AN INTRODUCTION TO WORKFLOWS WITH DAGMAN

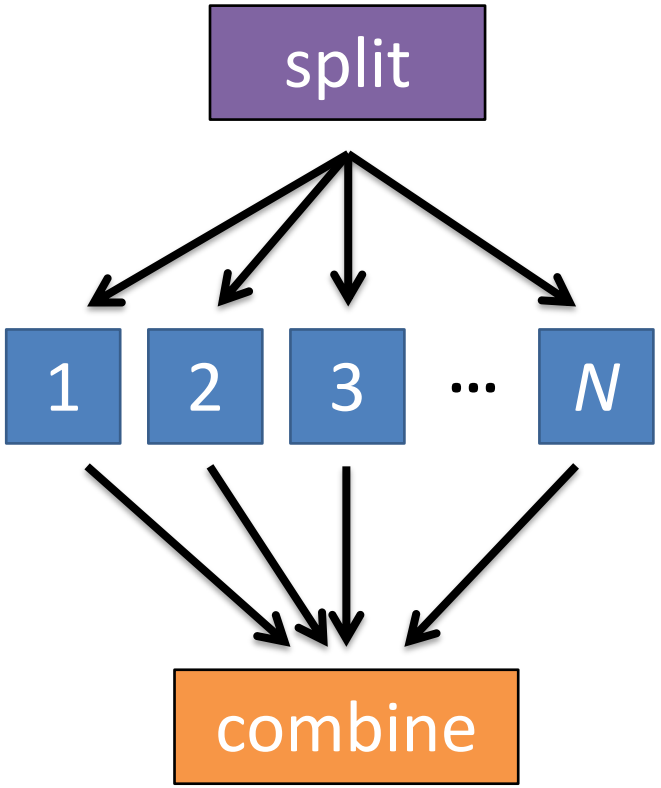
Presented by Lauren Michael

Covered In This Tutorial

- Why Create a Workflow?
- Describing workflows as *directed acyclic graphs* (DAGs)
- Workflow execution via DAGMan (DAG Manager)
- Node-level options in a DAG
- Modular organization of DAG components
- DAG-level control
- Additional DAGMan Features

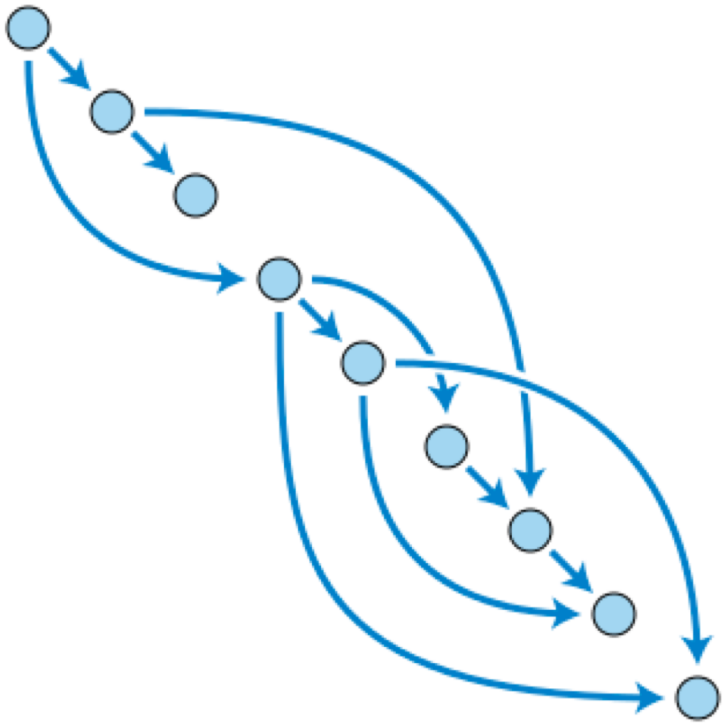
Automation!

- Objective: Submit jobs in a particular order, *automatically*.
- Especially if: Need to reproduce the same workflow multiple times.



DAG = ”directed acyclic graph”

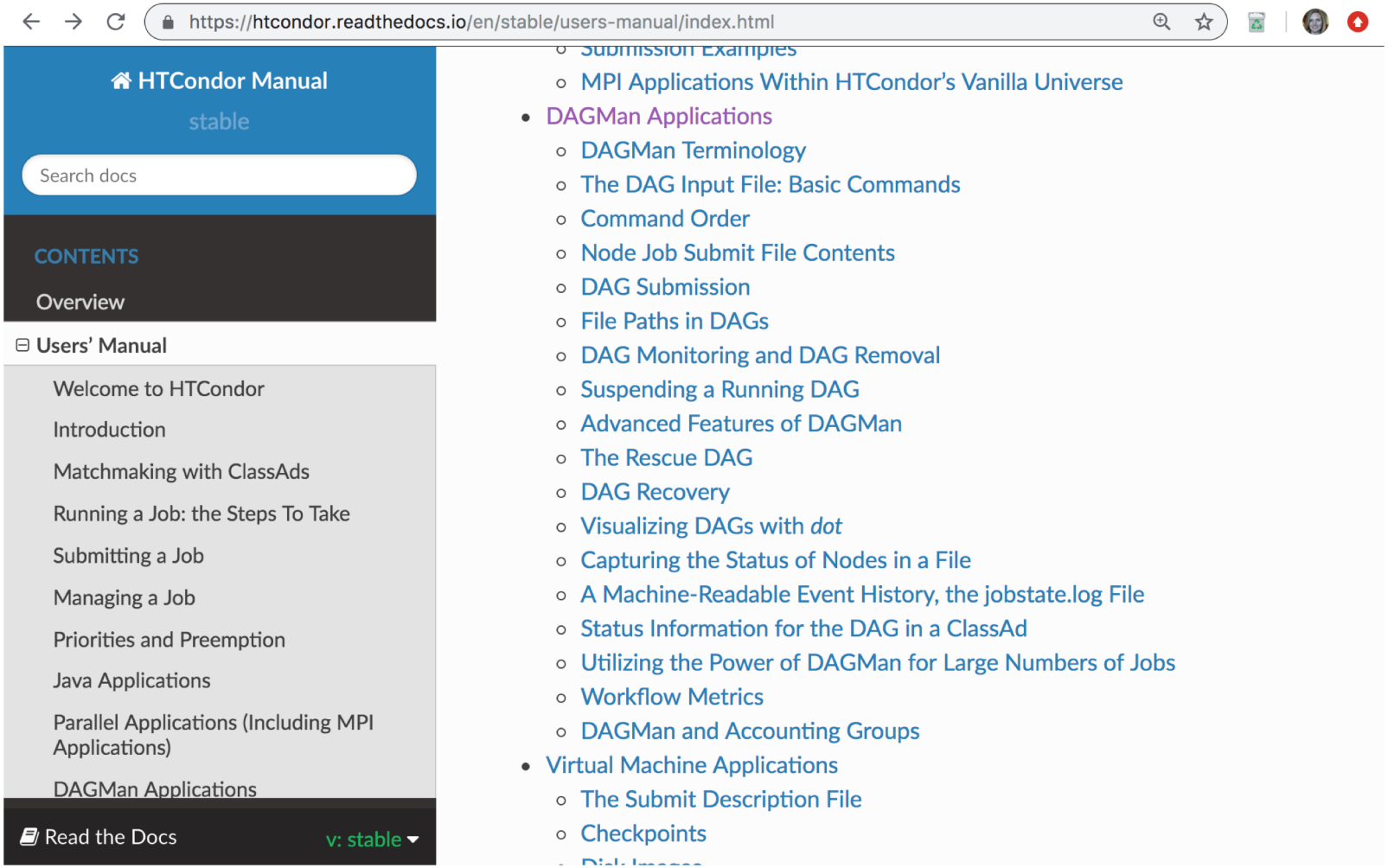
- topological ordering of vertices (“**nodes**”) is established by directional connections (“**edges**”)
- “acyclic” aspect requires a start and end, with no looped repetition
  - can contain cyclic subcomponents, covered in later slides for workflows



