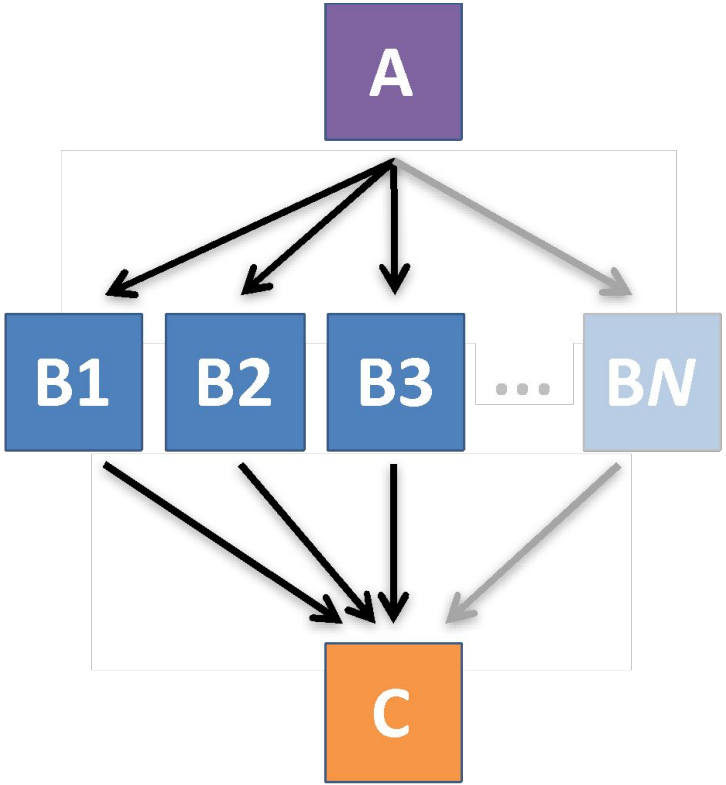


Basic DAG input file: *JOB* nodes, *PARENT-CHILD* edges

my.dag

```
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
```

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



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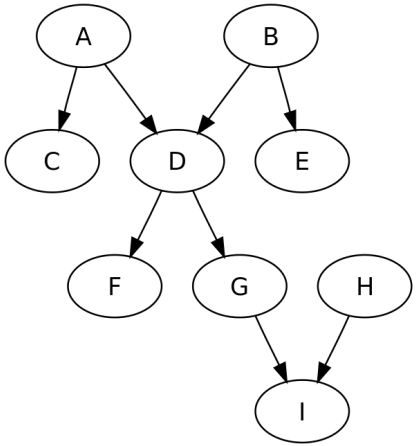
JOB B2 B2.sub
JOB B3 B3.sub
JOB C C.sub
PARENT A CHILD B1 B2 B3
PARENT B1 B2 B3 CHILD C
```

(dag_dir)/

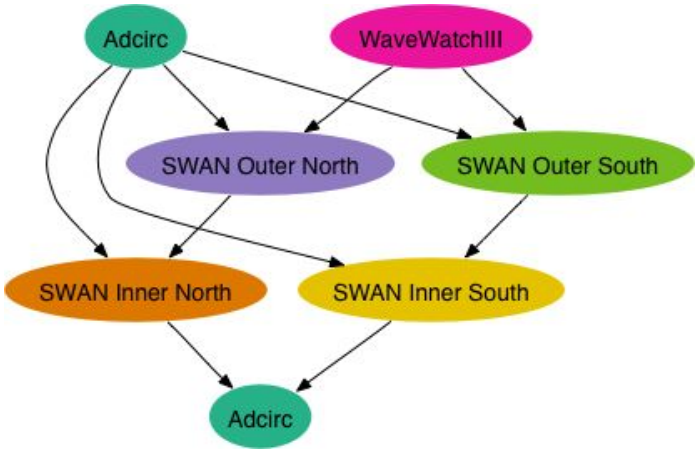
```
A.sub   B1.sub
B2.sub  B3.sub
C.sub   my.dag
(other job files)
```

