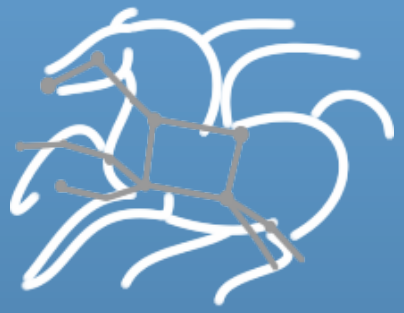


Scientific Workflows - How Pegasus can enhance your DAGMan experience

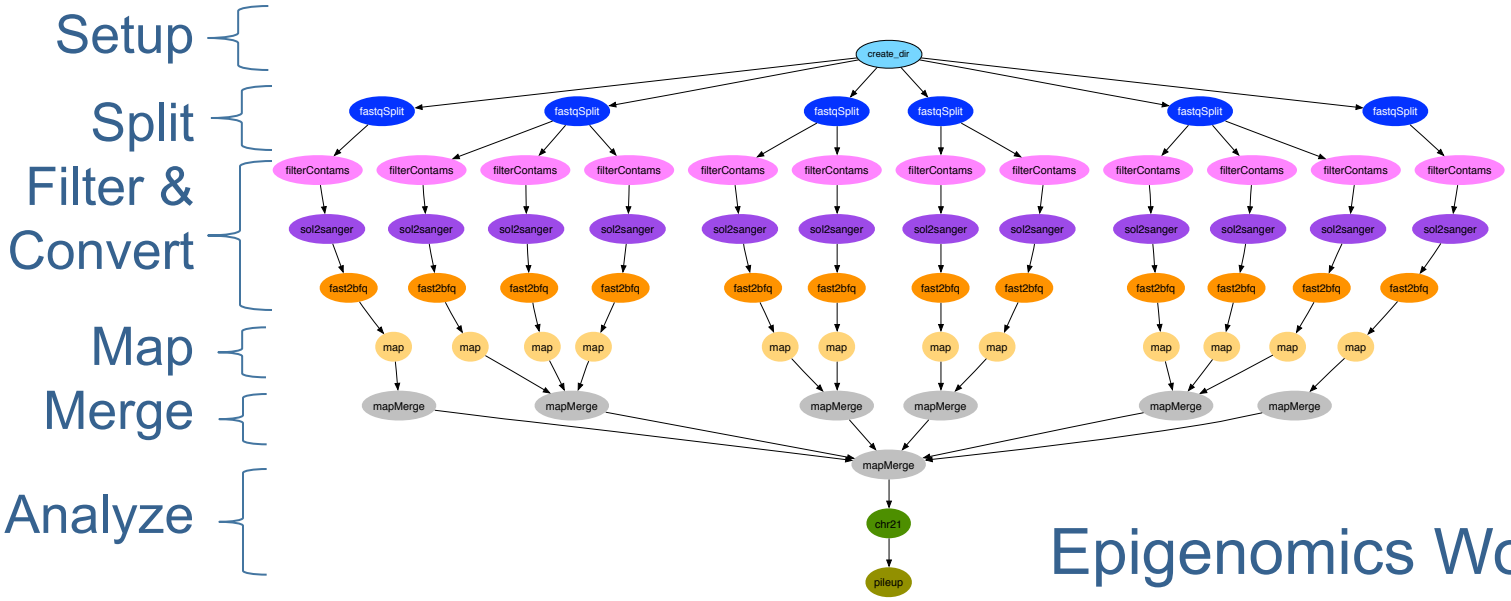
Karan Vahi

Science Automation Technologies Group

USC Information Sciences Institute

Scientific Workflows

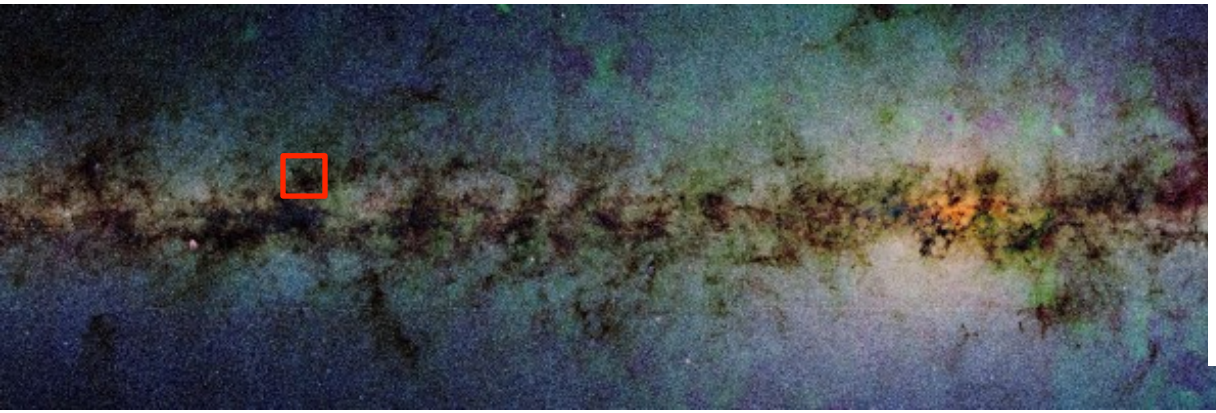
- Orchestrate complex, multi-stage scientific computations
- Often expressed as directed acyclic graphs (DAGs)
- Capture analysis pipelines for sharing and reuse
- Can execute in parallel on distributed resources