Wikimedia Commons

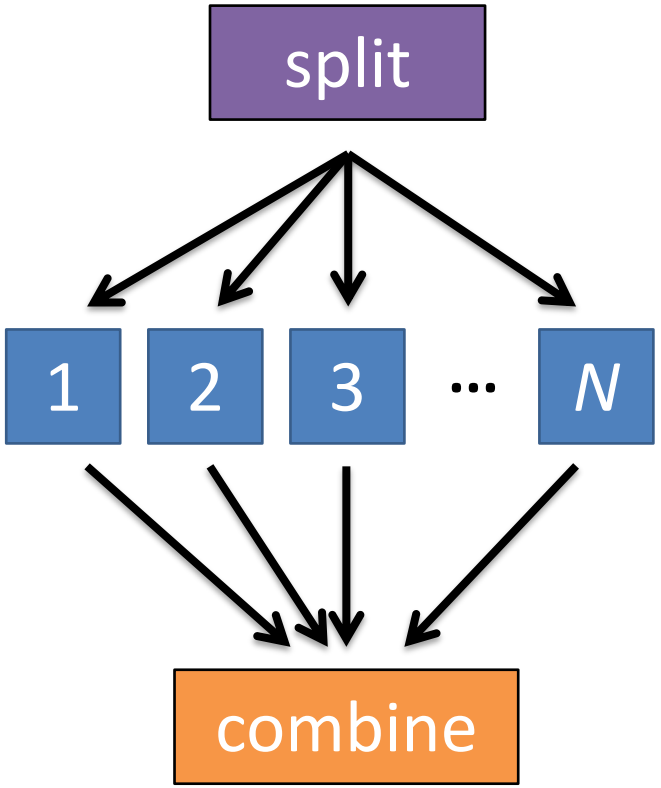
wikipedia.org/wiki/Directed_acyclic_graph

HTCondor has a *DAG Manager* (DAGMan)!



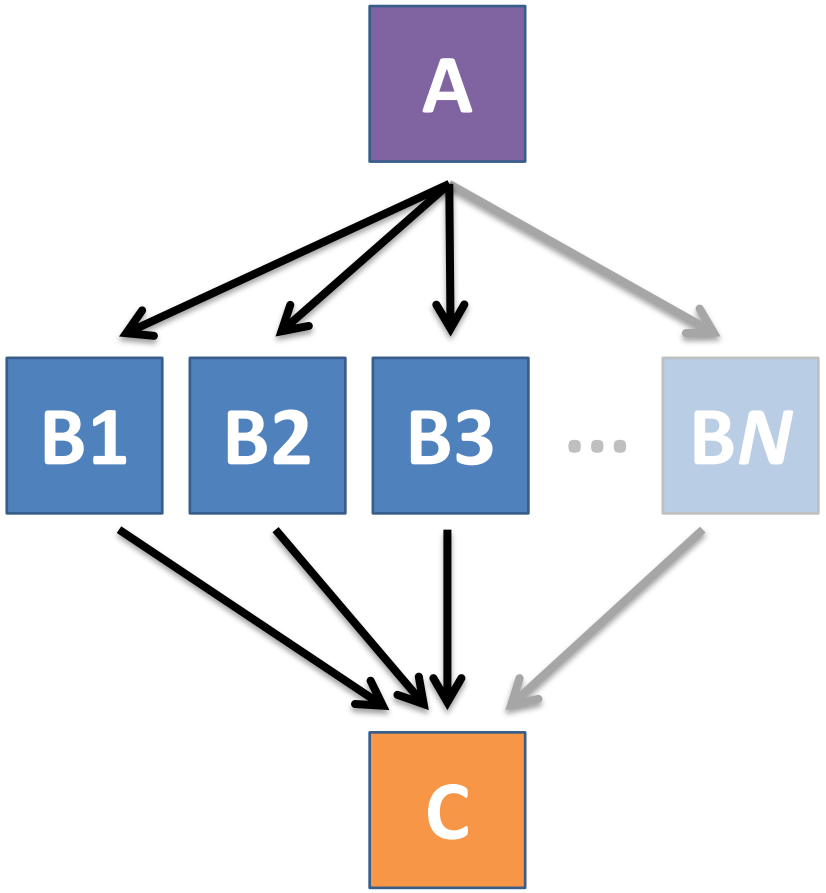
An Example HTC Workflow

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



Simple Example for this Tutorial

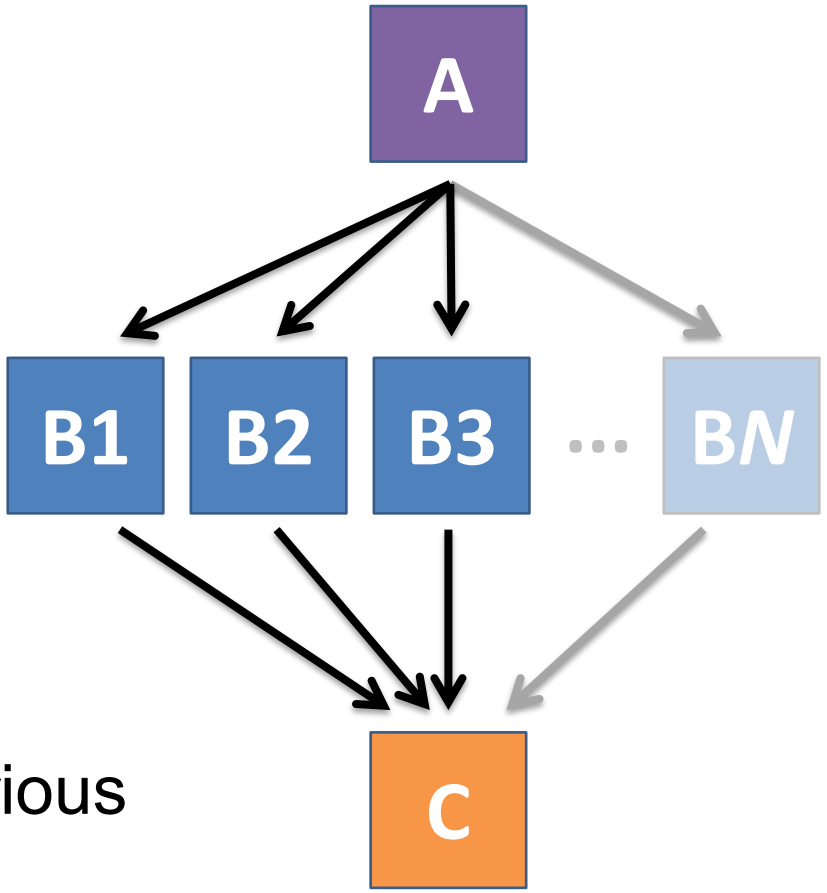
- **The DAG input file** communicates the "nodes" and directional "edges" of the DAG



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 are used by various DAG features to modify their execution by DAG Manager.

