Workflows

Rob Quick <rquick@iu.edu>
Chief Operations Officer - Open Science Grid
Manager High Throughput Computing

Some Slides Contributed by the University of Wisconsin HTCondor Team and Scot Kronenfeld

Before we begin…

- Any questions on the lectures or exercises up to this point?

Remember

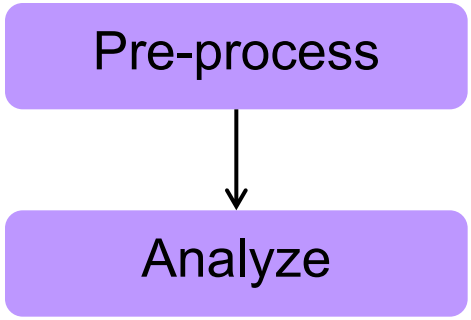
- All materials are available from: https://opensciencegrid.github.io/dosar/Materials/TriesteMaterials/

Workflows

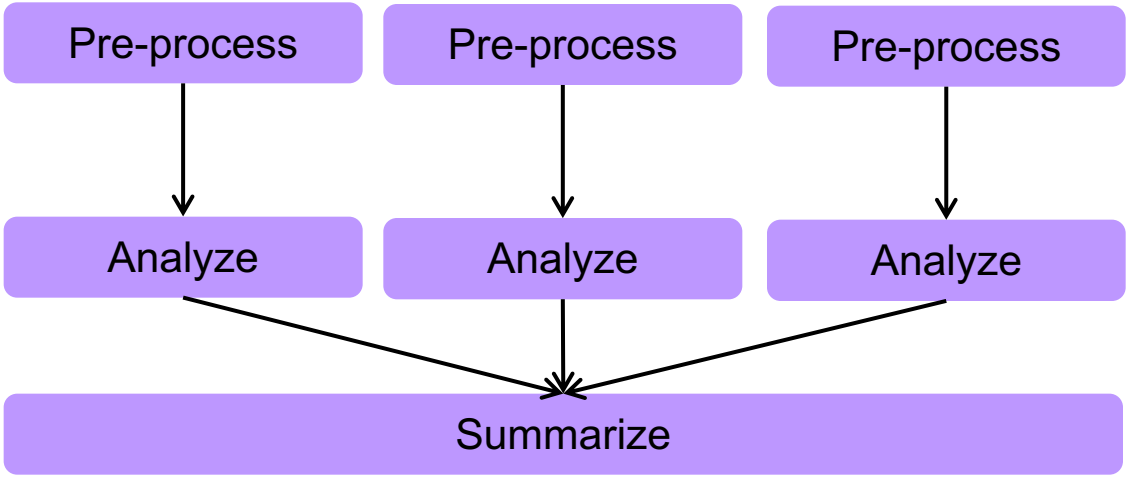
- What if you have a complex set of programs to run for your science?
- For example:
  - You want to analyze a set of images
  - Each image needs to be pre-processed
  - Each image needs to be analyzed
  - You need to summarize the results of all the analyses
  - Each of these is done with a separate application

Workflows

One Image:



Three Images:



Workflows: definition

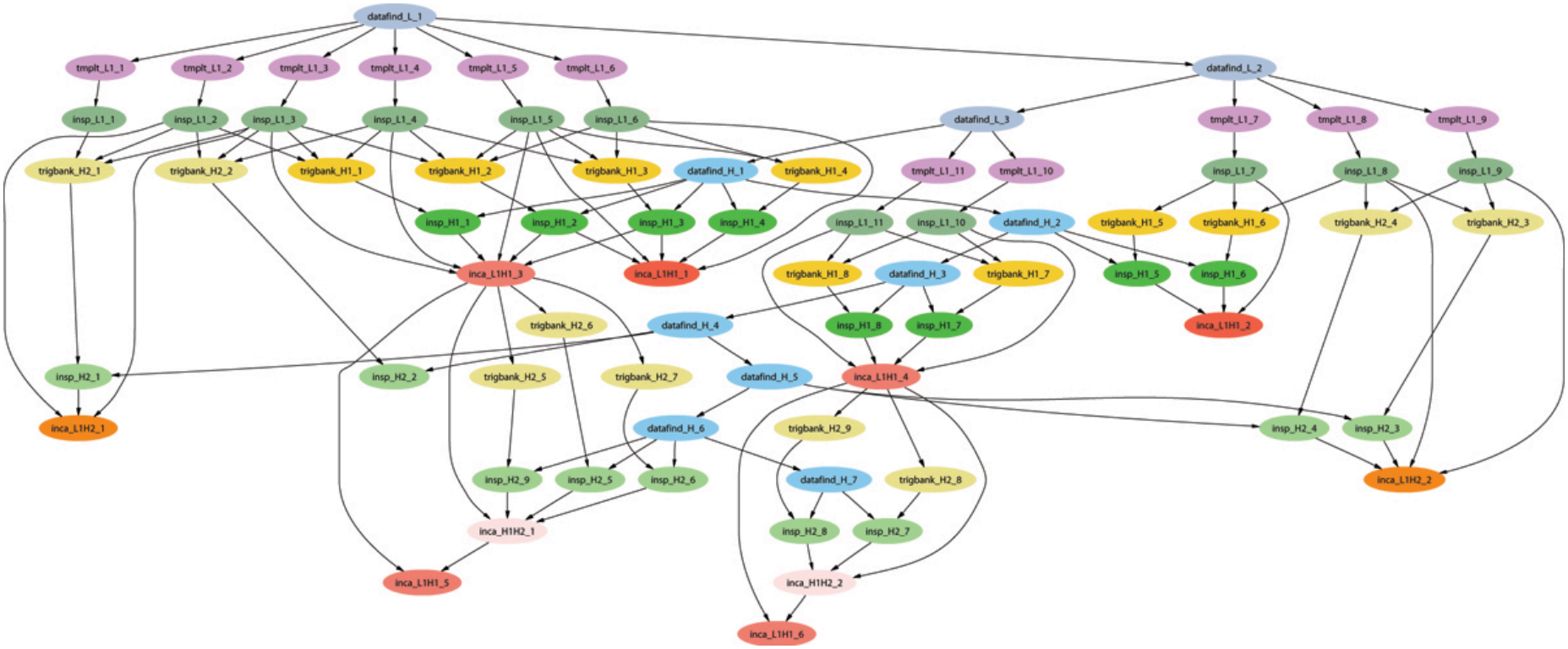
Definition 1:
A set of steps to complete a complex task

Definition 2:
A graph of jobs to run: some jobs need to run before others while other jobs can run in parallel

LIGO

LSC

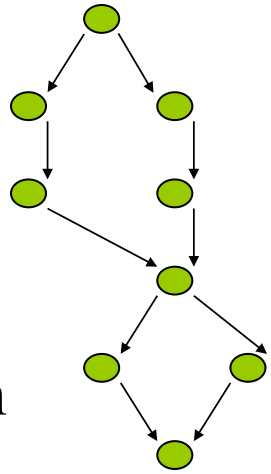
Example of a LIGO Inspiral DAG



INDIANA UNIVERSITY

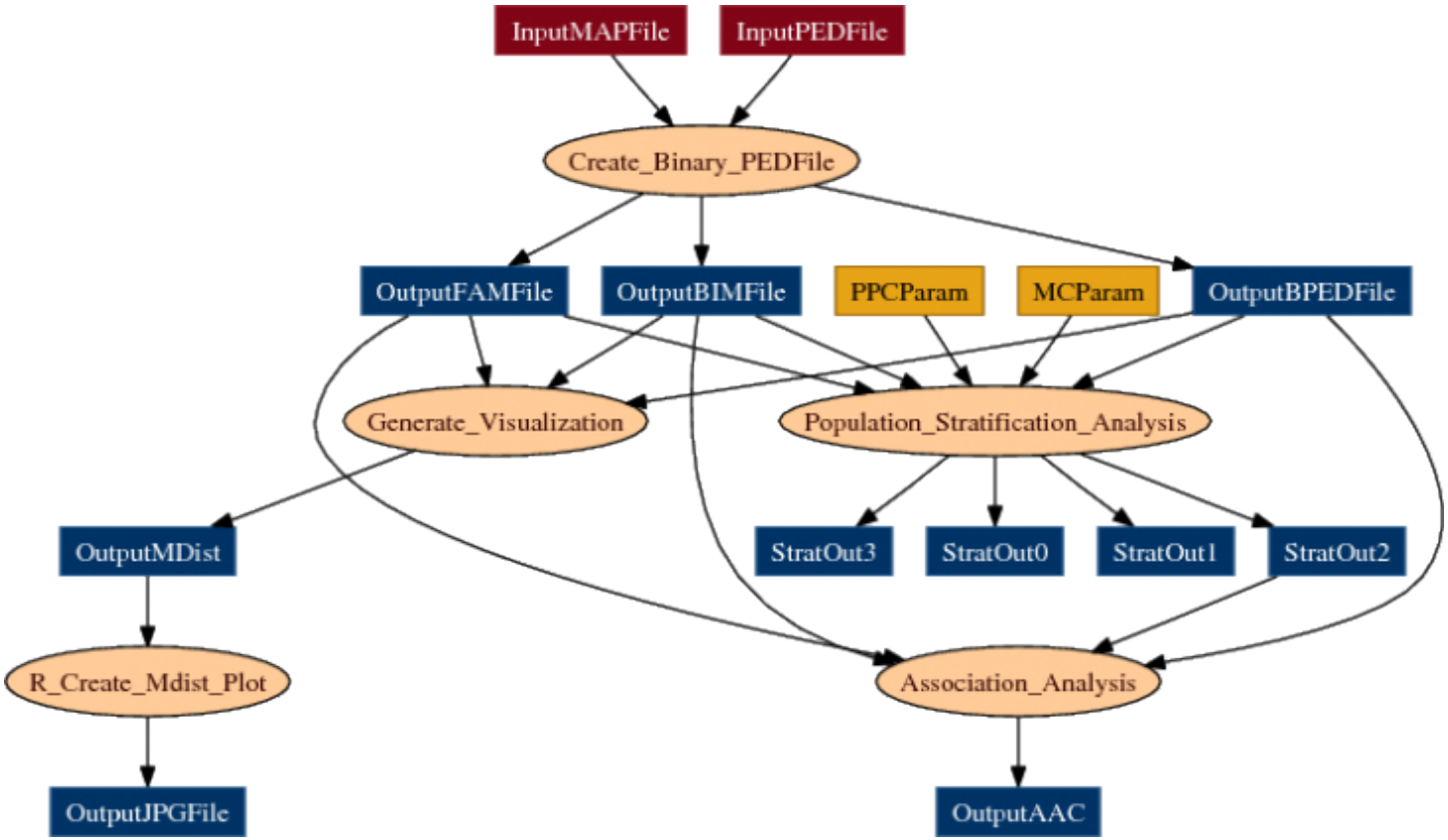
Use of Condor by the LIGO Scientific Collaboration