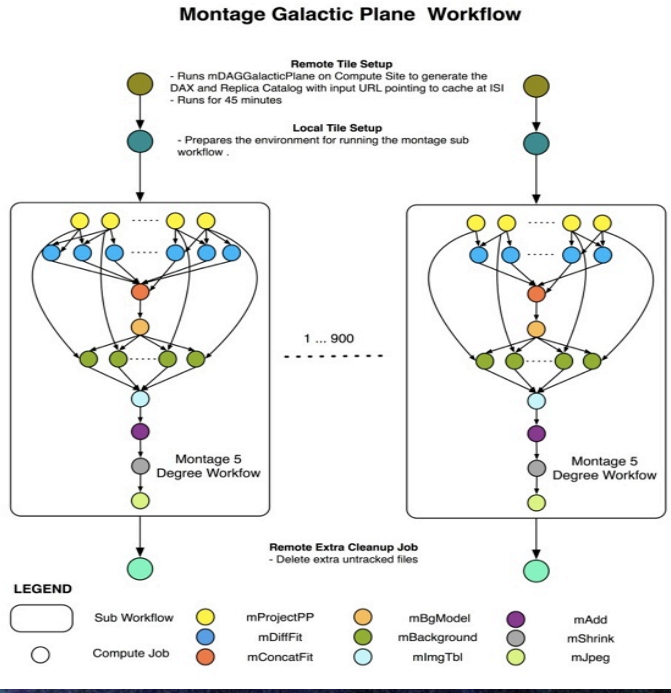


Epigenomics Workflow

Workflows can be simple

Some workflows are large-scale and data-intensive





John Good (Caltech)

- **Montage Galactic Plane Workflow**
  - 18 million input images (~2.5 TB)
  - 900 output images (2.5 GB each, 2.4 TB total)
  - 10.5 million tasks (34,000 CPU hours)

× 17

- **Need to support hierarchical workflows and scale**

HTCondor DAGMan

- **All the previous workflow pipeline are DAG based**
- **DAGMan is a reliable and a scalable workflow executor**
  - Sits on top of HTCondor Schedd
  - Can handle very large workflows (to order of million tasks)
- **Has useful reliability features in-built**
  - Automatic Job retries
  - Rescue DAG's (recover from where you left off in case of failures)
- **Throttling for jobs in a workflow**
- **Easy way to describe workflows**
  - Users can directly express their workflows as DAGMan Dags and condor submit files.

However - !

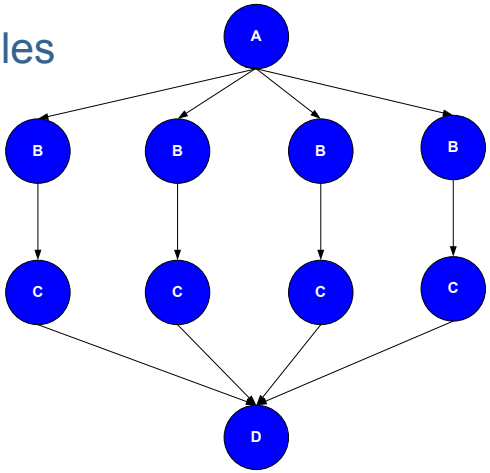
- **If you code directly against DAGMan**
  - **You are potentially limiting yourself to a single execution resource**
  - **You are responsible for figuring out how to access the data**
    - Where do the inputs for your pipeline exist and what file servers to use?
    - How do you ship in the small/large amounts data required by the workflows?
    - Can I use SRM? How about GridFTP? HTTP and Squid proxies?
    - Can I use Cloud based storage like S3 on EC2?
  - **How do you leverage underlying infrastructure setups**
    - E.g. On a HPC cluster in XSEDE, you can rely on the shared filesystem to store data, and use it for all jobs in the workflow
    - On OSG and in computational clouds each job needs to bring it's own inputs
  - **What happens if somebody wants setup your pipleine on their own resource?**
    - Can your pipeline on Amazon EC2 one day, and a PBS cluster the next?

Other Workflow Challenges

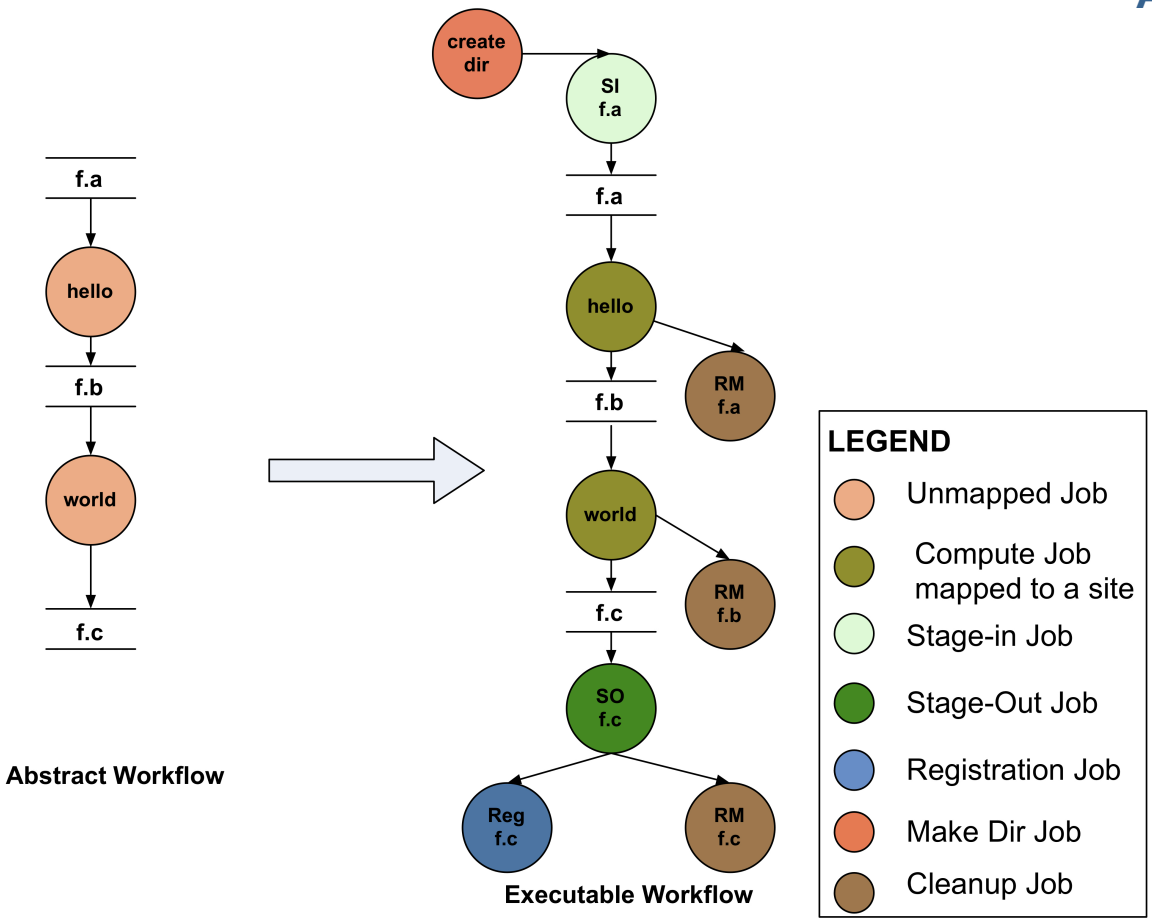
- **Provenance**
  - Can you go back and find out how and where data was produced?
- **Debug and Monitor Workflows**
  - Users need automated tools to go through the log files
  - Need to correlate data across lots of log files
  - Need to know what host a job ran on and how it was invoked
- **Restructure Workflows for Improved Performance**
  - Short running tasks?
  - Data placement?
- **Integrate with higher level tools such as HubZero and provisioning infrastructure**
  - such as GlideinWMS, BOSCO