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

my.dag

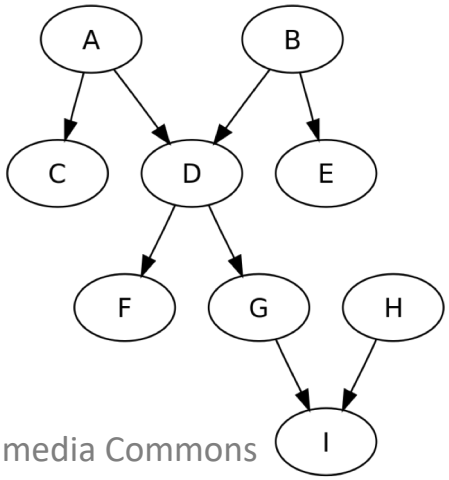
```
JOB A A.sub
JOB B1 B1.sub
JOB B2 B2.sub
JOB B3 B3.sub
JOB C C.sub
PARENT A CHILD B1 B2 B3
PARENT B1 B2 B3 CHILD C
```

(dag_dir)/

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

- Node names and filenames can be anything.
- Node name and submit filename do not have to match.

Endless Workflow Possibilities



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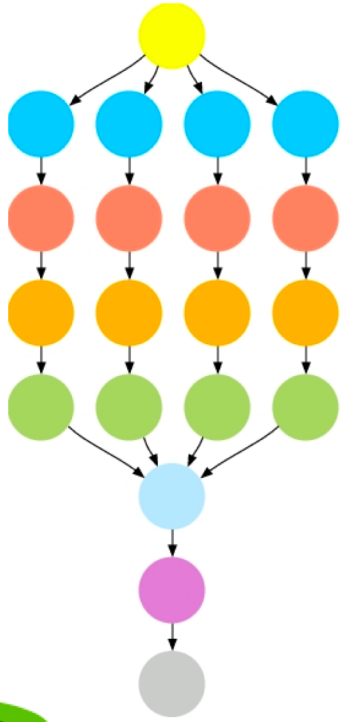
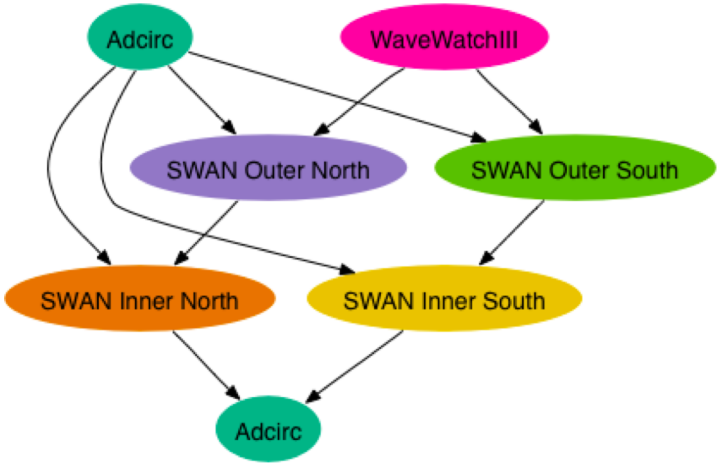
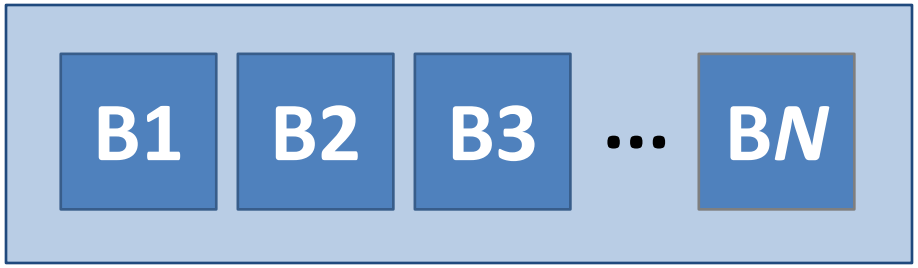




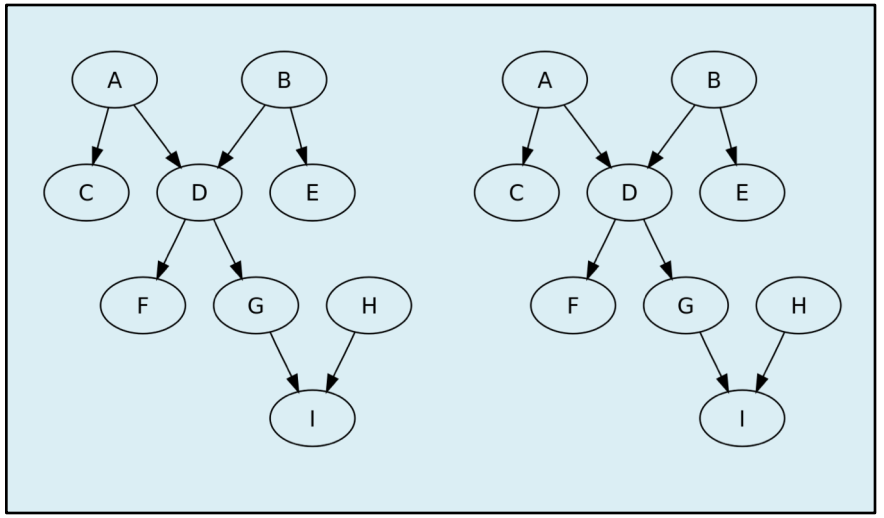
https://confluence.pegasus.isi.edu/display/pegasus/WorkflowGenerator

