AN INTRODUCTION TO WORKFLOWS WITH DAGMAN

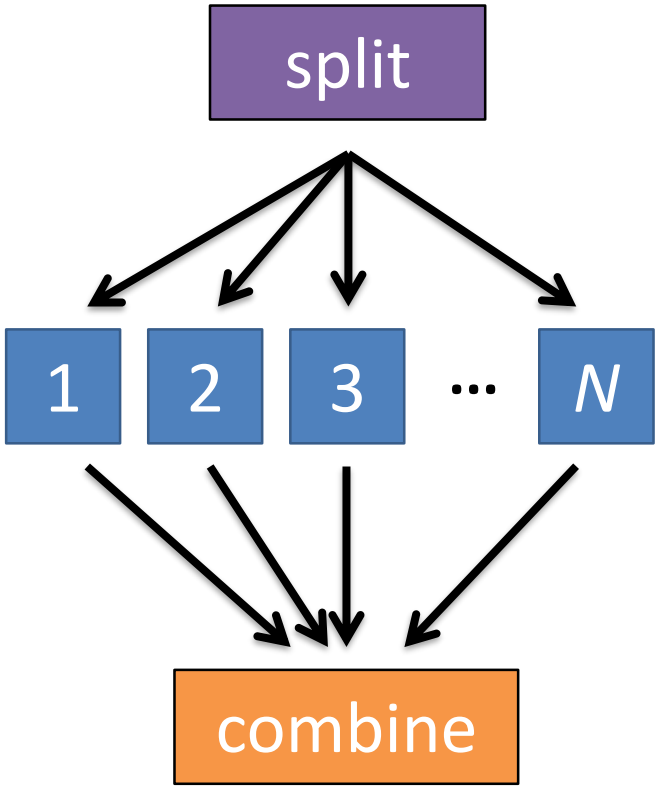
Presented by Lauren Michael

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

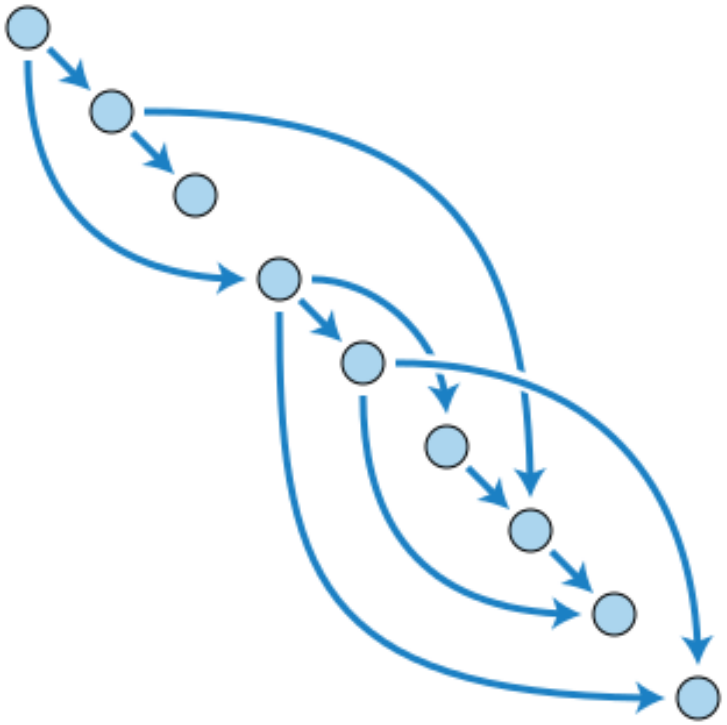
Automation!

- 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” with a distinct start and end
  - might contain cyclic subcomponents, covered later