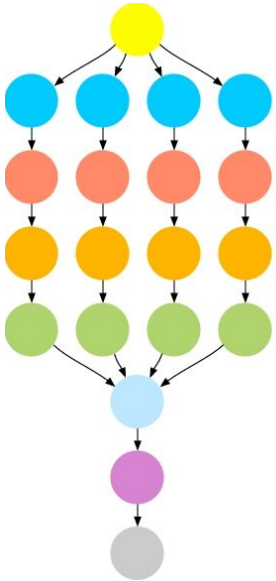
- Node names and filenames are your choice.
- Node name and submit filename do not have to match.

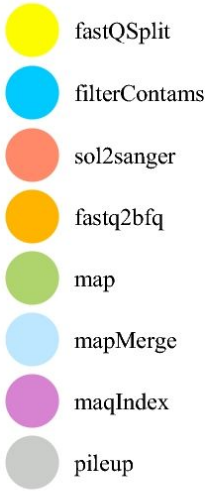
Endless Workflow Possibilities



Wikimedia Commons



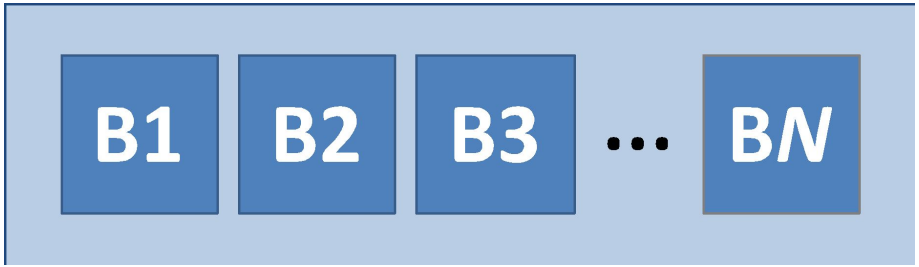




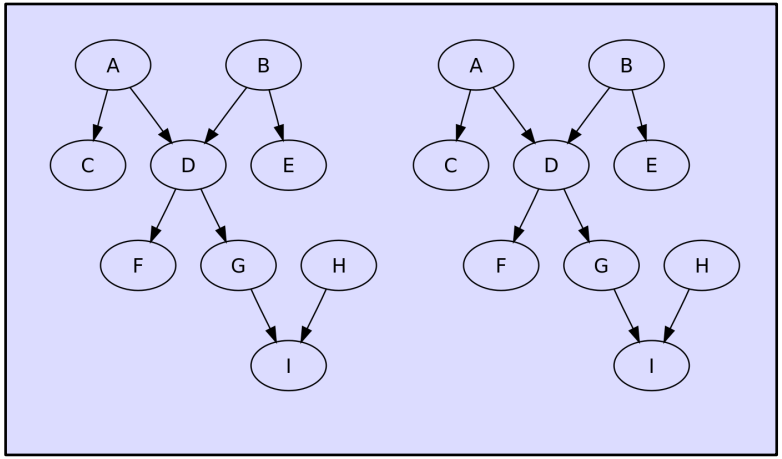
https://confluence.pegasus.isi.edu/display/pegasus/WorkflowGenerator

DAGs are also useful for non-sequential work

‘bag’ of HTC jobs



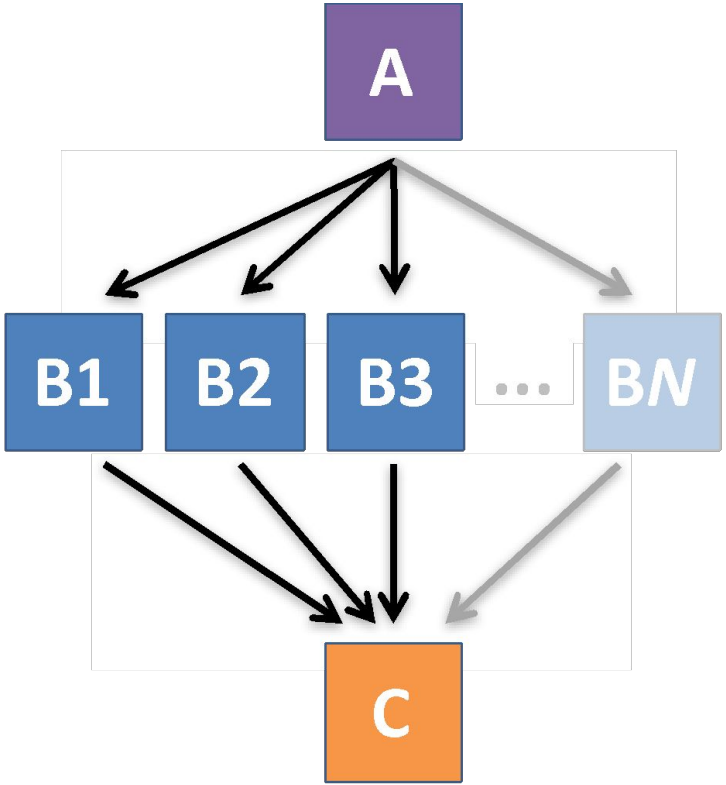
disjointed workflows



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