- Condor handles 10's of millions of jobs per year running on the LDG, and up to 500k jobs per DAG.
- Condor standard universe check pointing widely used, saving us from having to manage this.
- At Caltech, 30 million jobs processed using 22.8 million CPU hrs. on 1324 CPUs in last 30 months.
- For example, to search 1 yr. of data for GWs from the inspiral of binary neutron star and black hole systems takes ~2 million jobs, and months to run on several thousand ~2.6 GHz nodes.



(Statement from 2010—"last 30 months" isn't from now. Also, I think they do up to 1 million jobs per DAG now.)

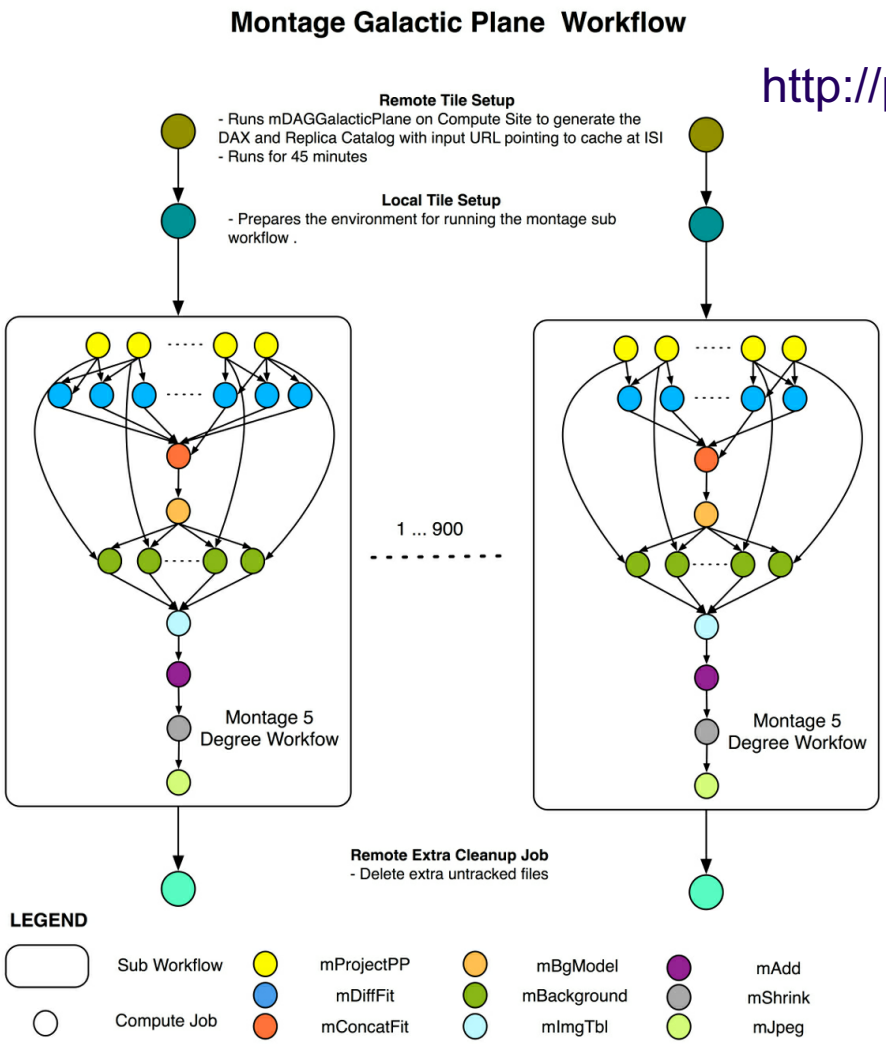
Example workflow: Bioinformatics



From Mason, Sanders, State (Yale)