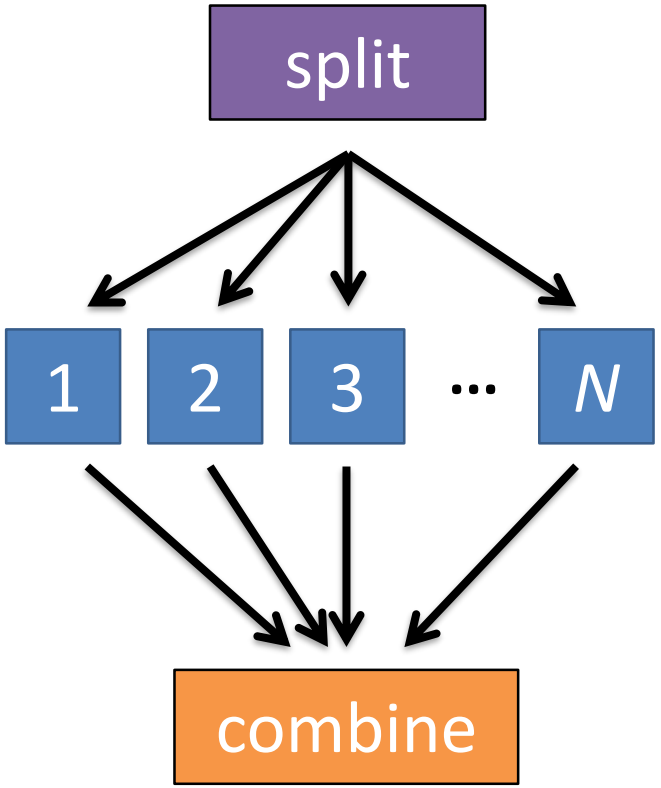


Wikimedia Commons

wikipedia.org/wiki/Directed_acyclic_graph

An Example HTC Workflow

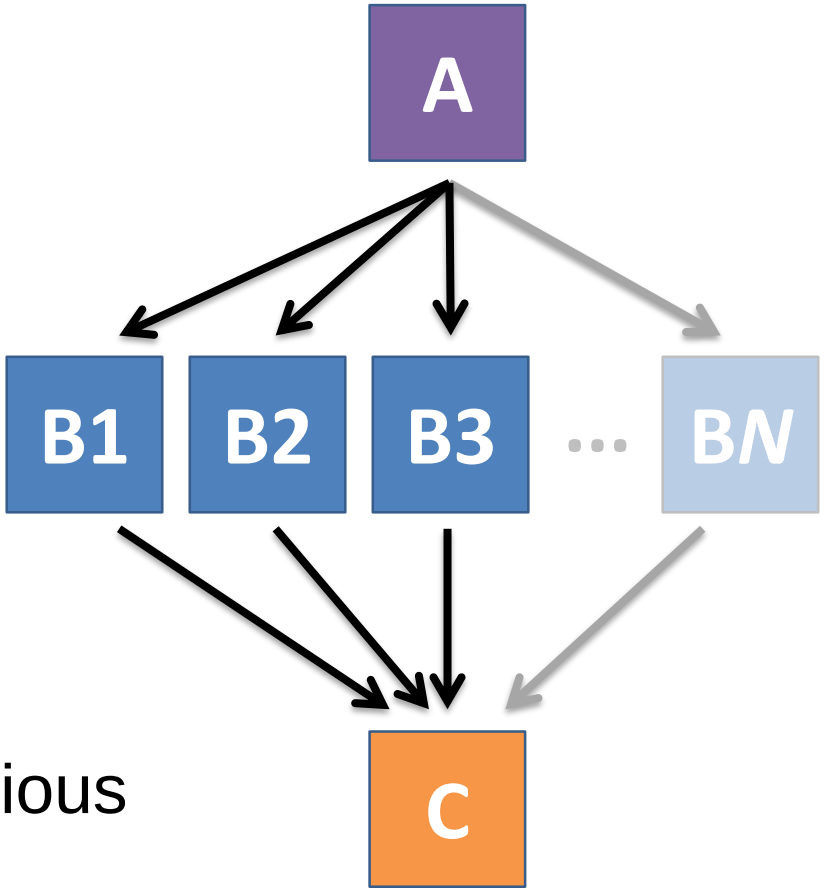
- User must communicate the "**nodes**" and directional "**edges**" of the DAG



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

Basic DAG input file: Data Organization

my.dag

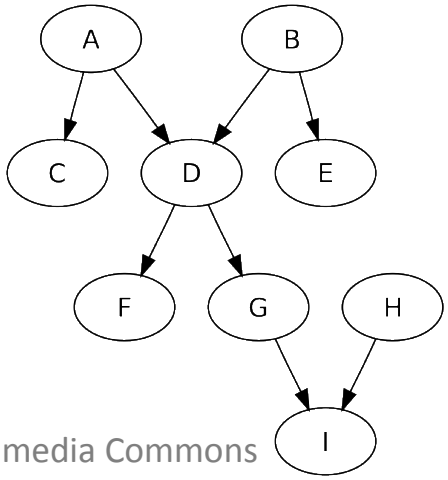
```
JOB A A.sub
JOB B1 B1.sub
JOB B2 B2.sub
JOB B3 B3.sub
JOB C C.sub
PARENT A CHILD B1 B2 B3
PARENT B1 B2 B3 CHILD C
```

(dag_dir)/

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

- Node name and submit filename do not have to match.
- Submit files expected in location *relative* to the submission of the DAG.

Endless Workflow Possibilities



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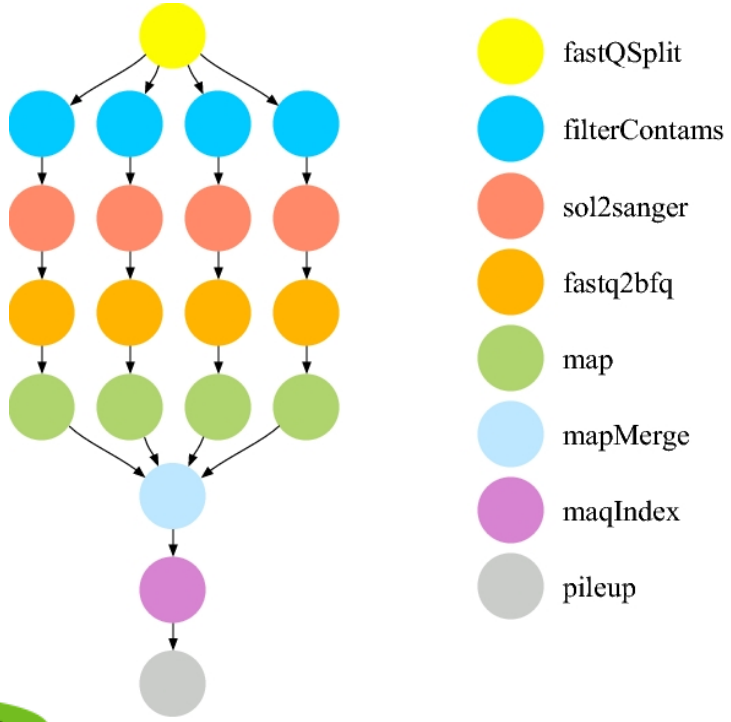
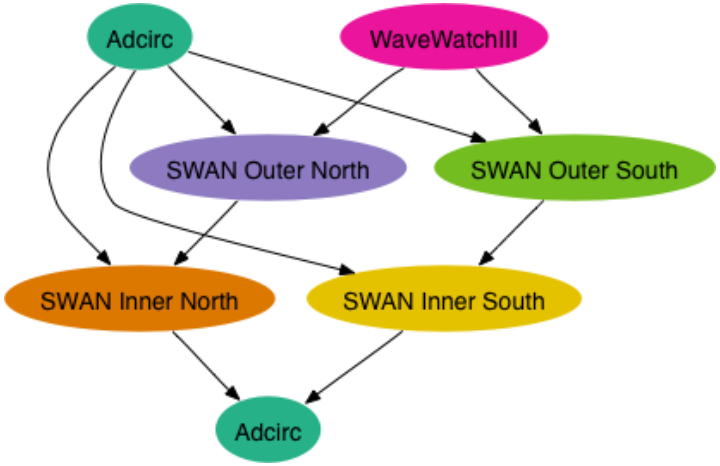
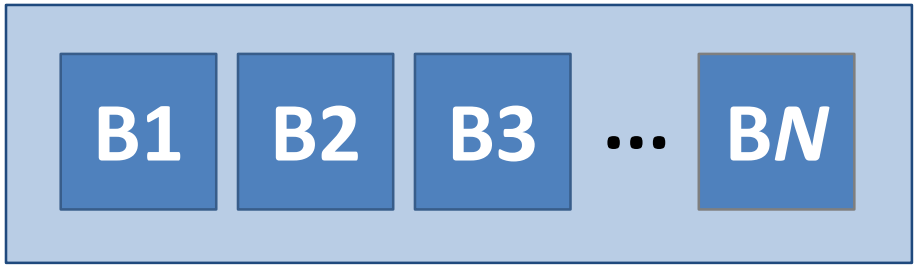