Pegasus Workflow Management System

- **NSF funded project since 2001**
  - Developed as a collaboration between USC Information Sciences Institute and the Condor Team at UW Madison
- **Builds on top of HTCondor DAGMan.**
- **Abstract Workflows - Pegasus input workflow description**
  - Workflow “high-level language”
  - Only identifies the computation, devoid of resource descriptions, devoid of data locations
  - File Aware – For each task you specify the input and output files
- **Pegasus is a workflow “compiler” (plan/map)**
  - Target is DAGMan DAGs and Condor submit files
  - Transforms the workflow for performance and reliability
  - Automatically locates physical locations for both workflow components and data
  - Collects runtime provenance



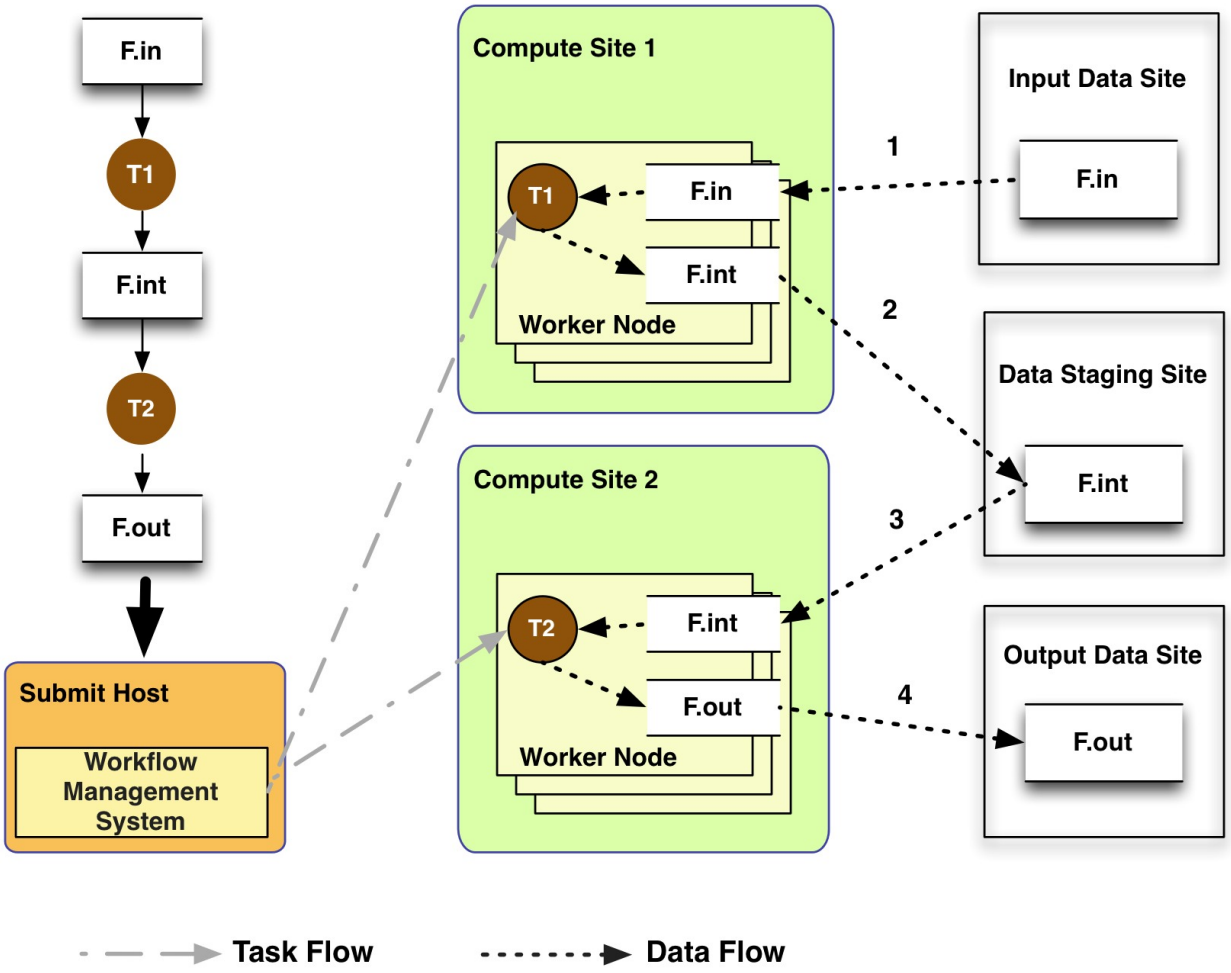
Abstract to Executable Workflow Mapping



- Abstraction provides
  - Ease of Use (do not need to worry about low-level execution details)
  - Portability (can use the same workflow description to run on a number of resources and/or across them)
  - Gives opportunities for optimization and fault tolerance
    - automatically restructure the workflow
    - automatically provide fault recovery (retry, choose different resource)

Pegasus Guarantee - Wherever and whenever a job runs it's inputs will be in the directory where it is launched.