http://pegasus.isi.edu/applications/association_test

Example workflow: Astronomy



From Berriman & Good (JPAC)

http://pegasus.isi.edu/applications/galactic-plane

DAGMan

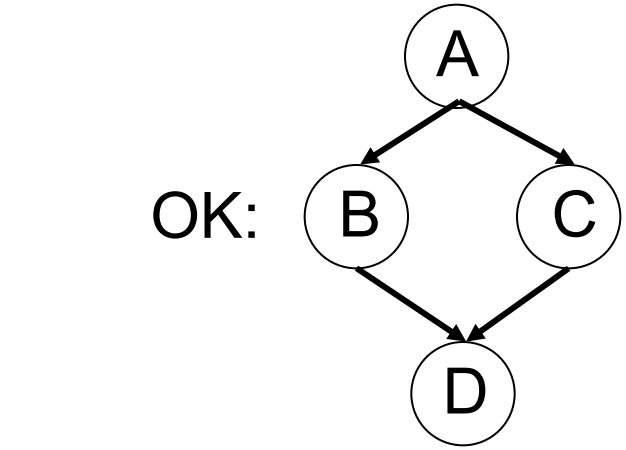
- DAGMan:
  - Directed Acyclic Graph (DAG)
  - Manager (Man)
- Allows you to specify the dependencies between your jobs
- Manages the jobs and their dependencies

- That is, it manages a workflow of jobs

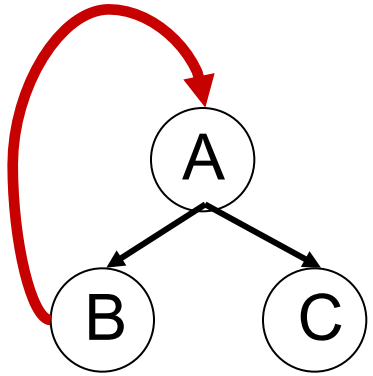
What is a DAG?

- A DAG is the structure used by DAGMan to represent these dependencies.
- Each job is a node in the DAG.
- Each node can have any number of "parent" or "children" nodes – as long as there are no loops!

OK:



Not OK:

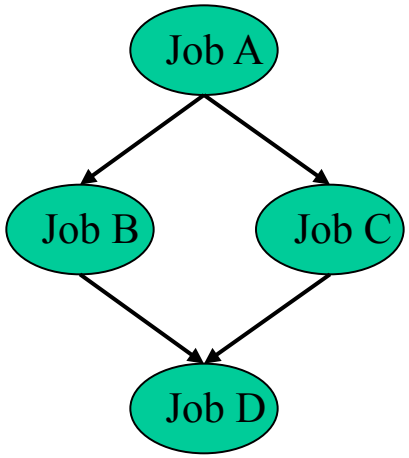


Defining a DAG

- A DAG is defined by a *.dag file*, listing each of its nodes and their dependencies. For example:

```
Job A a.sub
Job B b.sub
Job C c.sub
Job D d.sub

Parent A Child B C
Parent B C Child D
```



DAG Files….

- This complete DAG has five files

One DAG File:

```
Job A a.sub
Job B b.sub
Job C c.sub
Job D d.sub

Parent A Child B C
Parent B C Child D
```

Four Submit Files:

```
Universe = Vanilla
Executable = analysis…
```

```
Universe = …
```