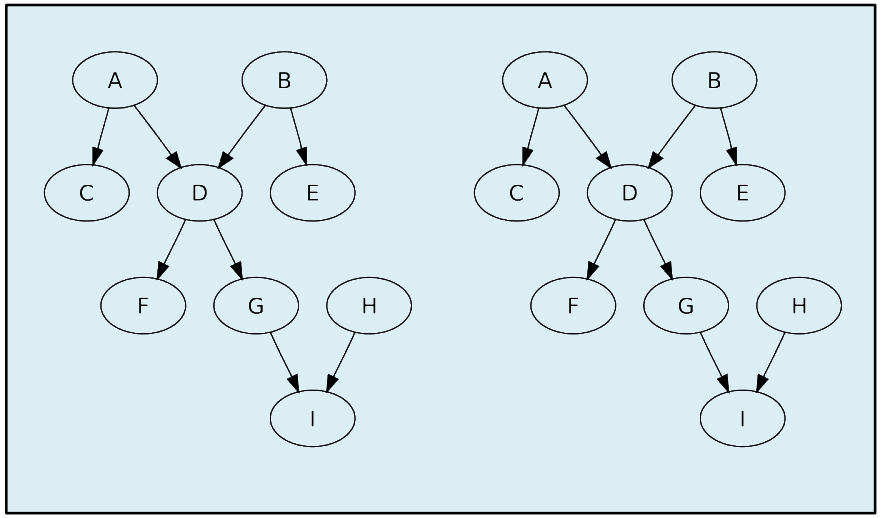
https://confluence.pegasus.isi.edu/display/pegasus/WorkflowGenerator

DAGs are also useful for non-sequential work

‘bag’ of HTC jobs



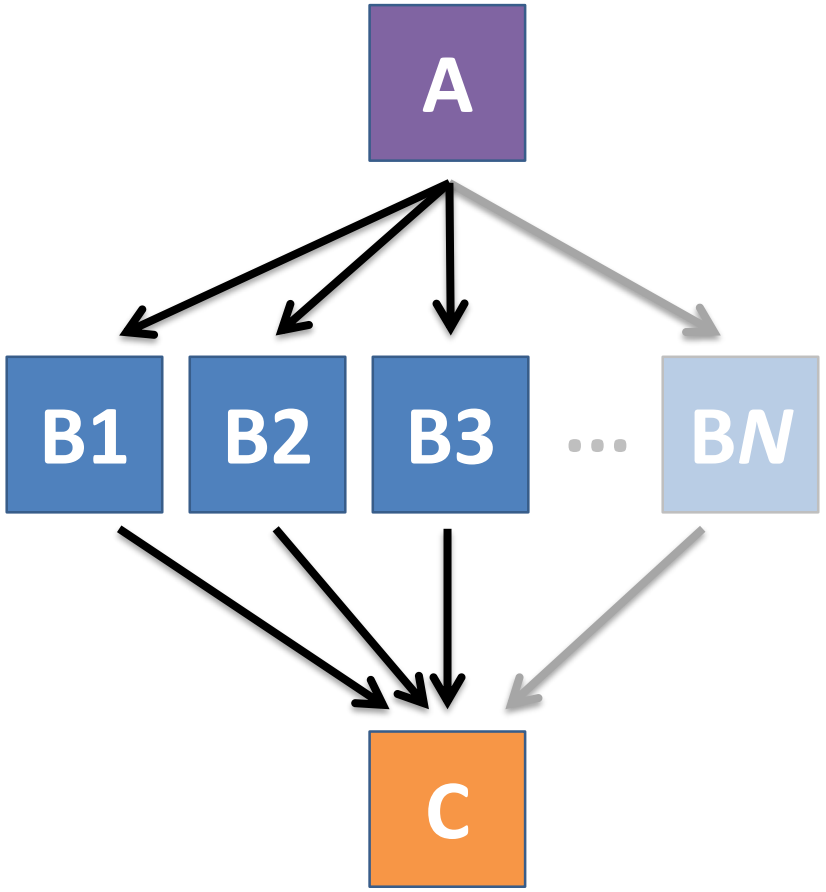
disjointed workflows



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
```



HTCondor Manual: DAGMan Applications > DAG Input File

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

DAGMan > DAG Monitoring and DAG Removal

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)

DAGMan > DAG Monitoring and DAG Removal

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
```

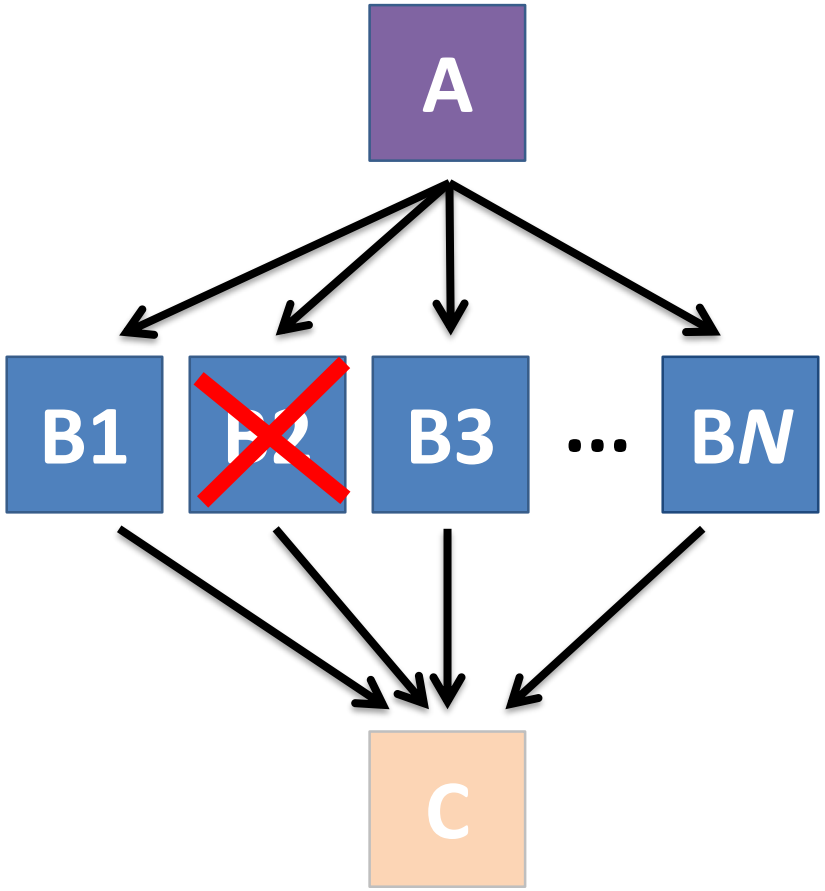
- Creates a **rescue file** so that only incomplete or unsuccessful NODES are repeated upon resubmission