DAGs are also useful for non-sequential work

‘bag’ of HTC jobs



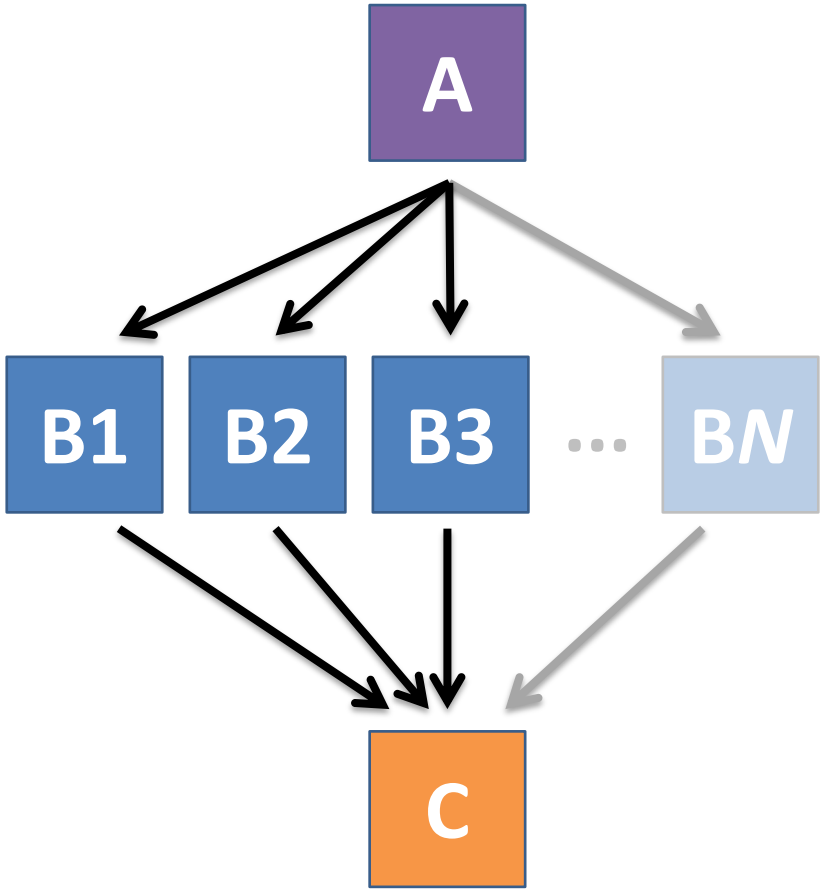
disjointed workflows



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           : my.dag.condor.sub
Log of DAGMan debugging messages                   : my.dag.dagman.out
Log of HTCondor library output                     : my.dag.lib.out
Log of HTCondor library error messages             : my.dag.lib.err
Log of the life of condor_dagman itself            : my.dag.dagman.log

Submitting job(s).
1 job(s) submitted to cluster 87274940.
------------------------------------------------------------------------
```


HTCondor Manual: DAGMan > DAG Submission

A submitted DAG creates a DAGMan job process in the queue

- DAGMan runs on the submit server, 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
```


DAGMan > DAG Monitoring and DAG Removal

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
```


DAGMan > DAG Monitoring and DAG Removal

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 18:28   0+00:00:00 I  0    0.3 B_run.sh
131.0   alice   4/30 18:28   0+00:00:00 I  0    0.3 B_run.sh
132.0   alice   4/30 18:28   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
```


DAGMan > DAG Monitoring and DAG Removal

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
```


DAGMan > DAG Monitoring and DAG Removal

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
- ***.dagman.out** has detailed 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 for all jobs (look to first for errors)

Removing a DAG from the queue

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

  `condor_rm` *`dagman_jobID`*

```
$ 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       6   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
```

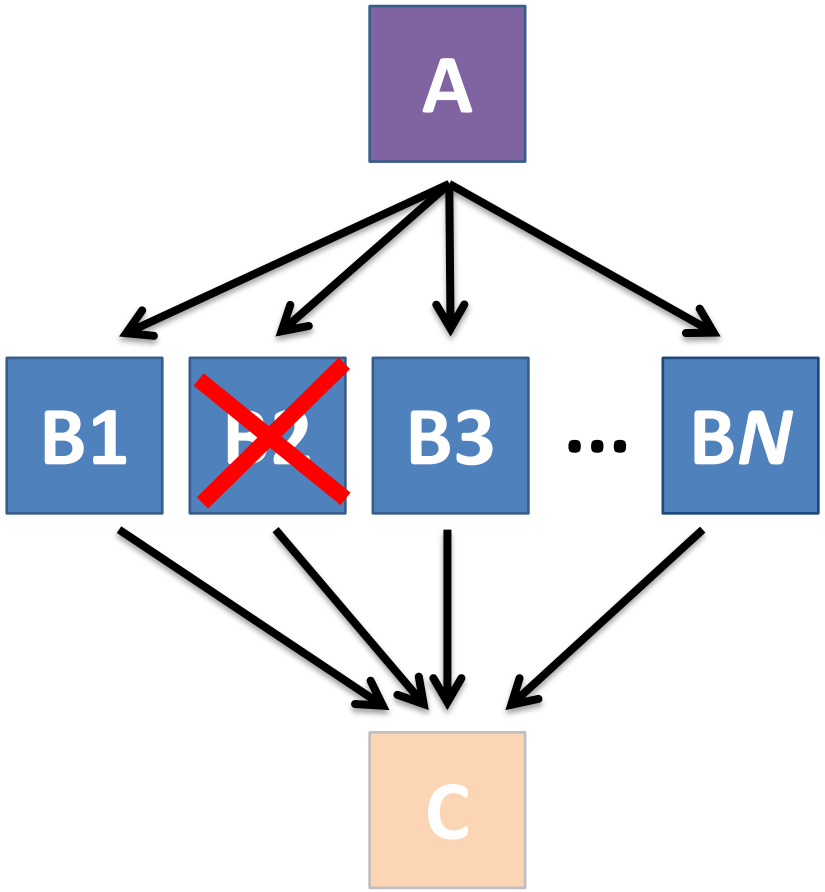
- Creates a **rescue file** so that only incomplete or unsuccessful NODES are repeated upon resubmission

DAGMan > DAG Monitoring and DAG Removal

DAGMan > The Rescue DAG

Node Failures Result in DAG Failure and Removal

- **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**

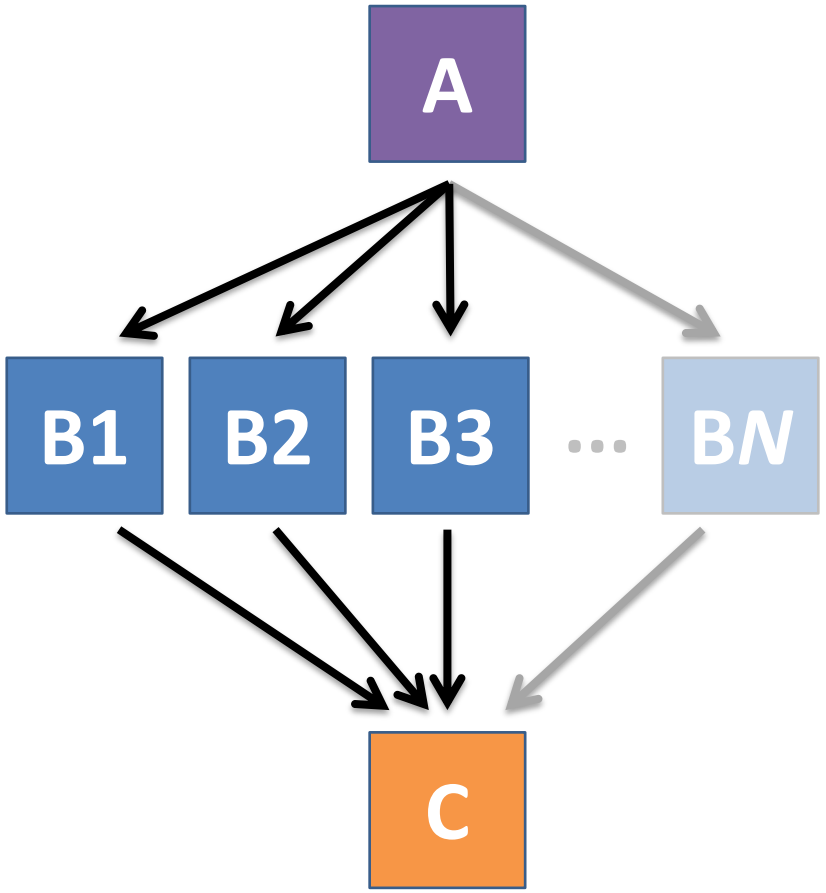


DAGMan > DAG Monitoring and DAG Removal

DAGMan > The Rescue DAG

Best Control Achieved with One Process per JOB Node

- While submit files can '`queue`' many processes, a ***single process per submit*** file is usually best for DAG JOBs
  - Failure of any process in a JOB node results in failure of the entire node and immediate removal of other processes in the node.
  - RETRY of a JOB node resubmits 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

DAGMan > DAG Monitoring and DAG Removal

Beyond the Basic DAG: Node-level Modifiers

By default, JOB files are relative to the DAG submission directory

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 different JOB node files in different directories?

Designate different submission directories with DIR

- combine DIR with submit file contents (file paths) to achieve your desired organization

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
```