Submitting a DAG

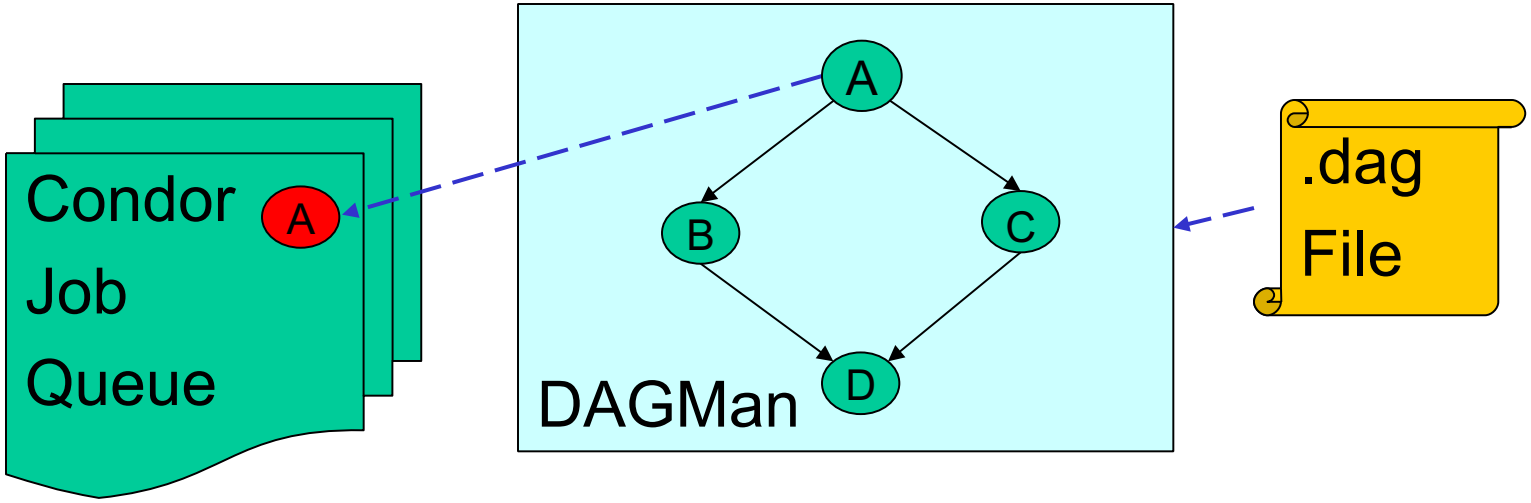
- To start your DAG, just run **`condor_submit_dag`** with your .dag file, and Condor will start a DAGMan process to manage your jobs:

```
% condor_submit_dag diamond.dag
```

- condor_submit_dag submits a Scheduler Universe job with DAGMan as the executable
- Thus the DAGMan daemon itself runs as a Condor job, so you don't have to baby-sit it

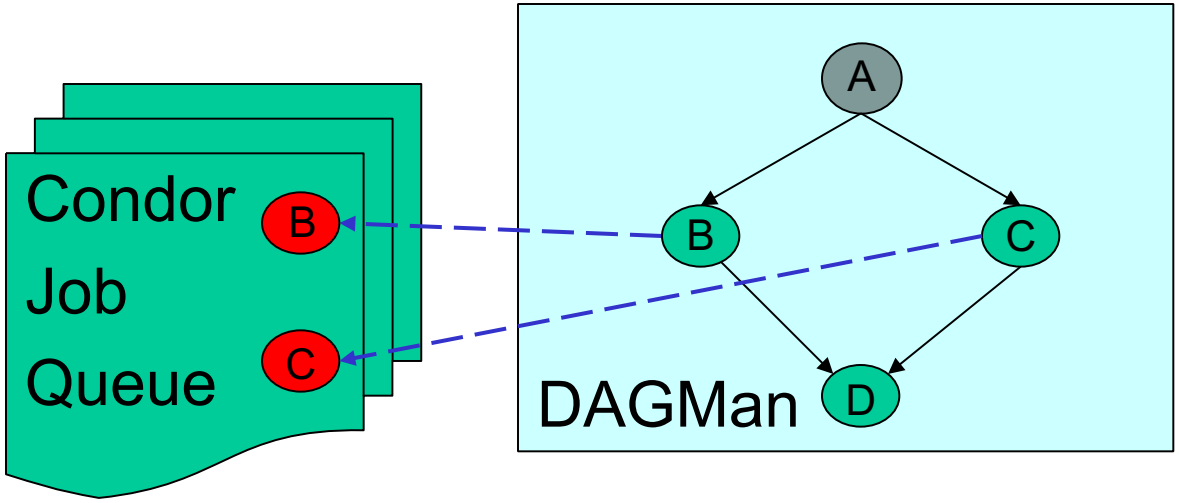
Running a DAG

- DAGMan acts as a scheduler, managing the submission of your jobs to Condor based on the DAG dependencies