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**

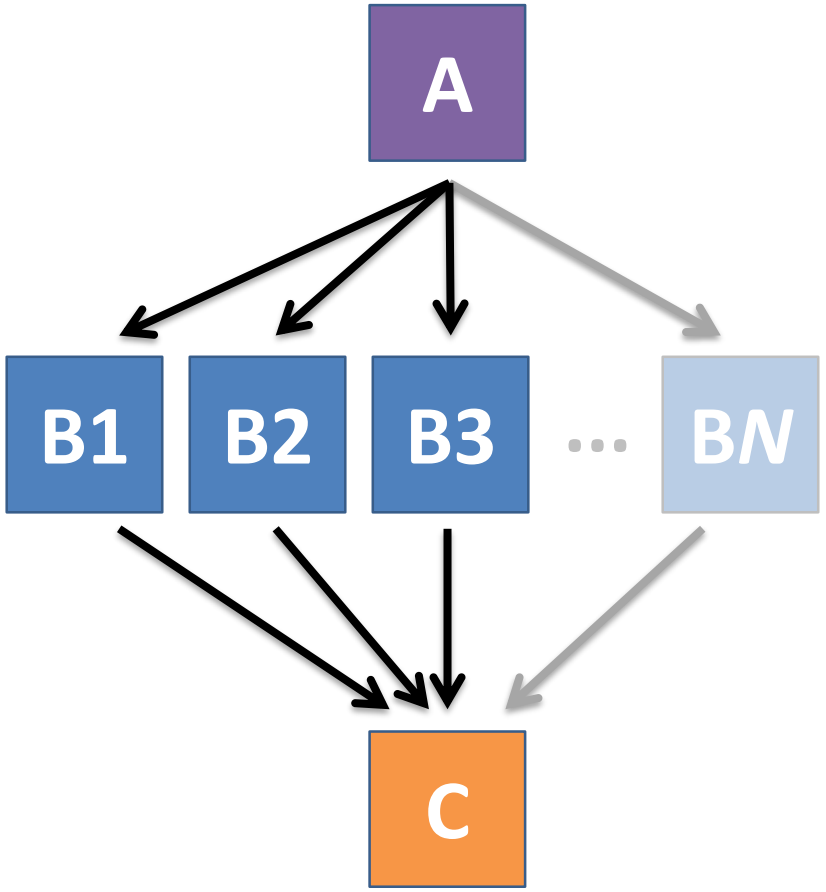


DAGMan > DAG Monitoring and DAG Removal

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.



HTCondor Manual: DAGMan Applications > DAG Input 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?

HTCondor Manual: DAGMan Applications > File Paths in DAGs

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)/

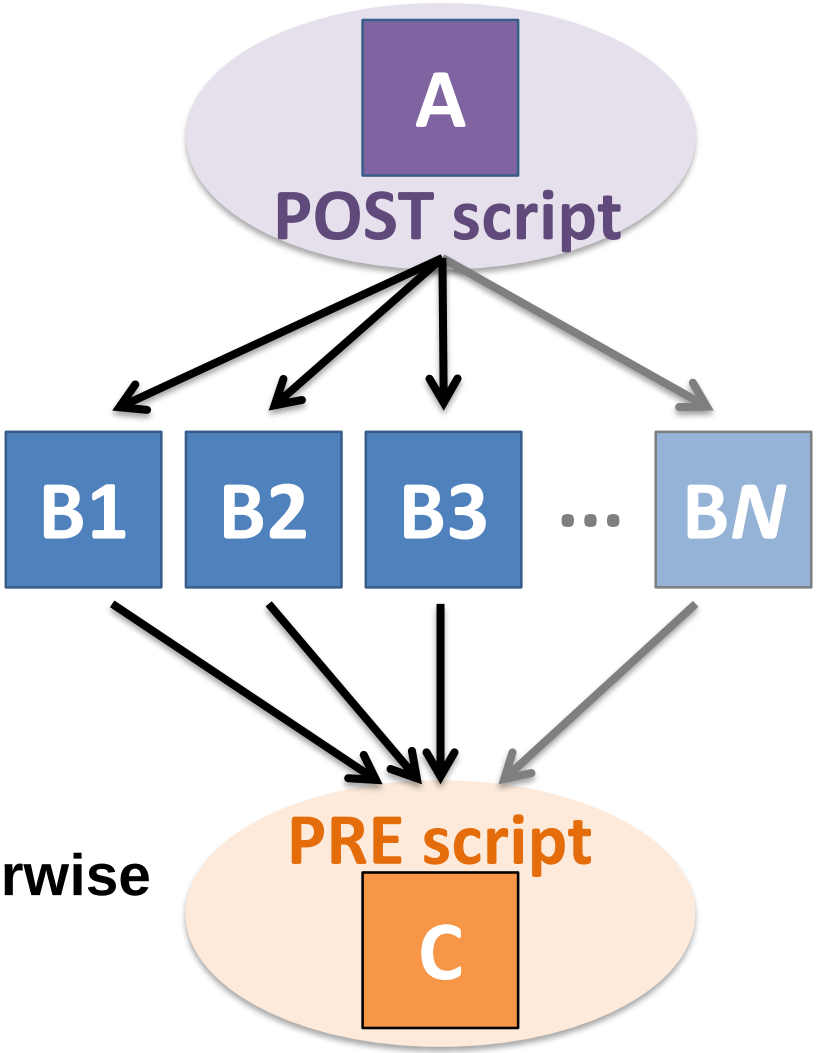
```
my.dag
A/  A.sub    (A job files)
B/  B1.sub   B2.sub
    B3.sub   (B job files)
C/  C.sub    (C job files)
```