```
$ 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)/

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.nodes.log		

- ***.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)/

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.nodes.log	**my.dag.dagman.metrics**	

- ***.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:

`condor_rm dagman_jobID`

- Creates a **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   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.logmy.dag.rescue001
```

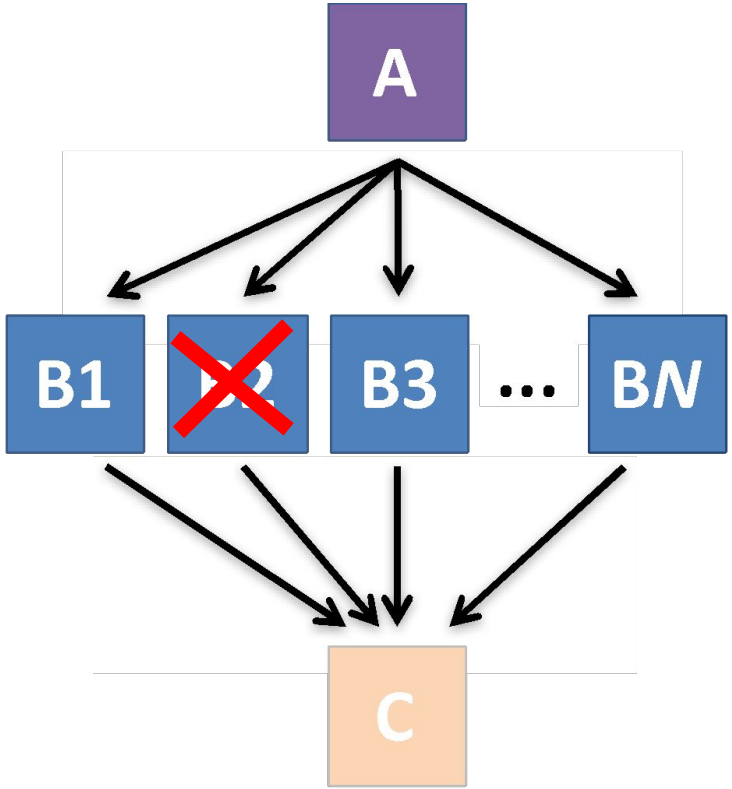
- Named ***dag_file.rescue001***
  - increments if more rescue DAG files are created
- Records which NODES have completed successfully
  - does not contain the actual DAG structure

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`

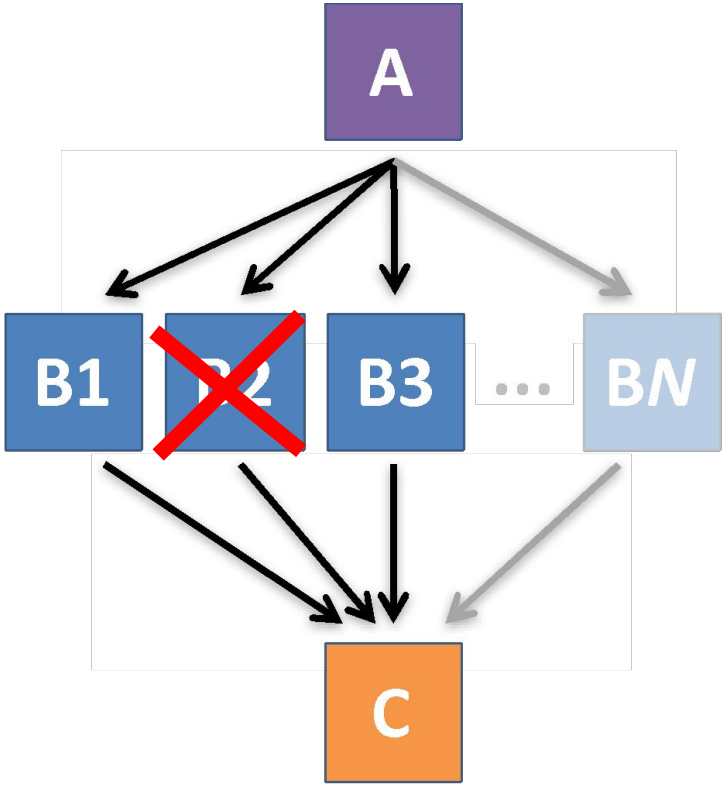
Node Failures Result in DAG Failure

- 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