General Workflow Execution Model



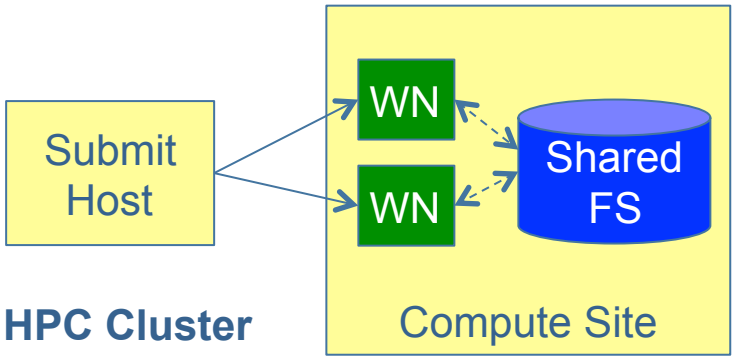
- Most of the tasks in scientific workflow applications require POSIX file semantics
  - Each task in the workflow opens one or more input files
  - Read or write a portion of it and then close the file.

- Input Data Site, Compute Site and Output Data Sites can be co-located
  - Example: Input data is already present on the compute site.

Supported Data Staging Approaches - I

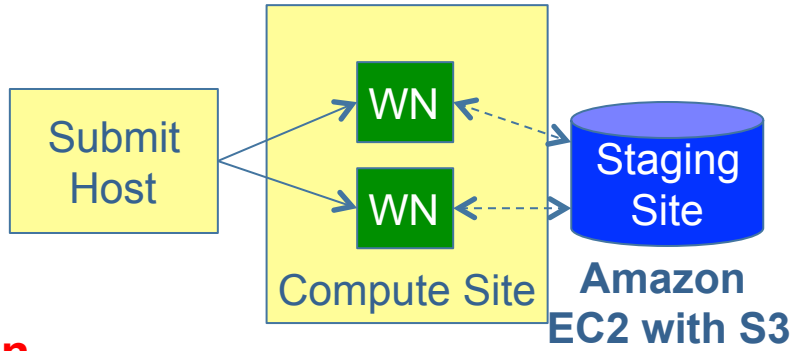
Shared Filesystem setup (typical of XSEDE and HPC sites)

- Worker nodes and the head node have a shared filesystem, usually a parallel filesystem with great I/O characteristics
- Can leverage symlinking against existing datasets
- Staging site is the shared-fs.



Non-shared filesystem setup with staging site (typical of OSG and EC 2)

- Worker nodes don't share a filesystem.
- Data is pulled from / pushed to the existing storage element.
- A separate staging site such as S3.



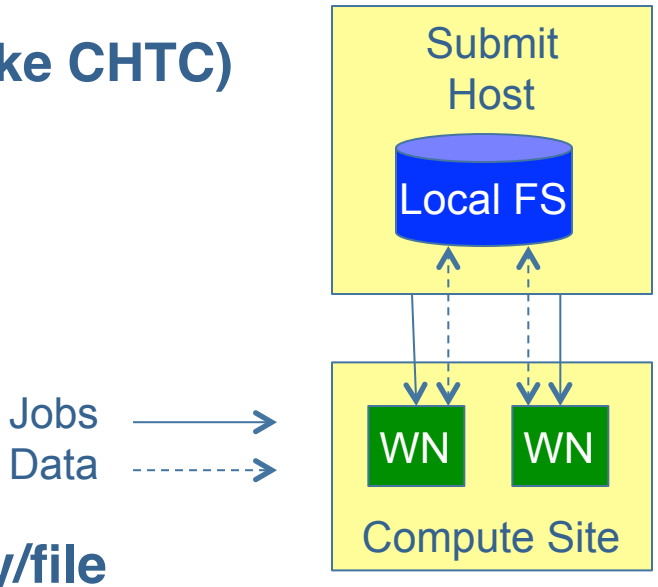
HubZero uses Pegasus to run a single application worklow across sites, leveraging shared filesystem at local PBS cluster and non shared filesystem setup at OSG!

Jobs →
Data - - - - - - - - →

Supported Data Staging Approaches - II

Condor IO (Typical of large Condor Pools like CHTC)

- Worker nodes don't share a filesystem
- Symlink against datasets available locally
- Data is pulled from / pushed to the submit host via Condor file transfers
- Staging site is the submit host.