HTCondor Manual: DAGMan Applications > DAG Input File

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
```

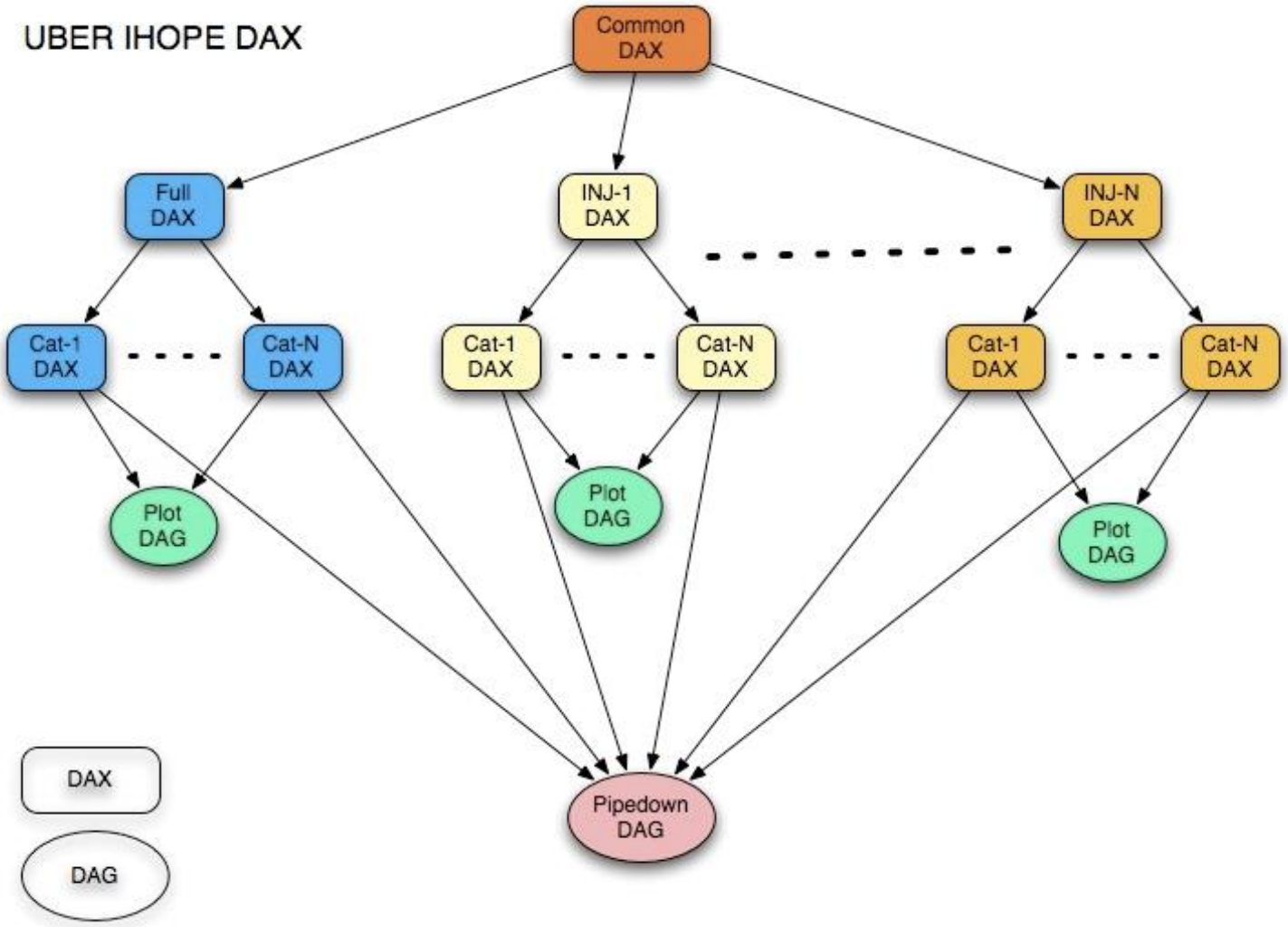


- **Use sparingly for light work; otherwise include work in submitted jobs**

DAGMan Applications > DAG Input File > SCRIPT

Modular Organization and Control of DAG Components

Repeating DAG Components!!



https://confluence.pegasus.isi.edu/display/pegasus/LIGO+IHOPE

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
```

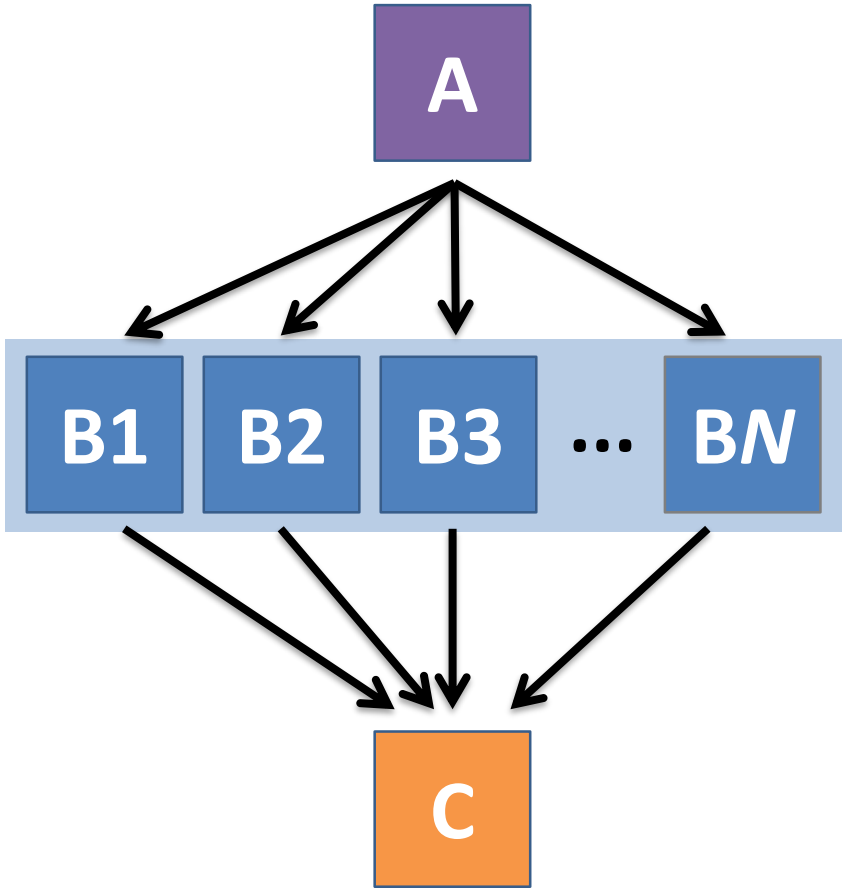
SPLICE subsets of the DAG to simplify lengthy DAG files