```
$ 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 H  0    0.3 B_run.sh
131.0    alice   4/30 18:18   0+00:00:00 H  0    0.3 B_run.sh
132.0    alice   4/30 18:18   0+00:00:00 H  0    0.3 B_run.sh
4 jobs; 0 completed, 0 removed, 0 idle, 1 running, 3 held, 0 suspended
```

- 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!)

BEYOND THE BASIC DAG: NODE-LEVEL MODIFIERS

Default File Organization

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
```

(dag_dir)/

```
A.sub          B1.sub
B2.sub         B3.sub
C.sub          my.dag
(other job files)
```

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

Node-specific File Organization with *DIR*

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

my.dag

```
JOB A A.sub DIR A
JOB B1 B1.sub DIR B
JOB B2 B2.sub DIR B
JOB B3 B3.sub DIR B
JOB C C.sub DIR C
PARENT A CHILD B1 B2 B3
PARENT B1 B2 B3 CHILD C
```

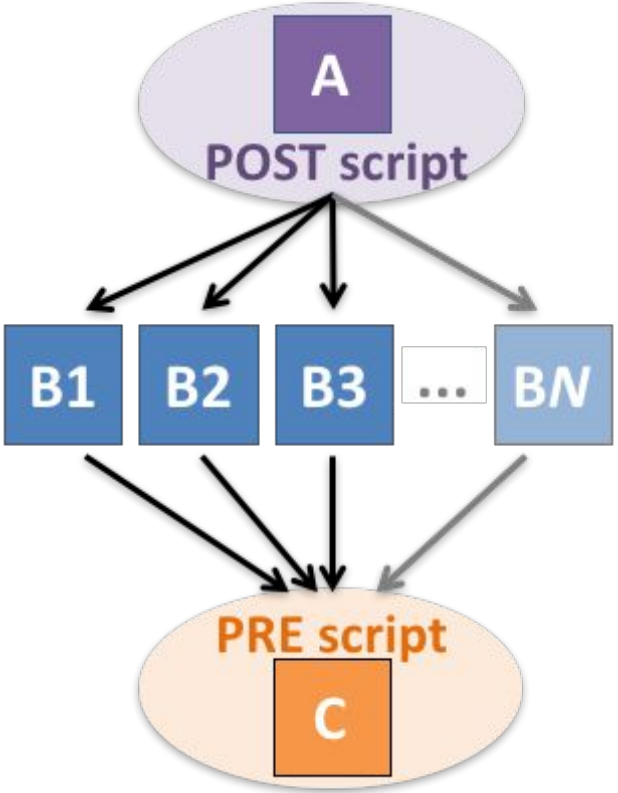
(dag_dir)/

```
my.dag
A/  A.sub    (A job files)
B/  B1.sub   B2.sub
    B3.sub   (B job files)
C/  C.sub    (C job files)
```

