



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?







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

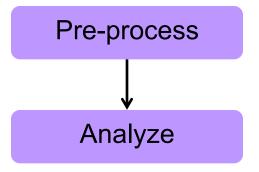




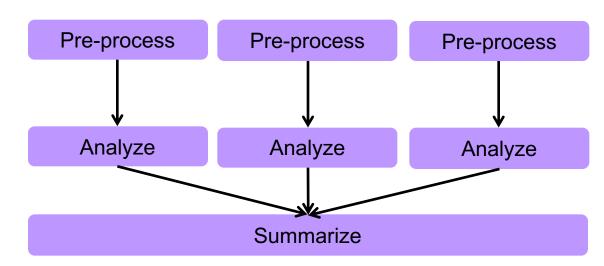
Workflows



One Image:



Three Images:







Workflows: definition



Definition 1:

A set of steps to complete a complex task

Definition 2:

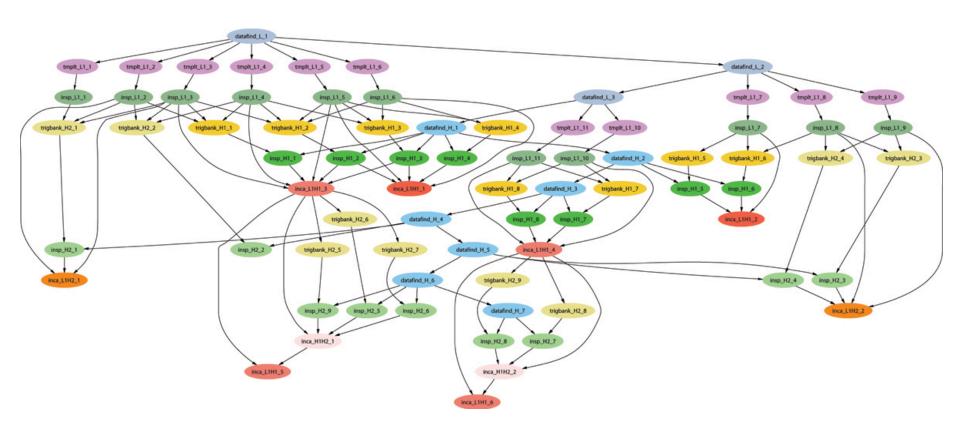
A graph of jobs to run: some jobs need to run before others while other jobs can run in parallel







Example of a LIGO Inspiral DAG





LIGO

Use of Condor by the LIGO Scientific Collaboration



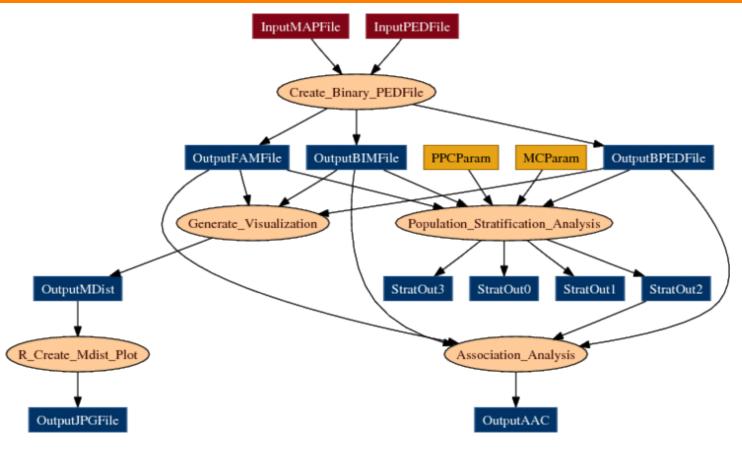
- Condor handles 10's of millions of jobs per year running on the LDG, and up to 500k jobs per DAG.
- Condor standard universe check pointing widely used, saving us from having to manage this.
- At Caltech, 30 million jobs processed using 22.8 million CPU hrs. on 1324 CPUs in last 30 months.
- For example, 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