my.dag

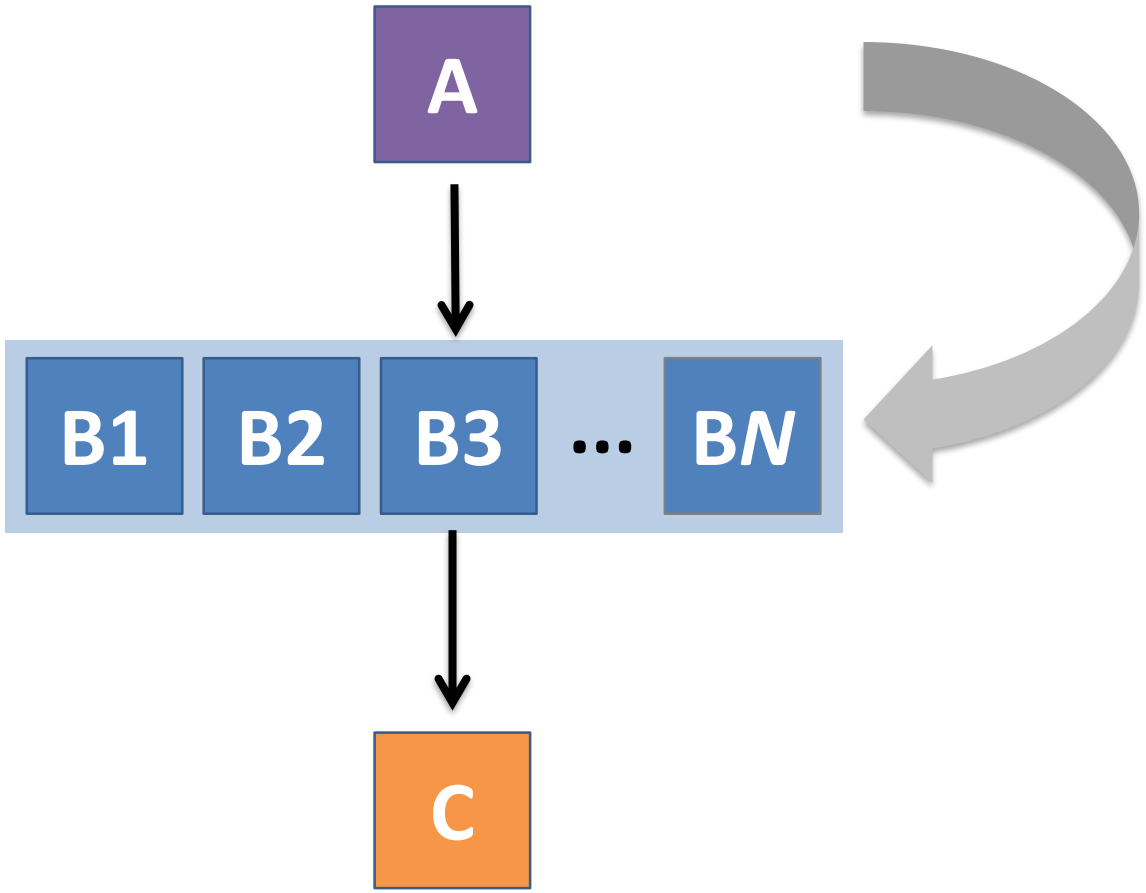
```
JOB A A.sub
SPLICE B B.spl
JOB C C.sub
PARENT A CHILD B
PARENT B CHILD C
```

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) …

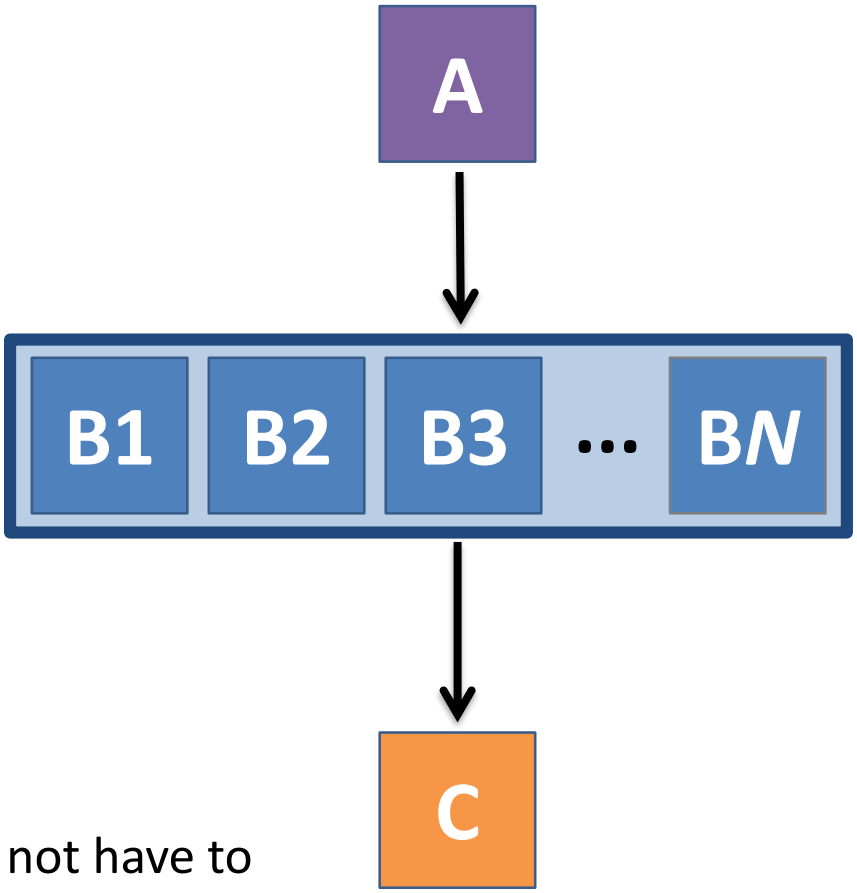
A SUBDAG within a DAG

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.

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

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

QUESTIONS?