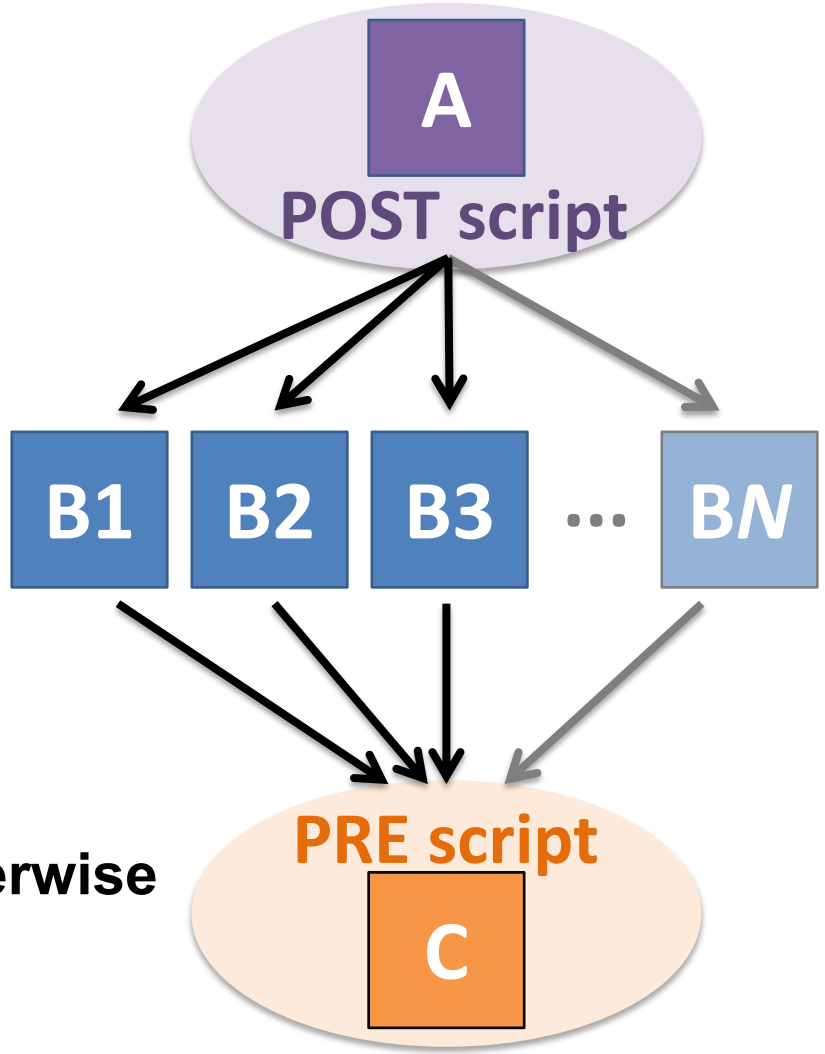
(dag_dir)/

```
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 submit server, 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 light work; otherwise include work in submitted jobs**

RETRY failed nodes to overcome transient errors

- Retry a node up to *N* times if it fails (the job 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
```

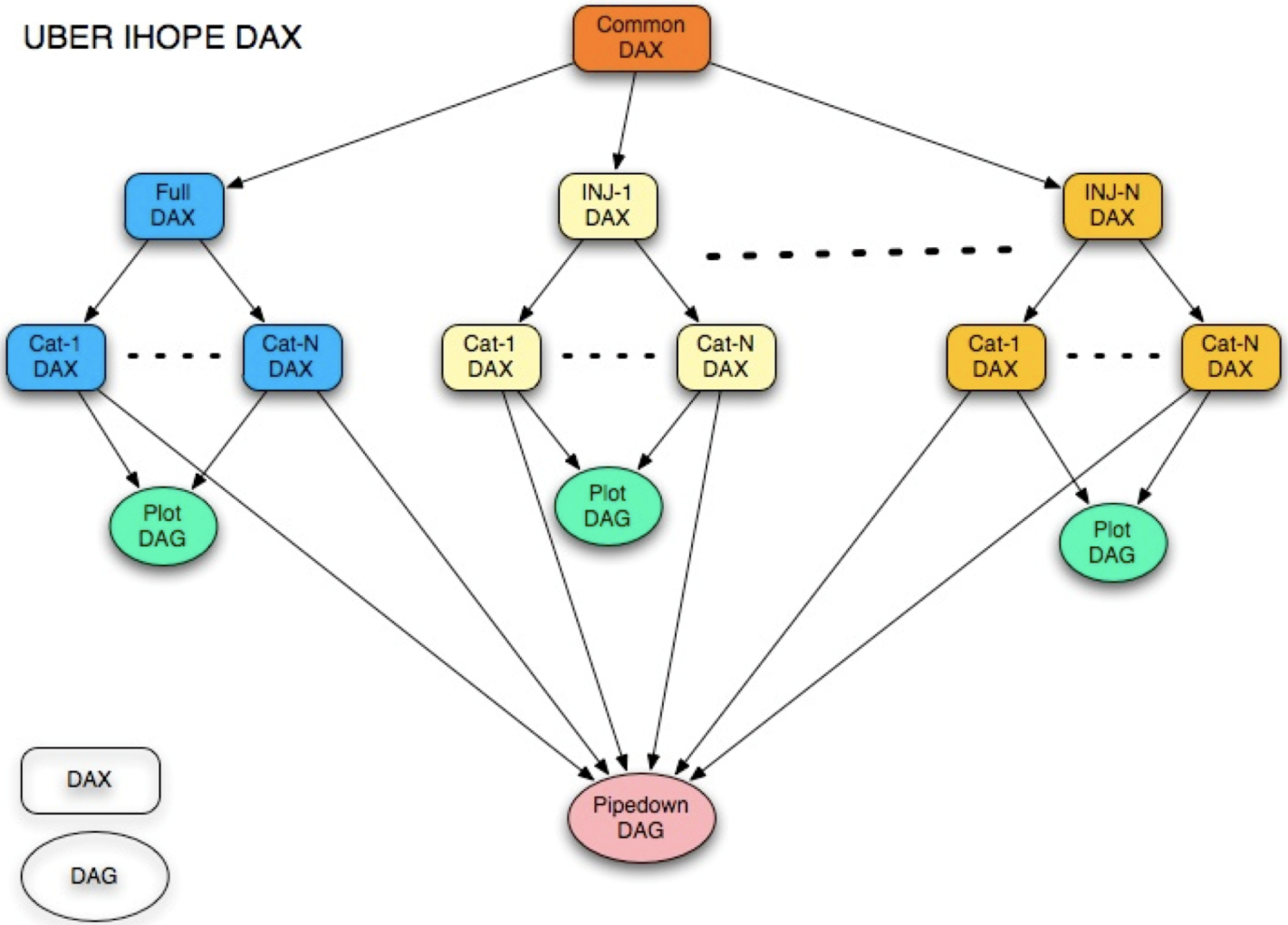
- See also: retry except for a particular exit code (`UNLESS-EXIT`)
- **Note:** `max_retries` in the submit file are preferable for simple cases