Supported Transfer Protocols – for directory/file creation and removal, file transfers

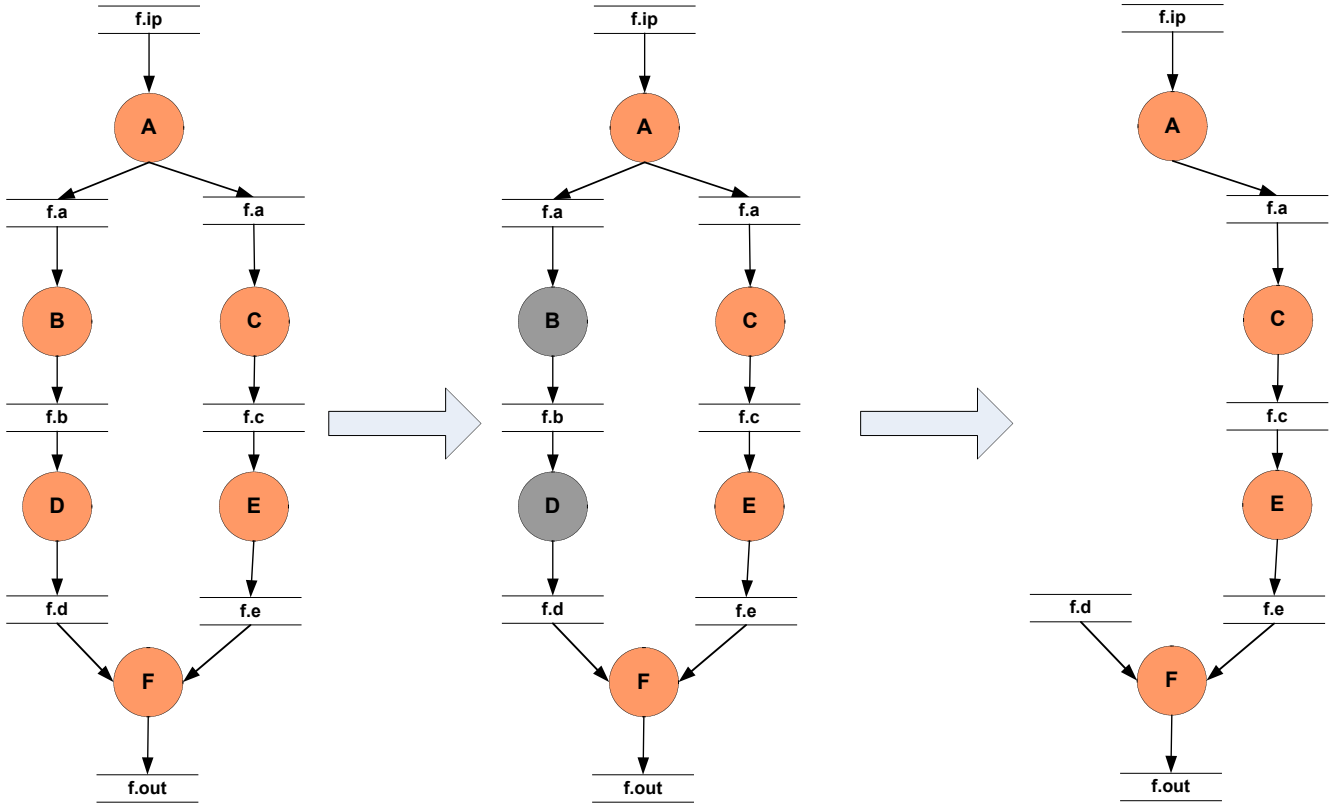
- HTTP
- SCP
- GridFTP
- IRODS
- S3 / Google Cloud Storage
- Condor File IO
- File Copy
- OSG Stash

Using Pegasus allows you to move from one deployment to another without changing the workflow description!

Pegasus Data Management Tools

pegasus-transfer, pegasus-create-dir, pegasus-cleanup support client discovery, parallel transfers, retries, and many other things to improve transfer performance and reliability

Workflow Reduction (Data Reuse)



Abstract Workflow

File f.d exists somewhere.
Reuse it.
Mark Jobs D and B to delete

Delete Job D and Job B

Useful when you have done a part of computation and then realize the need to change the structure. Re-plan instead of submitting rescue DAG!

File cleanup

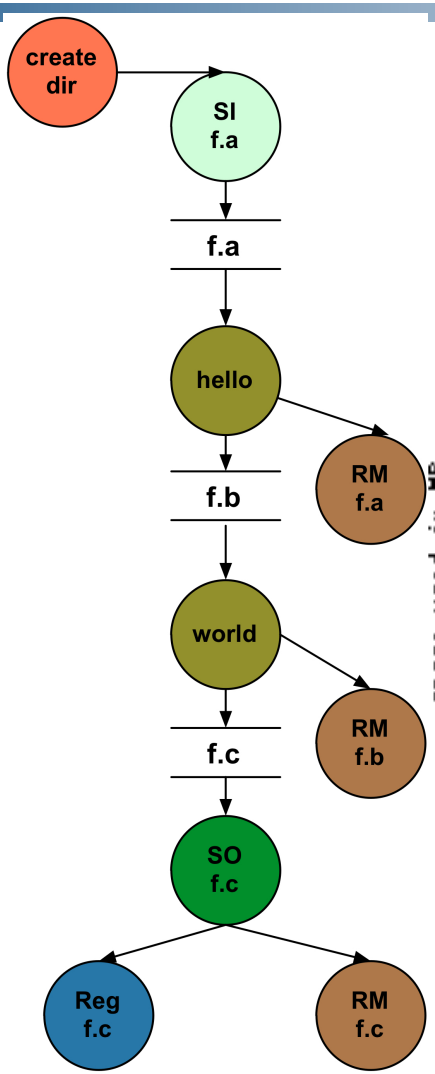
- **Problem: Running out of disk space during workflow execution**