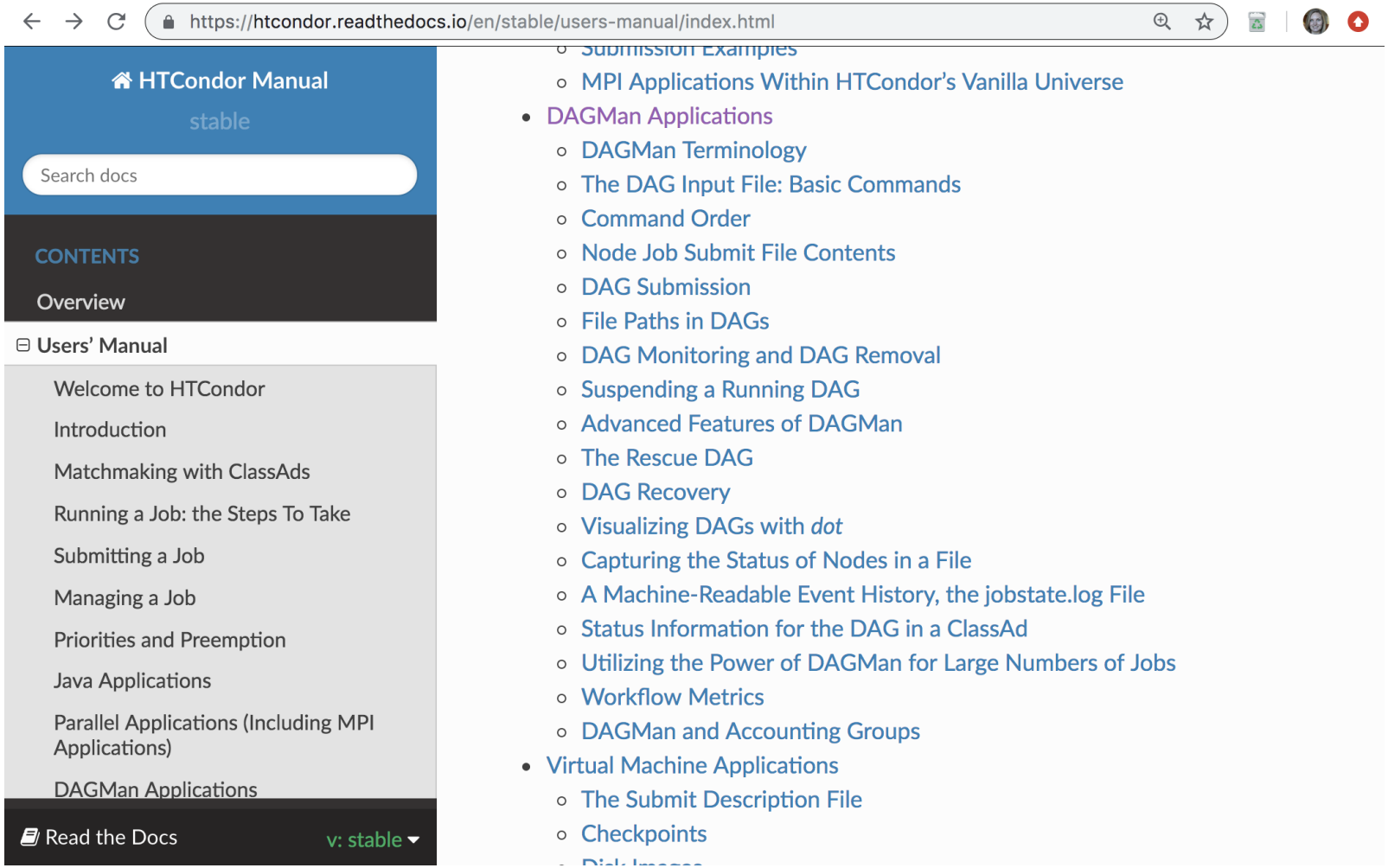
htcondor-users@cs.wisc.edu

lmichael@wisc.edu

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**

HTCondor has a *DAG Manager* (DAGMan)!



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

Beyond the Basic DAG: Node-level Modifiers

RETRY failed nodes to overcome transient errors

- Retry (or iterate!) 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 is preferable for simple cases

DAGMan Applications > Advanced Features > Retrying

DAGMan Applications > DAG Input File > SCRIPT

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

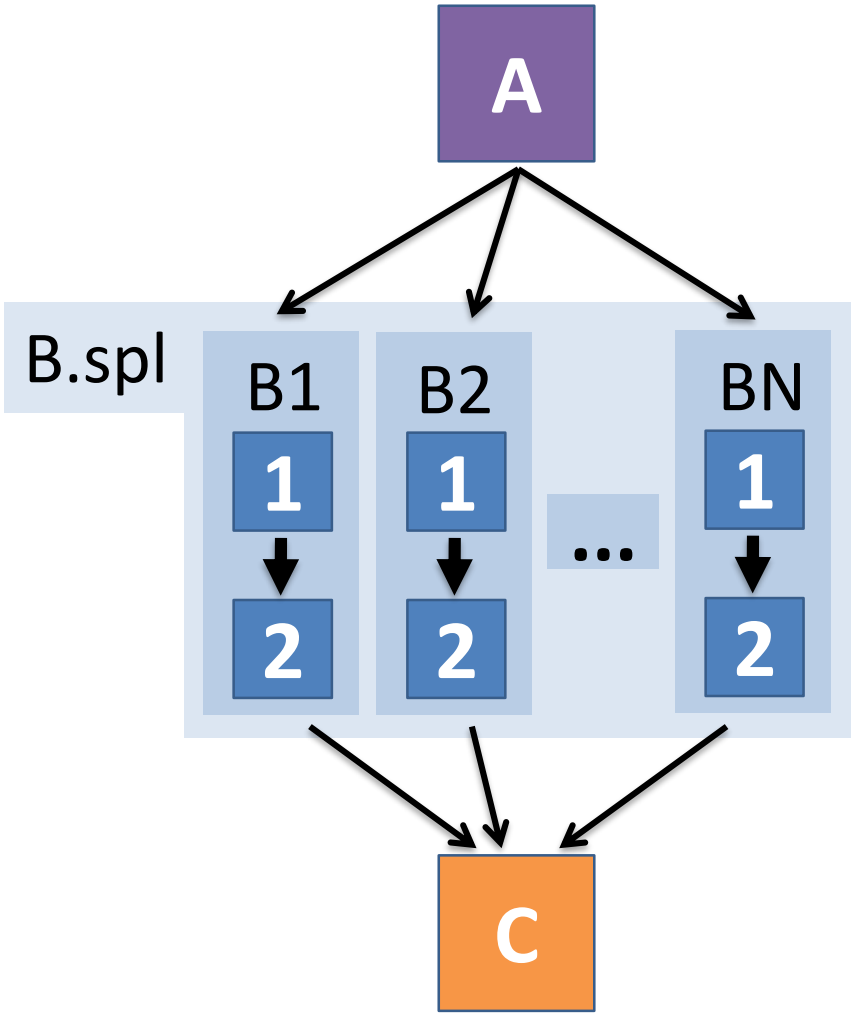
```
JOB A A.sub DIR A
SPLICE B B.spl DIR B
JOB C C.sub DIR C
PARENT A CHILD B
PARENT B CHILD C
```