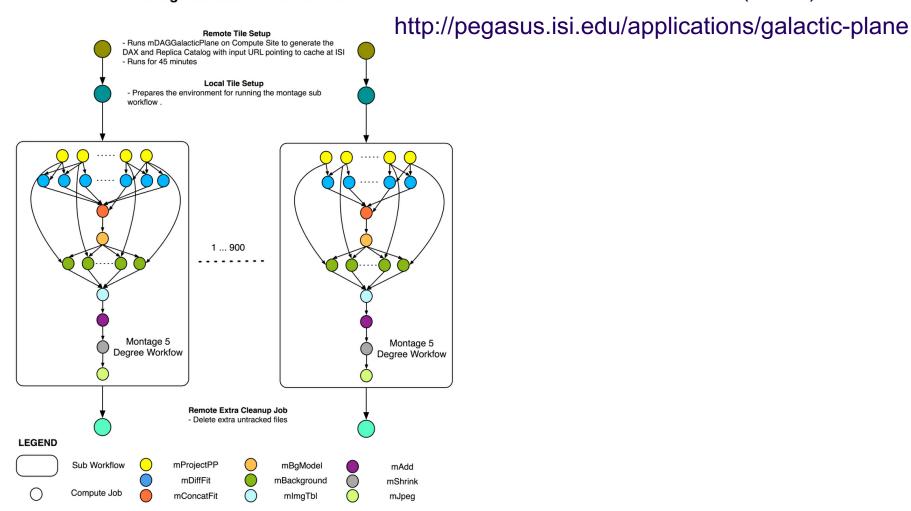


Example workflow: Astronomy



Montage Galactic Plane Workflow

From Berriman & Good (JPAC)





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

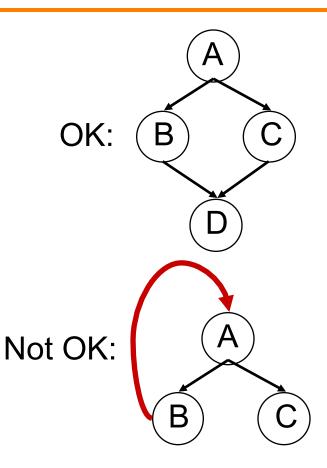




What is a DAG?



- 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!



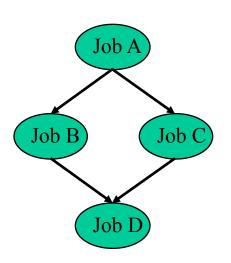




Defining a DAG



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







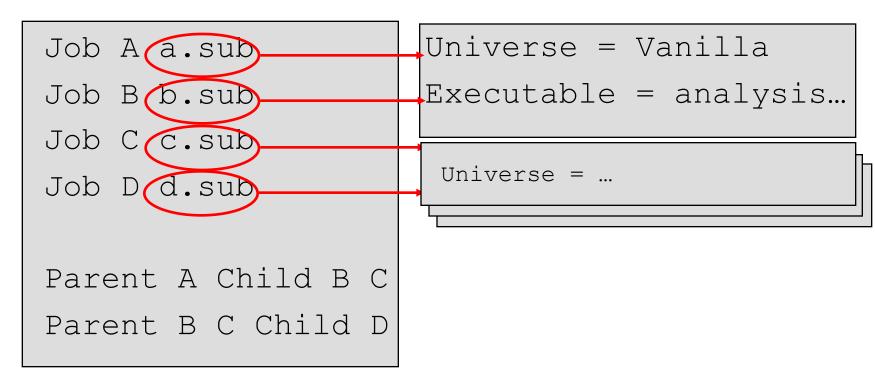
DAG Files....



This complete DAG has five files

One DAG File:

Four Submit Files:







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

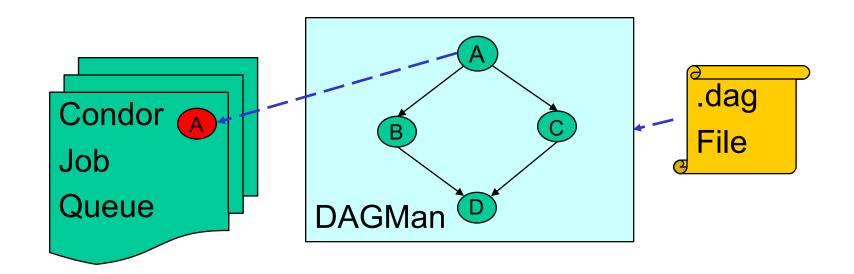




Running a DAG



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



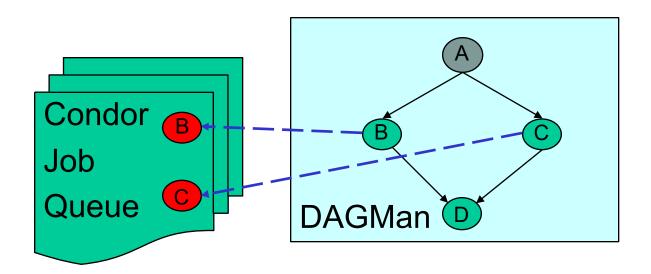




Running a DAG (cont'd)