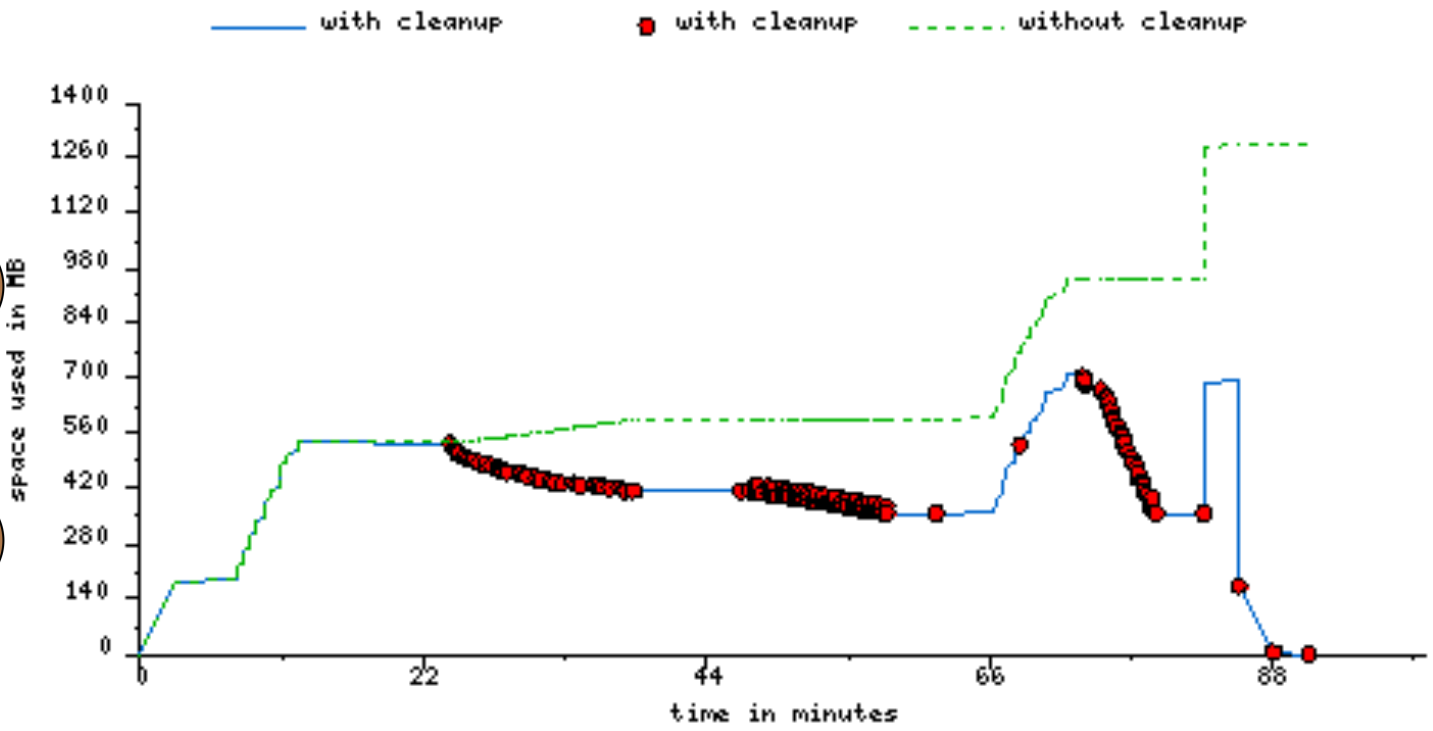
- **Why does it occur**
  - Workflows could bring in huge amounts of data
  - Data is generated during workflow execution
  - Users don't worry about cleaning up after they are done

- **Solution**
  - **Do cleanup after workflows finish**
    - Add a leaf Cleanup Job (Available in 4.4 Release onwards)
  - **Interleave cleanup automatically during workflow execution.**
    - Requires an analysis of the workflow to determine, when a file is no longer required
  - **Cluster the cleanup jobs by level for large workflows**
  - In 4.6 release, users should be able to specify maximum disk space that should not be exceeded. Pegasus will restructure the workflow accordingly.

Real Life Example: Used by a UCLA genomics researcher to delete TB's of data automatically for long running workflows!!

File cleanup (cont)





Montage 1 degree workflow run with cleanup

Job Checkpoint Files

- **A job can specify that it uses one or more checkpoint files**
- **Checkpoint files are both input files and output files**
  - Recommended - application code should create checkpoint files periodically.
- **Users specify checkpoint.time (the time at which the job creates a checkpoint file) and the maxwalltime of a site.**
- **Pegasus will stage-out these files in the case that job fails**
  - Typically due to a timeout on long-running jobs
  - They are sent a TERM signal at checkpoint.time associated with the jobs.
  - A KILL signal is sent K seconds after the TERM signal (where K is (maxwalltime – checkpoint.time)/2
- **Pegasus will stage-in these files before retrying the job**
  - They will appear in the working directory of the job

Works for Grid Universe not just vanilla!

Used by LIGO to run long running inspiral jobs on VIRGO compute resources, where maxwalltime is 12 hours per site policy.

Workflow and Task Notifications

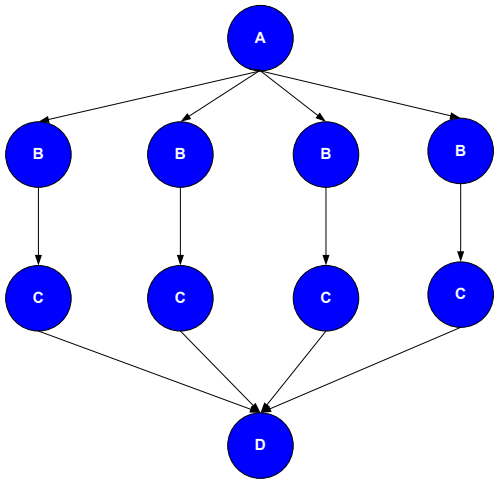
- **Users want to be notified at certain points in the workflow or on certain events.**

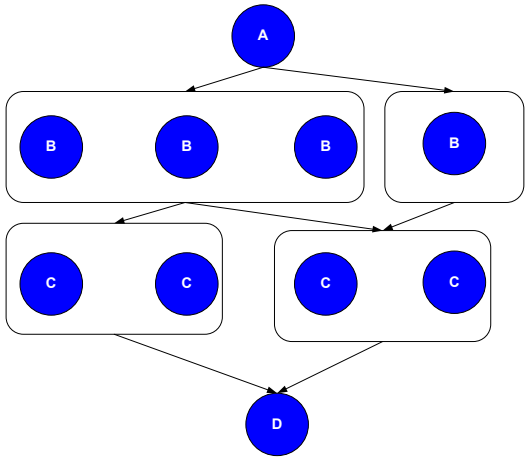
- **Support for adding notification to workflow and tasks**