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).
- SPLICEs are not treated like nodes.
  - no PRE/POST scripts or RETRIES

More on SUBDAG Behavior

- Yes, you can have DAGs of DAGs of DAGs, but …
- **Each SUBDAG EXTERNAL is a DAGMan job** running *on the submit host*, and too many can overwhelm the queue or node resources.
  - **WARNING:** SUBDAGs should only be used when absolutely necessary! (consider SPLICEs first)

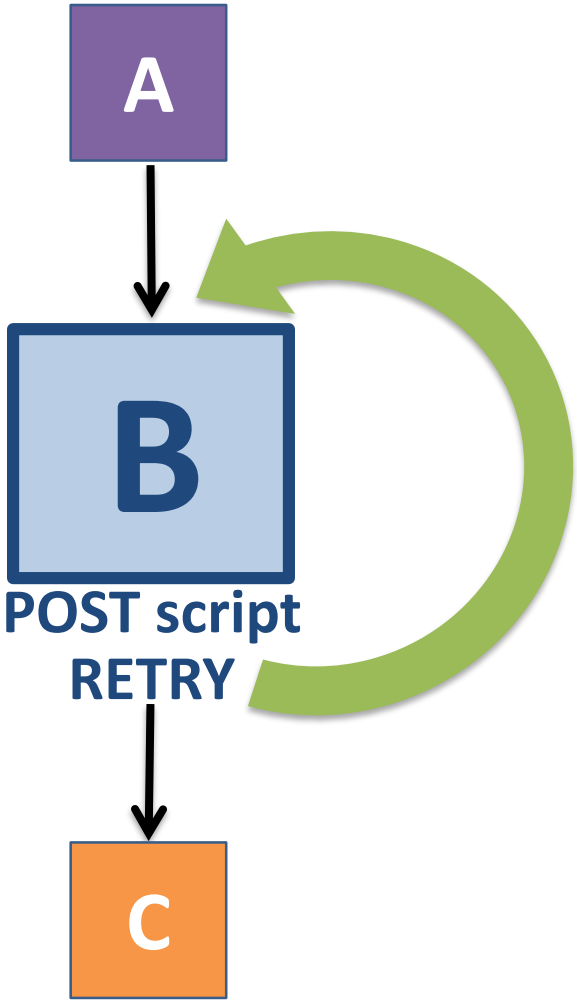
- **SUBDAGs *<u>are nodes</u>*** within the outer DAG (can have PRE/POST scripts, retries, etc.)

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

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
```



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

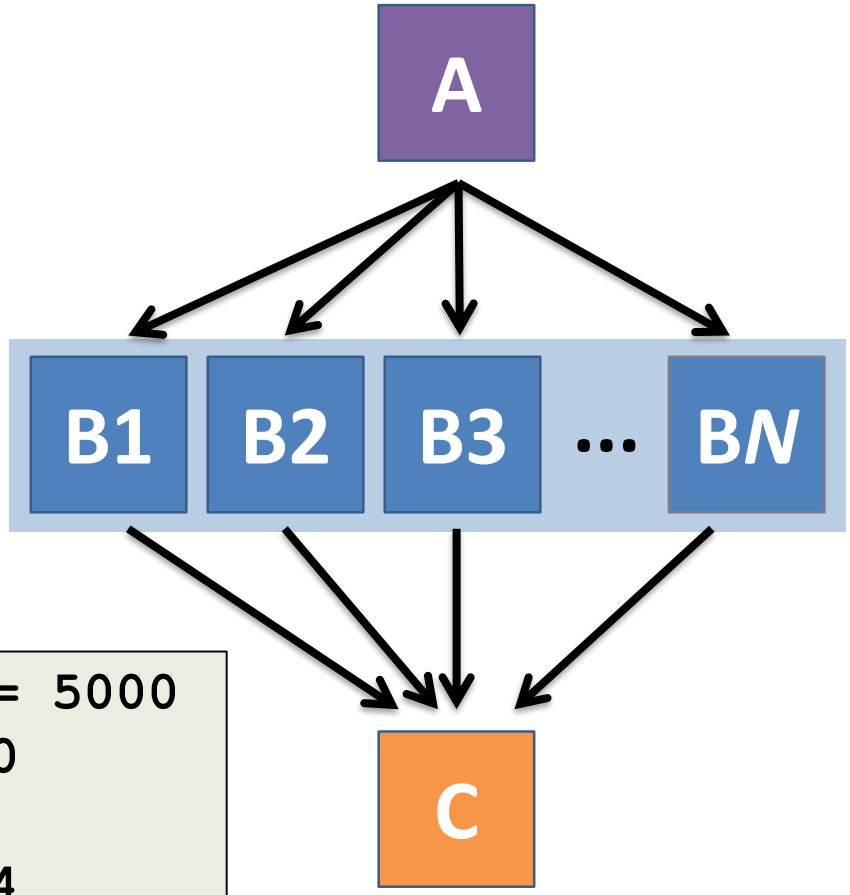
- **If a DAG has *many* (thousands or more) jobs**, submit server and queue performance can be assured by limiting:
  - Number of jobs in the queue
  - Number of jobs idle (waiting to run)
  - Number of PRE or POST scripts running
- Limits can be specified in a DAG-specific **CONFIG** file (recommended)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

DAGMan > Advanced Features > Configuration Specific to a 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
```


DAGMan > Advanced Features > Configuration Specific to a DAG

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