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



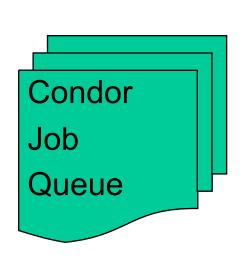


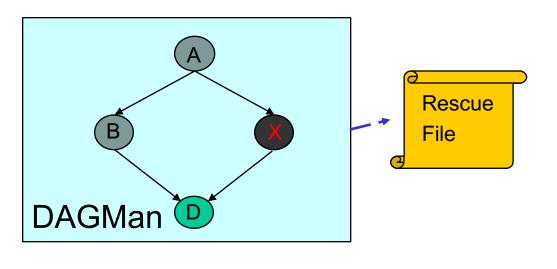


Running a DAG (cont'd)



- 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





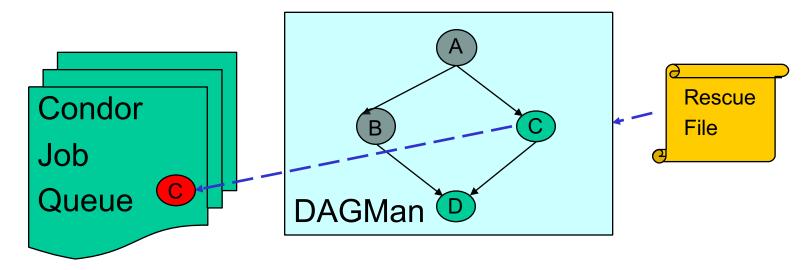




Recovering a DAG



- 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!



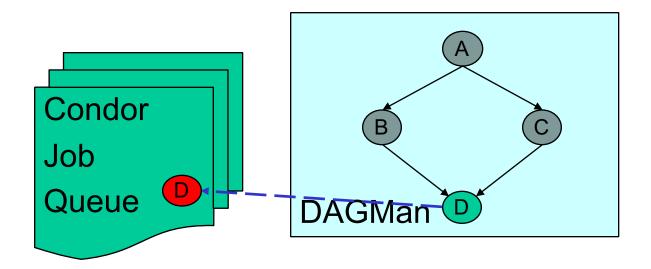




Recovering a DAG (cont'd)



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



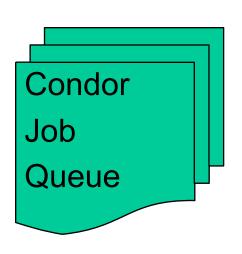


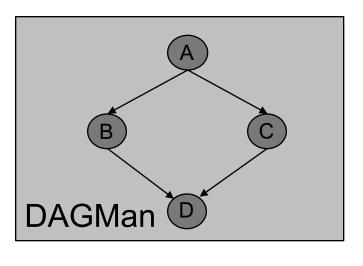


Finishing a DAG



 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



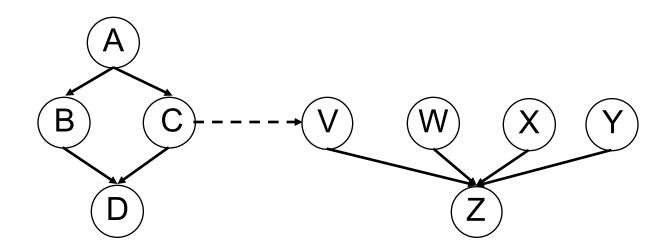
- Idea: any given DAG node can be another DAG
 - SUBDAG External Name DAG-file
- DAG node will not complete until sub-dag finishes
- Interesting idea: A previous node could generate this DAG node
- Why?
 - Simpler DAG structure
 - Implement a fixed-length loop
 - Modify behavior on the fly





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

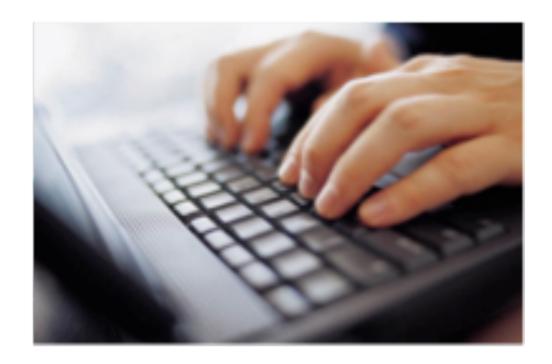




Let's try it out!



Exercises with DAGMan.







Questions?



Questions? Comments?

 Feel free to ask me questions now or later:

Rob Quick - rquick@iu.edu