- **Event based callouts**
  - On Start, On End, On Failure, On Success
  - Provided with email and jabber notification scripts
  - Can run any user provided scripts
  - Defined in the DAX

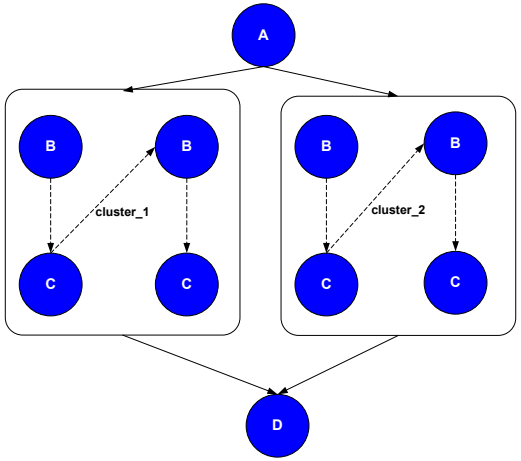
Workflow Restructuring to improve application performance

- **Cluster small running jobs together to achieve better performance**
- **Why?**
  - Each job has scheduling overhead – need to make this overhead worthwhile
  - Ideally users should run a job on the grid that takes at least 10/30/60/? minutes to execute
  - Clustered tasks can reuse common input data – less data transfers





Horizontal clustering



Label-based clustering

Workflow Monitoring - Stampede

- **Leverage Stampede Monitoring framework with DB backend**
  - Populates data at runtime. A background daemon monitors the logs files and populates information about the workflow to a database
  - Stores workflow structure, and runtime stats for each task.

- **Tools for querying the monitoring framework**
  - **pegasus-status**
    - Status of the workflow
  - **pegasus-statistics**
    - Detailed statistics about your finished workflow

```
------------------------------------------------------------------------------
Type           Succeeded Failed  Incomplete  Total     Retries   Total+Retries
Tasks          135002    0       0           135002    0         135002
Jobs           4529      0       0           4529      0         4529
Sub-Workflows  2         0       0           2         0         2
------------------------------------------------------------------------------

Workflow wall time                                : 13 hrs, 2 mins, (46973 secs)
Workflow cumulative job wall time                 : 384 days, 5 hrs, (33195705 secs)
Cumulative job walltime as seen from submit side : 384 days, 18 hrs, (33243709 secs)
```


Workflow Debugging Through Pegasus

- **After a workflow has completed, we can run pegasus-analyzer to analyze the workflow and provide a summary of the run**

- **pegasus-analyzer's output contains**
  - **a brief summary section**
    - showing how many jobs have succeeded
    - and how many have failed.
  - **For each failed job**
    - showing its last known state
    - exitcode
    - working directory
    - the location of its submit, output, and error files.
    - any stdout and stderr from the job.

Alleviates the need for searching through large DAGMan and Condor logs!

Workflow Monitoring Dashboard: pegasus-dashboard

- **A python based online workflow dashboard**
  - Uses the FLASK framework
  - Packaged with Pegasus 4.5 release.
  - Queries the STAMPEDE database
- **Lists all the user workflows on the home page and are color coded.**
  - Green indicates a successful workflow,
  - Red indicates a failed workflow
  - Blue indicates a running workflow
- **Explore Workflow and Troubleshoot (Workflow Page)**
  - Has identifying metadata about the workflow
  - Tabbed interface to
    - List of sub workflows
    - Failed jobs
    - Running jobs
    - Successful jobs.

Workflow Wall Time	7 mins 9 secs
Workflow Cumulative Job Wall Time	2 mins 51 secs
Cumulative Job Walltime as seen from Submit Side	5 mins 49 secs
Workflow Retries	0

▸ Workflow Statistics

▾ Job Breakdown Statistics

Workflow Statistics

Show 10 entries Search:

Transformation	Count	Succeeded	Failed	Min	Max	Mean	Total
dagman::post	32	32	0	5	5	5	160
mAdd:3.3	1	1	0	1.284	1.284	1.284	1.284
mBackground:3.3	32	32	0	0.119	0.211	0.174	5.562
mBgModel:3.3	1	1	0	16.949	16.949	16.949	16.949
mConcatFit:3.3	1	1	0	1.022	1.022	1.022	1.022
mDiffFit:3.3	73	73	0	0.088	0.370	0.192	14.044
mImgtbl:3.3	1	1	0	0.128	0.128	0.128	0.128
mJPEG:3.3	1	1	0	0.529	0.529	0.529	0.529
mProjectPP:3.3	32	32	0	1.875	2.040	1.945	62.246
mShrink:3.3	1	1	0	0.488	0.488	0.488	0.488

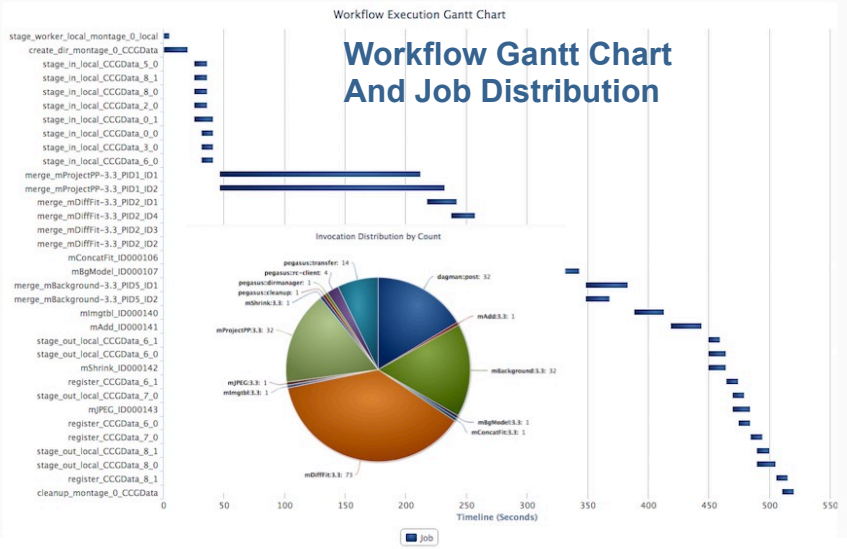
Showing 1 to 10 of 14 entries First Previous 1 2 Next Last