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

my.dag

```
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:

`RETRY node_name N`

Example:

```
JOB A A.sub
RETRY A 5
JOB B B.sub
PARENT A CHILD B
```

- **Note:** Unnecessary for nodes (jobs) that can use `max_retries` in the submit file
- See also: retry except for a particular exit code (`UNLESS-EXIT`), or retry scripts (`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
```

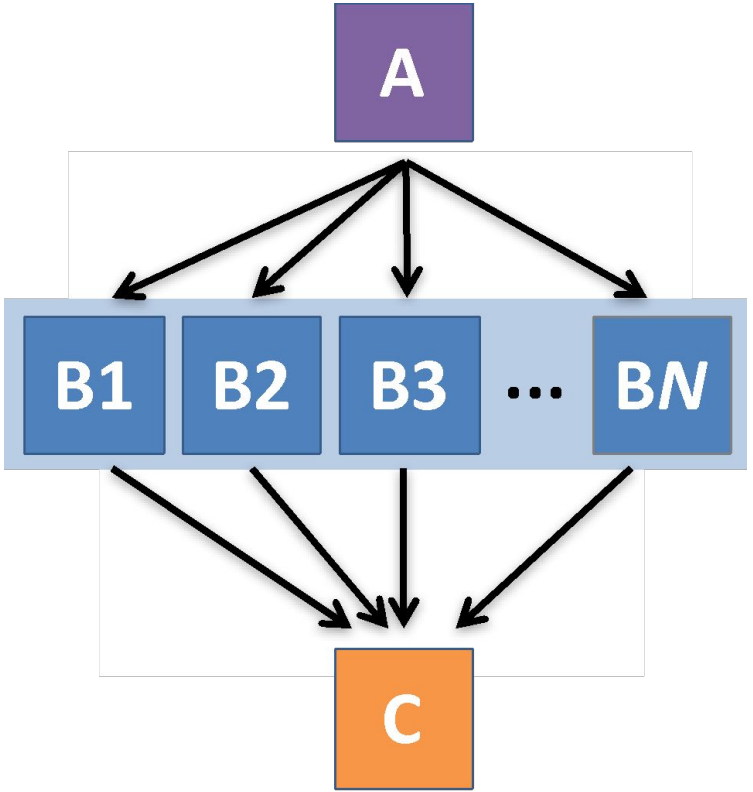
SPLICE subsets of a DAG to simplify lengthy DAG files