DAGMan Applications > Advanced Features > Retrying

DAGMan Applications > DAG Input File > SCRIPT

Modular Organization and Control of DAG Components

Repeating 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
```

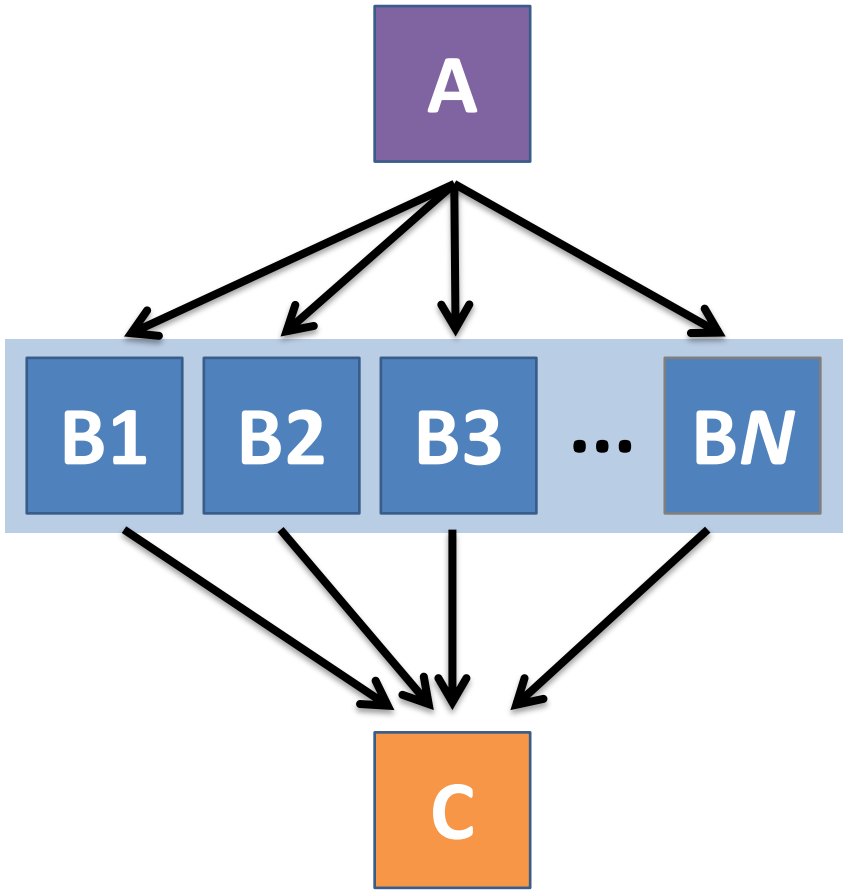
SPLICE subsets of the DAG to simplify lengthy DAG files

my.dag

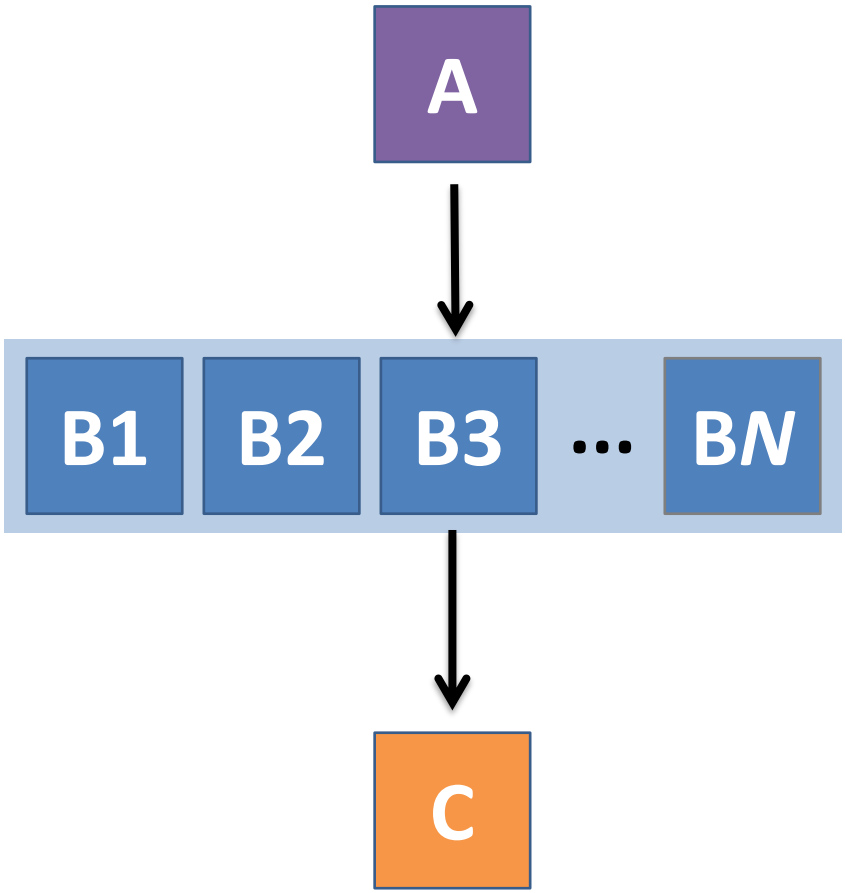
```
JOB A A.sub
SPLICE B B.spl
JOB C C.sub
PARENT A CHILD B
PARENT B CHILD C
```

B.spl

```
JOB B1 B1.sub
JOB B2 B2.sub
…
JOB BN BN.sub
```



What if some DAG components can't be known ahead of time?



e.g. If the value of ***N*** can only be determined as part of the work of the prior node (**A**) …

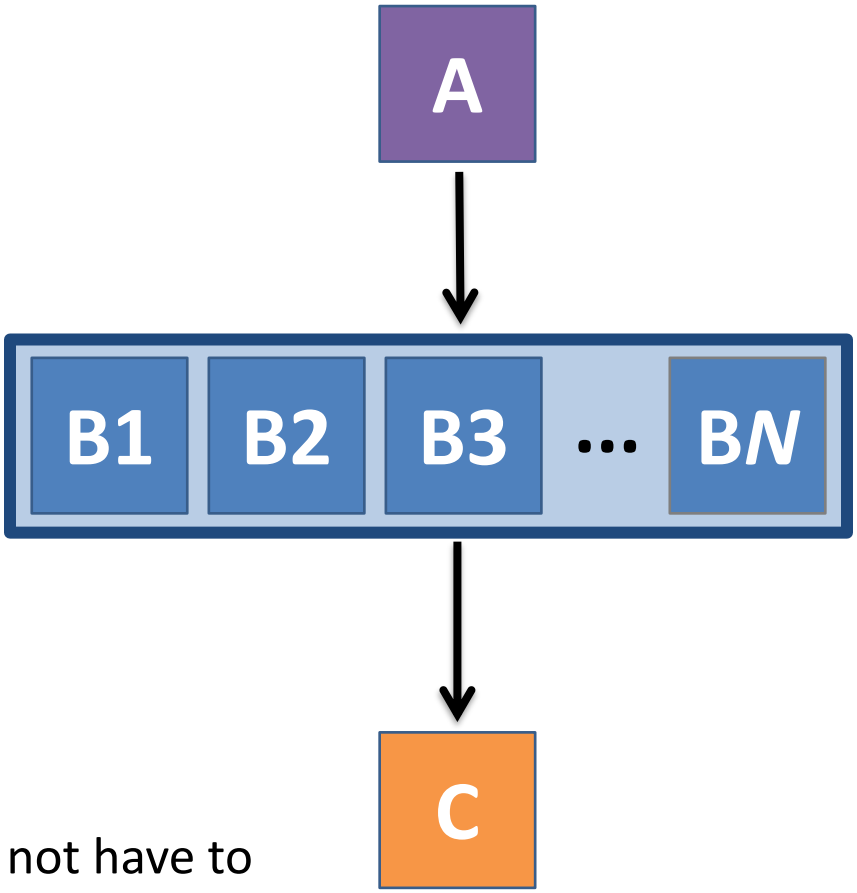
A SUBDAG within a DAG

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
```