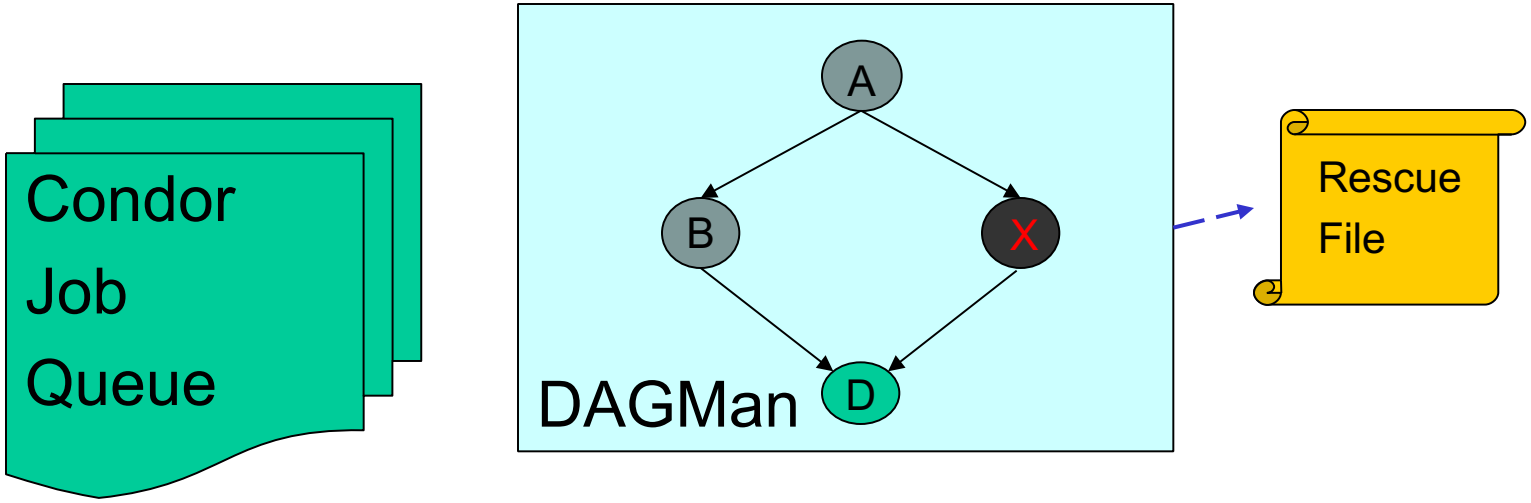
Running a DAG (cont'd)

- DAGMan submits jobs to Condor at the appropriate times
- For example, after A finishes, it submits B & C



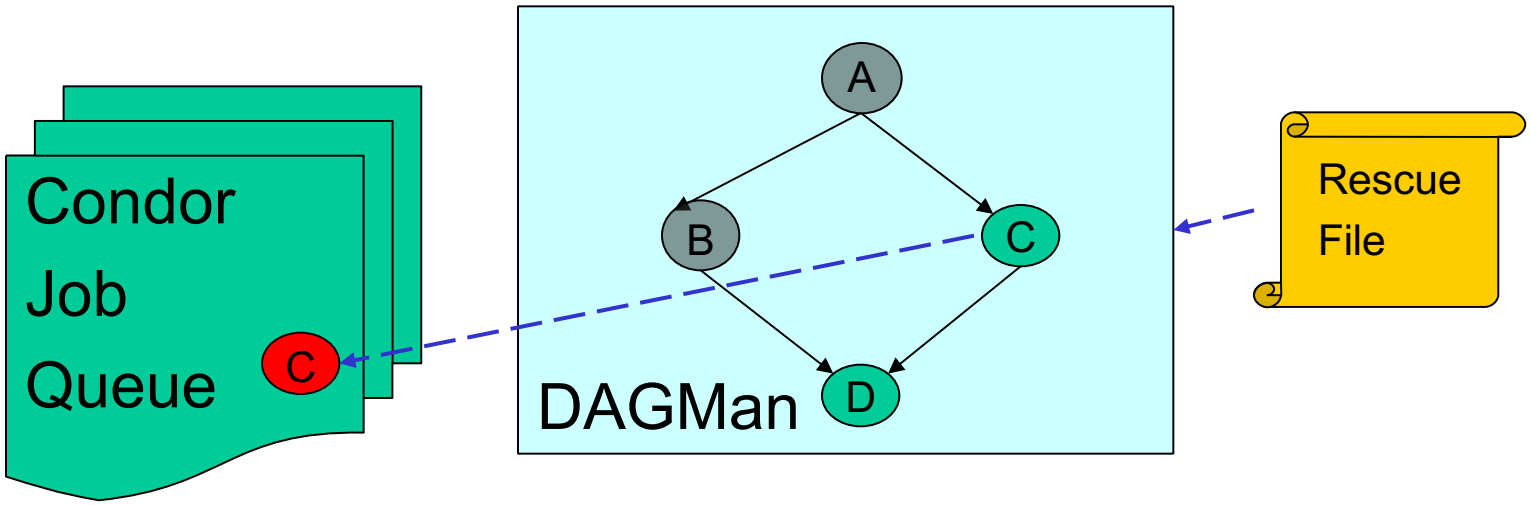
Running a DAG (cont'd)

- A job *fails* if it exits with a non-zero exit code
- In case of a job failure, DAGMan runs other jobs until it can no longer make progress, and then creates a *"rescue" file* with the current state of the DAG