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

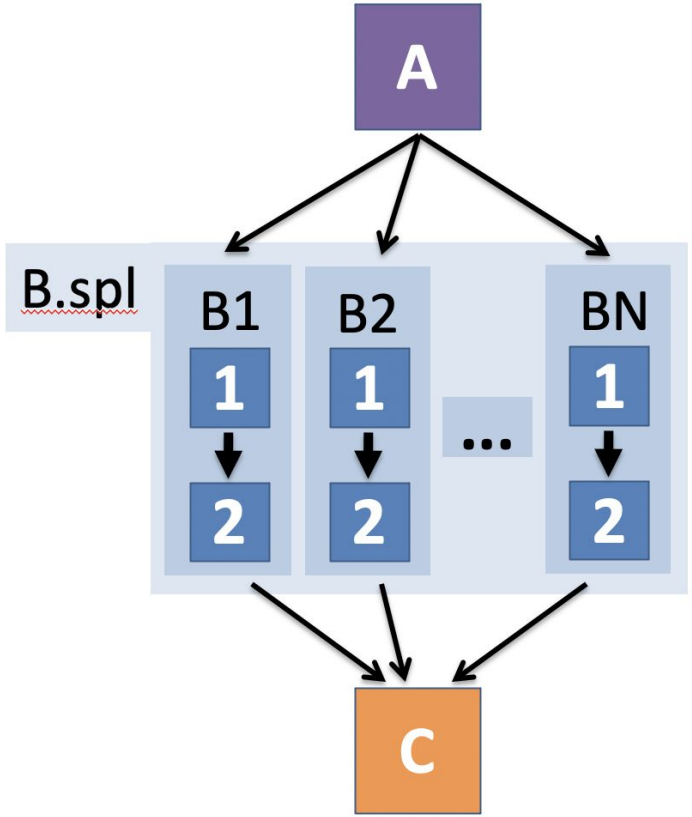
```
JOB A A.sub DIR A
SPLICE B B.spl DIR B
JOB C C.sub DIR C
PARENT A CHILD B
PARENT B CHILD C
```

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
```

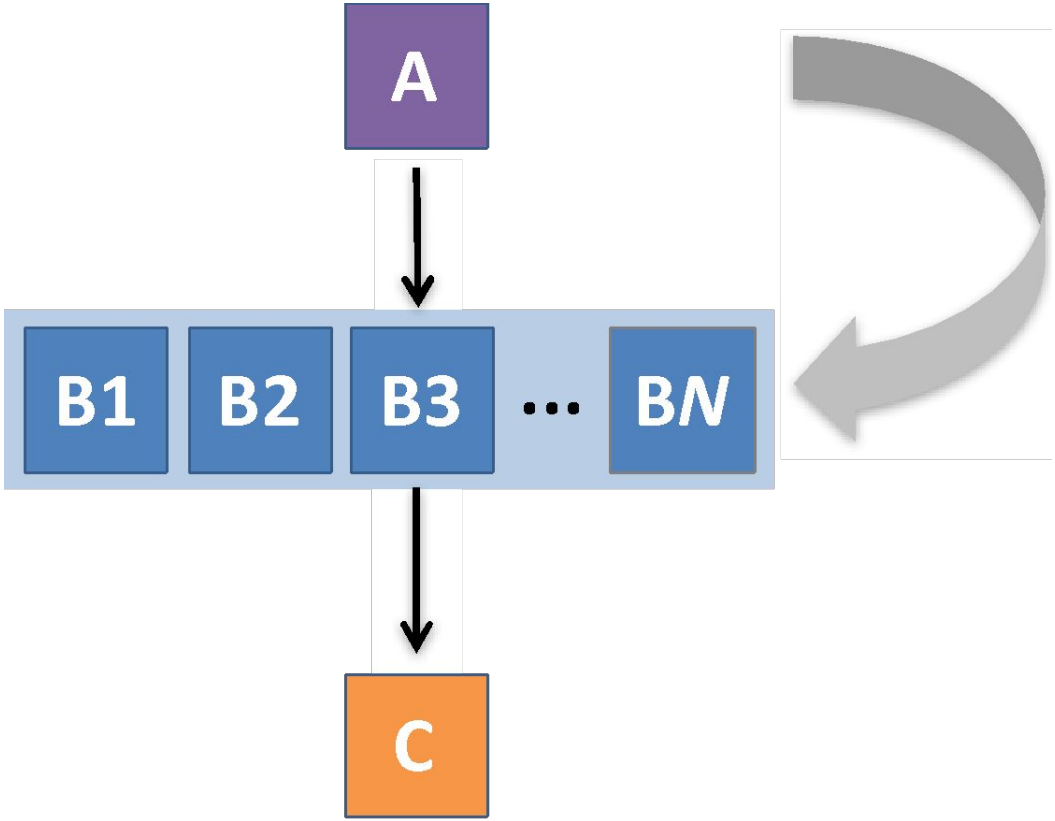
inner.spl