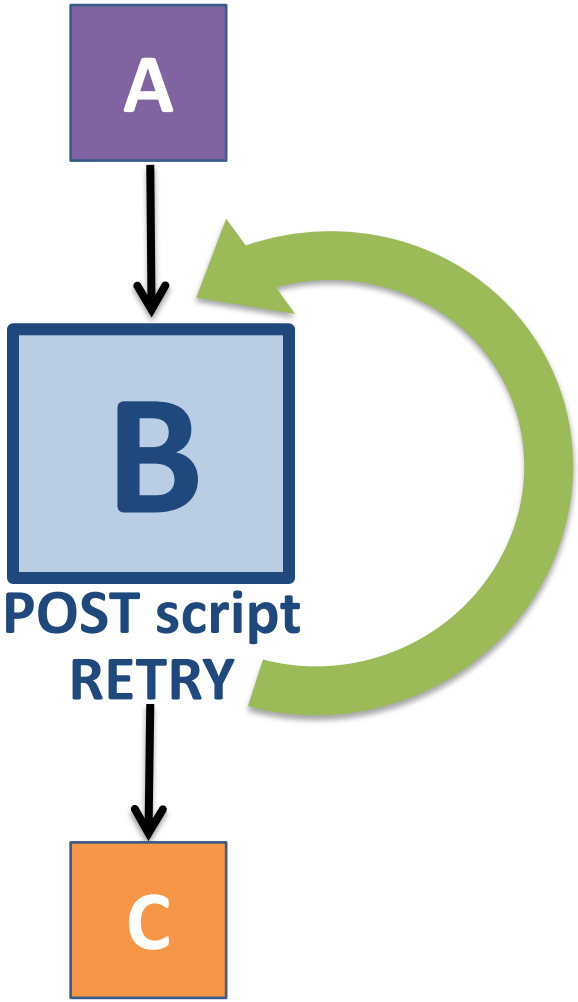
A SUBDAG is not submitted (so contents do not have to exist) until prior nodes in the outer DAG have completed.

Use a SUBDAG to achieve Cyclic Components 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 100
JOB C C.sub
PARENT A CHILD B
PARENT B CHILD C
```



More at the end of this presentation and in the HTCondor Manual!!!

https://htcondor.readthedocs.io/en/stable/users-manual/dagman-applications.html

Covered in Later Slides

- Why Create a Workflow?
- Describing workflows as *directed acyclic graphs* (DAGs)
- Workflow execution via DAGMan (DAG Manager)
- **Node-level options in a DAG (cont…)**
- **Modular organization of DAG components (…)**
- **DAG-level control (…)**
- **Additional DAGMan Features**

QUESTIONS?

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Beyond the Basic DAG: Node-level Modifiers

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 (**or need for iteration**)

Example:

```
SCRIPT PRE A download.sh
JOB A A.sub
SCRIPT POST A checkA.sh
RETRY A 5
```

DAGMan Applications > Advanced Features > Retrying

DAGMan Applications > DAG Input File > SCRIPT

SCRIPT Arguments and Argument Variables

```
JOB A A.sub
SCRIPT POST A checkA.sh my.out $RETURN
RETRY A 5
```

$JOB: node name

$JOBID: *cluster.proc*

$RETURN: exit code of the node

$PRE_SCRIPT_RETURN: exit code of PRE script

$RETRY: current retry ('iteration') count

(more variables described in the manual)

DAGMan Applications > Advanced Features > Retrying

DAGMan Applications > DAG Input File > SCRIPT

Other Node-Level Controls

- Set the **PRIORITY** of JOB nodes with:

  `PRIORITY` ***`node_name priority_value`***

- Use a **PRE_SKIP** to skip a node and mark it as successful, if the PRE script exits with a specific exit code:

  `PRE_SKIP` ***`node_name exit_code`***

DAGMan Applications > Advanced Features > Setting Priorities

DAGMan Applications > The DAG Input File > PRE_SKIP

Modular Organization and Control of DAG Components

Use nested SPLICEs with DIR for repeating workflow components

my.dag

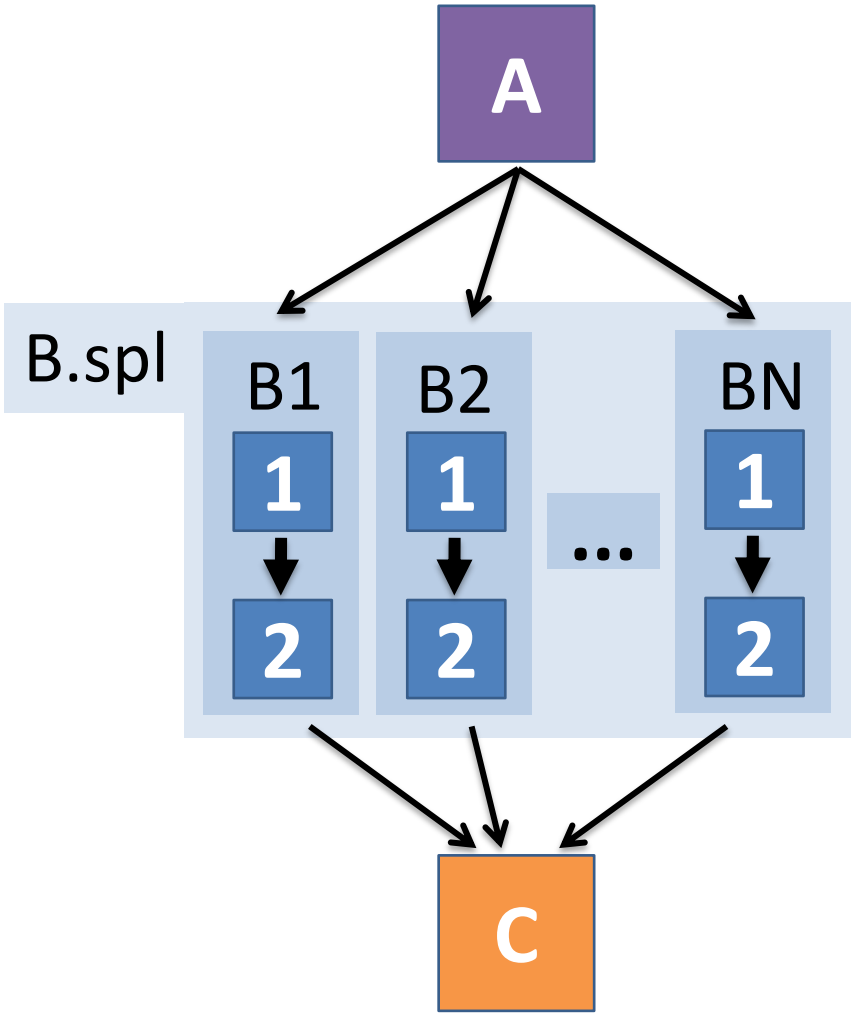
```
JOB A A.sub DIR A
SPLICE B B.spl DIR B
JOB C C.sub DIR C
PARENT A CHILD B
PARENT B CHILD C
```

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 for repeating workflow components

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)
```