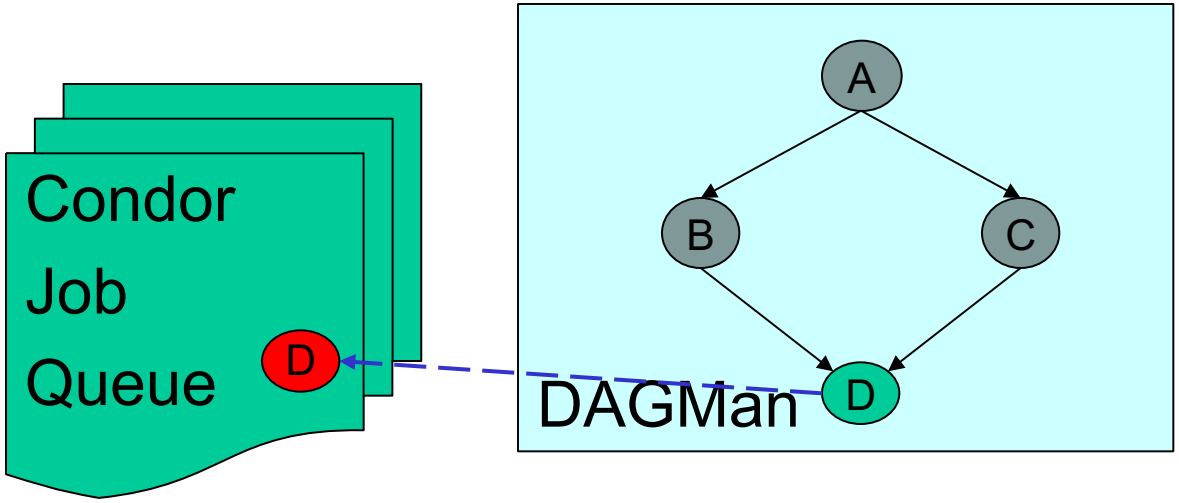
Recovering a DAG

- Once the failed job is ready to be re-run, the rescue file can be used to restore the prior state of the DAG
  - Another example of reliability for HTC!



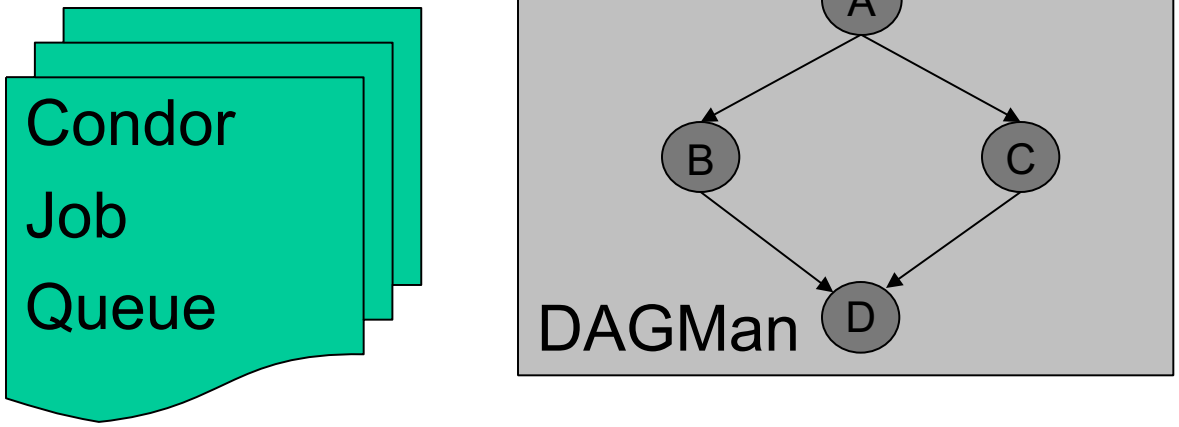
Recovering a DAG (cont'd)

- Once that job completes, DAGMan will continue the DAG as if the failure never happened



Finishing a DAG

- Once the DAG is complete, the DAGMan job itself is finished, and exits



DAGMan & Fancy Features

- DAGMan doesn't have a lot of "fancy features"
  - No loops
  - Not much assistance in writing very large DAGs (script it yourself)
- Focus is on solid core
  - Add the features people need in order to run large DAGs well
  - People build systems on top of DAGMan

Related Software

Pegasus: http://pegasus.isi.edu/

- Writes DAGs based on abstract description
- Runs DAG on appropriate resource (Condor, OSG, EC2…)
- Locates data, coordinates execution
- Uses DAGMan, works with large workflows

Makeflow: http://nd.edu/~ccl/software/makeflow/

- User writes *make* file, not DAG
- Works with Condor, SGE, Work Queue…
- Handles data transfers to remote systems
- Does not use DAGMan

DAGMan: Reliability

- For each job, Condor generates a log file
- DAGMan reads this log to see what has happened
- If DAGMan dies (crash, power failure, etc…)
  - Condor will restart DAGMan
  - DAGMan re-reads log file
  - DAGMan knows everything it needs to know
  - Principle: DAGMan can recover state from files and without relying on a service (Condor queue, database…)
- Recall: HTC requires reliability!