```
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)
```

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** …

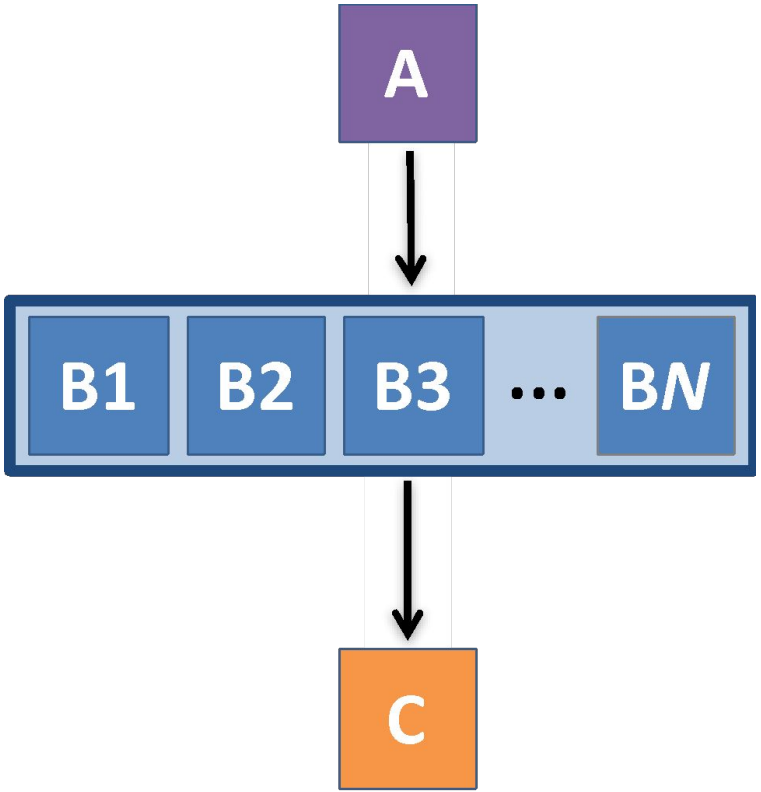
A *SUBDAG* within a DAG

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
```

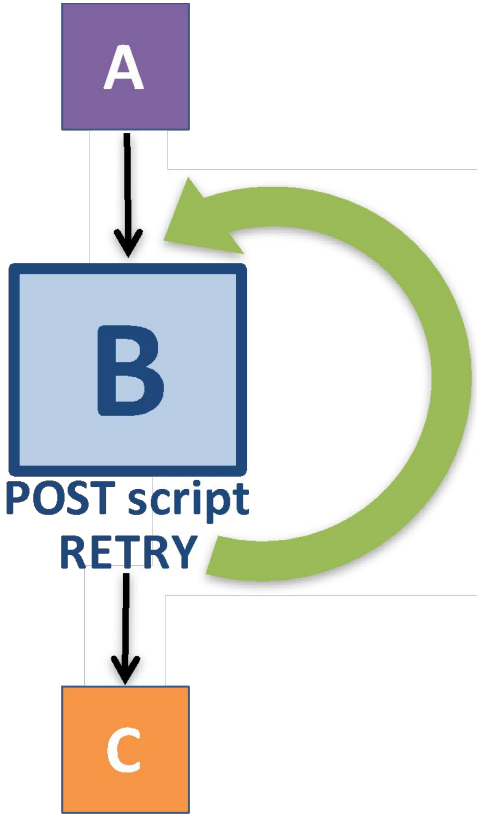


Use a *SUBDAG* to achieve a Cyclic Component within a DAG

- 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!