More on SPLICE Behavior

- **HTCondor takes in a DAG and its SPLICEs as a single, large DAG file.**
  - SPLICEs simply allow the user to simplify and modularize the DAG expression using separate files
  - A single DAGMan job is queued with single set of status files.
- Great for gradually testing and building up a large DAG (since a SPLICE file can be submitted by itself, without its outer DAG).
- SPLICE lines are not treated like nodes.
  - no PRE/POST scripts or RETRIES

More on SUBDAG Behavior

- **Each SUBDAG EXTERNAL is a DAGMan job** running in the queue, and too many can overwhelm the queue.
  - **WARNING:** SUBDAGs should only be used (rather than SPLICES) when absolutely necessary!
- **SUBDAGs *are nodes*** (can have PRE/POST scripts, retries, etc.)

Other Modular Controls

- Append **NOOP** to a JOB definition so that its JOB process isn't run by DAGMan
  - Test DAG structure without running jobs (node-level)
  - Simplify combinatorial PARENT-CHILD statements (modular)
- Communicate DAG features separately with **INCLUDE**
  - e.g. separate files for JOB nodes and for VARS definitions, as part of the same DAG
- Define a **CATEGORY** of JOB nodes to throttle only a specific subset

DAGMan Applications > The DAG Input File > JOB
DAGMan Applications > Advanced Features > INCLUDE
DAGMan Applications > Advanced > Throttling by Category

DAG-level Control

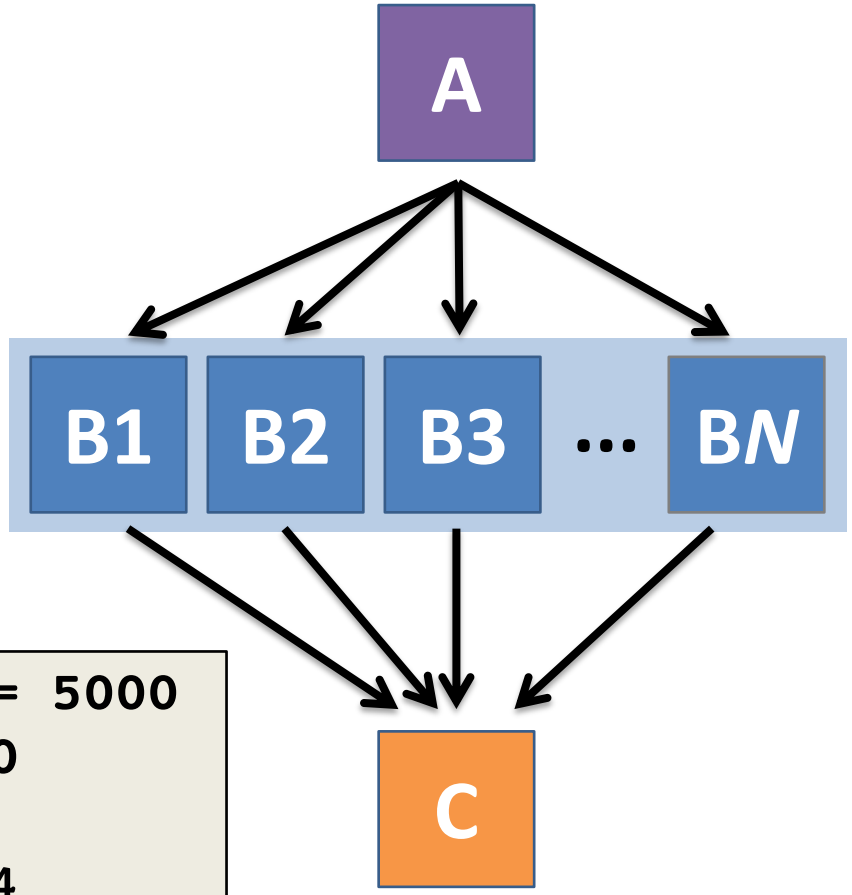
Throttle job nodes of large DAGs via DAG-level configuration

- **If a DAG has *many* (thousands or more) jobs**, submit server and queue performance can be assured by limiting:
  - Number of jobs in the queue
  - Number of jobs idle (waiting to run)
  - Number of PRE or POST scripts running
- Limits can be specified in a DAG-specific **CONFIG** file (recommended) or as arguments to `condor_submit_dag`

DAG-specific throttling via a CONFIG file

my.dag

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



my.dag.config

```
DAGMAN_MAX_JOBS_SUBMITTED = 5000
DAGMAN_MAX_JOBS_IDLE = 1000
DAGMAN_MAX_PRE_SCRIPTS = 4
DAGMAN_MAX_POST_SCRIPTS = 4
```

Removal of a DAG results in 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

DAGMan > DAG Monitoring and DAG Removal

DAGMan > The Rescue DAG

Rescue Files For Resuming a Failed DAG

- A **rescue file** is created any time a DAG is removed from the queue by the user (condor_rm) or automatically:
  - a node fails, and after DAGMan advances through any other possible nodes
  - the DAG is **aborted** (covered later)
  - the DAG is **halted** and not unhalted (covered later)
- The **rescue file** will be used (if it exists) when the original DAG file is resubmitted
  - override: **`condor_submit_dag` *`dag_file -f`***

DAGMan > The Rescue DAG

Pause (then resume) a DAG by holding it

- Hold the DAGMan job process:

  `condor_hold` *`dagman_jobID`*

- Pauses the DAG
  - No new node jobs submitted
  - Queued node jobs continue to run (including SUBDAGs), but no PRE/POST scripts
  - DAG resumes when released (**`condor_release` *`dagman_jobID`***)

DAGMan > Suspending a Running DAG

Cleanly quit a DAG with a halt file

- Create a file named ***`DAG_file.halt`*** in the same directory as the submitted DAG file
- Allows the DAG to complete nodes in-progress
  - No new node jobs submitted
  - Queued node jobs and SUBDAGs (including POST scripts) continue to run, but not PRE scripts
  - After all queued jobs have completed, the DAG creates a rescue DAG file and exits.
- If the DAG hasn't yet exited and the file is deleted, then the DAG resumes

DAGMan > Suspending a Running DAG

DAGMan > The Rescue DAG

Other DAG-Level Controls

- Replace the ***node_name*** with **ALL_NODES** to apply a DAG feature to all nodes of the DAG

- Abort the entire DAG if a specific node exits with a specific exit code:

  ABORT-DAG-ON *node_name exit_code*

- Define a **FINAL** node that will always run, even in the event of DAG failure (to clean up, perhaps).

  FINAL *node_name submit_file*

DAGMan Applications > Advanced > ALL_NODES
DAGMan Applications > Advanced > Stopping the Entire DAG
DAGMan Applications > Advanced > FINAL Node