Advanced DAGMan Tricks

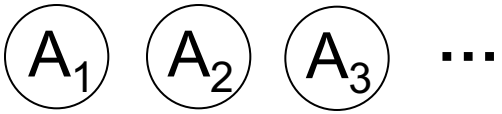
- Throttles
- DAGs without dependencies
- Sub-DAGs
- Pre and Post scripts: editing your DAG

Throttles

- Failed nodes can be automatically retried a configurable number of times
  - Helps recover from jobs that crash some percentage of the time
- Throttles to control job submissions
  - Max jobs submitted
  - Max scripts running
  - These are important when working with large DAGs

DAGs without dependencies

- Submit DAG with:
  - 200,000 nodes
  - No dependencies

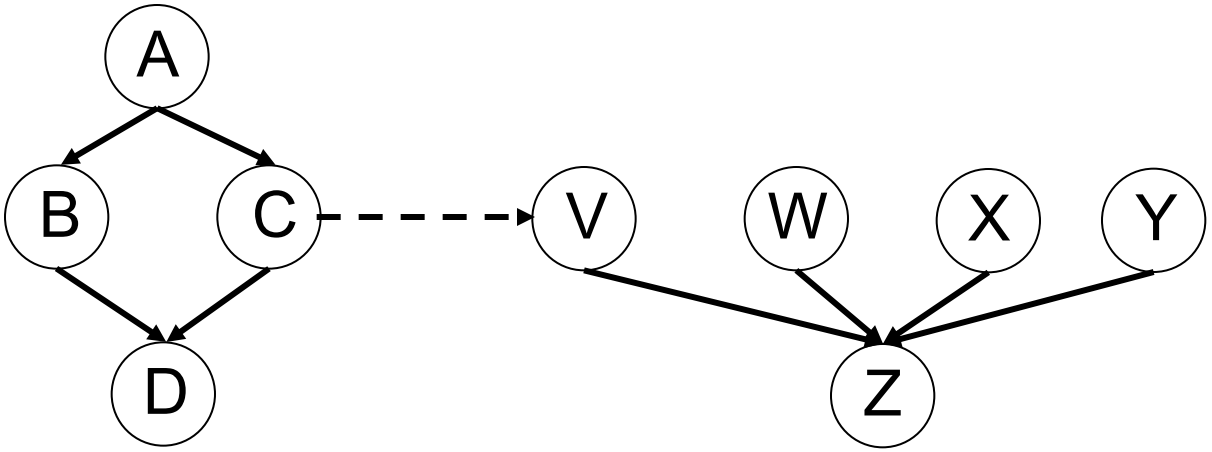


- Use DAGMan to throttle the job submissions:
  - Condor is scalable, but it will have problems if you submit 200,000 jobs simultaneously
  - DAGMan can help you with scalability even if you don't have dependencies

Sub-DAG

- Idea: any given DAG node can be another DAG
  - SUBDAG External Name DAG-file
- DAG node will not complete until sub-dag finishes
- Interesting idea: A previous node could *generate* this DAG node
- Why?
  - Simpler DAG structure
  - Implement a fixed-length loop
  - Modify behavior on the fly

Sub-DAG



DAGMan scripts

- DAGMan allows pre & post scripts
  - Run before (pre) or after (post) job
  - Run on the same computer you submitted from
  - Don't have to be scripts: any executable
- Syntax:

```
JOB A a.sub
SCRIPT PRE A before-script $JOB
SCRIPT POST A after-script $JOB $RETURN
```

So What?

- Pre script can make decisions
  - Where should my job run? (Particularly useful to make job run in same place as last job.)
  - What should my job do?
  - Generate Sub-DAG
- Post script can change return value
  - DAGMan decides job failed in non-zero return value
  - Post-script can look at {error code, output files, etc} and return zero or non-zero based on deeper knowledge.

Quick UNIX Refresher Before We Start

- `$`
- `nano, vi, emacs, cat >, etc.`
- `module, scp, cp, watch, cat, ls, rm`

Let's try it out!

- Exercises with DAGMan.

Questions?

- Questions? Comments?

- Feel free to ask me questions now or later:

  Rob Quick - rquick@iu.edu

Materials available from:
https://opensciencegrid.github.io/dosar/Materials/TriesteMaterials/