Charts

▸ Job Distribution

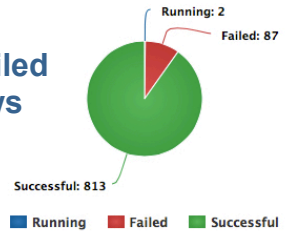
▸ Time Chart

▾ Gantt Chart



Workflow Gantt Chart And Job Distribution

Workflow Listing Page Shows Successful, Failed and Running Workflows

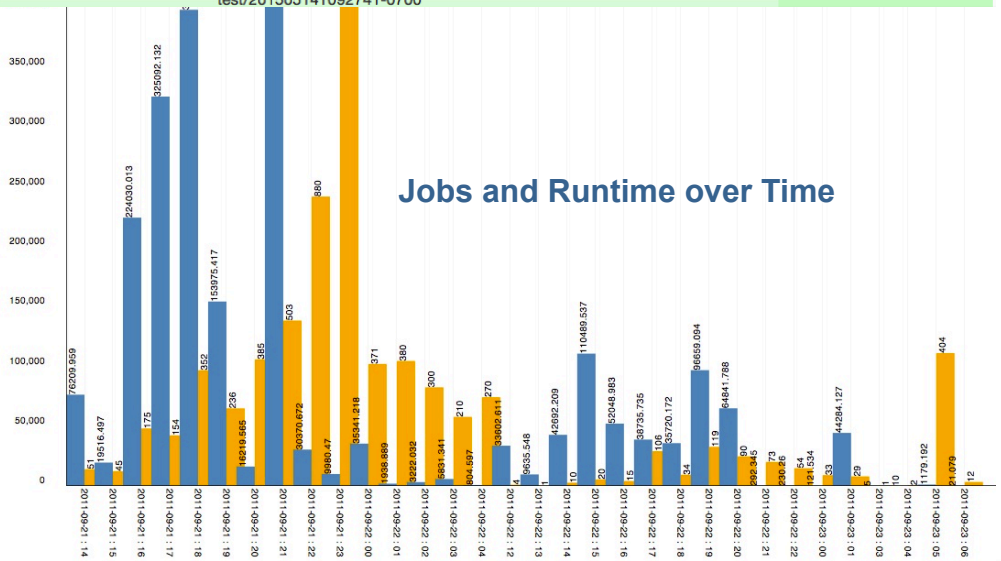


Pegasus Dashboard

Show results for last week

Show 10 entries Search:

Workflow Label	Submit Host	Submit Directory	State	Submitted On
blackdiamond	cartman	/lfs1/software/bamboo/data/xml-data/build-dir/PEGASUS-WT-T19A/test/core/019-black-label/work/bamboo/pegasus/blackdiamond/20150514T092718-0700	Successful	Thu, 14 May 2015 09:27:18
rosetta	cartman	/lfs1/software/bamboo/data/xml-data/build-dir/PEGASUS-WT-SSHFTP030/test/core/030-pegasuslite-sshftp/work/bamboo/pegasus/rosetta/20150514T092732-0700	Failed	Thu, 14 May 2015 09:27:32
horizontal-clustering-test	cartman	/lfs1/software/bamboo/data/xml-data/build-dir/PEGASUS-WT-T10D/test/core/010-runtime-clustering/work/submit/bamboo/pegasus/horizontal-clustering-test/20150514T092741-0700	Successful	Thu, 14 May 2015 09:27:41



Home Planner Metrics DAGMan Metrics Downloads Maps Admin May 20, 2015

Show results from start of May / 2014 to end of May / 2015 Update

Showing 2014-04-30 17:00:00 to 2015-05-31 17:00:00

Metametrics

Number of raw objects	259,898
Number of invalid objects	5
Number of processed objects	259,893

Planner Metrics

Workflows Planned	230,673
Tasks Planned	1,288,322,926
Jobs Planned	234,209,972
Errors Reported	5,883

DAGMan Metrics

Workflow Runs	27,446
Total Jobs	2,928,140
Jobs Submitted	1,954,608
Jobs Succeeded	1,939,640
Jobs Failed	14,968
Total Runtime (hrs)	0.00

Download Metrics

Number of downloads	1,751

Metrics Usage May 2014-May2015

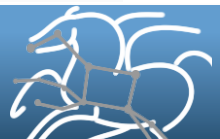
DAGMan metrics reporting only in 4.5 onwards

Top Planner Domains

Domain	Workflows	Tasks	Jobs
isi.edu	50,028	289,840,396	128,095,184
nanohub.org	45,948	71,070	272,610
mps.mpg.de	40,960	1,300,183	1,626,657
opensciencegrid.org	23,629	501,008,491	33,269,886
grid.iu.edu	18,906	372,352,884	10,851,866

Top Planner Hosts

Host	Workflows	Tasks	Jobs
cartman.isi.edu	45,270	279,893,163	122,228,810
seismo3.mps.mpg.de	40,914	1,299,455	1,625,707
scatter.nanohub.org	34,109	47,405	188,697
xd-login.opensciencegrid.org	23,629	501,008,491	33,269,886
osg-xsede.grid.iu.edu	18,906	372,352,884	10,851,866



Summary – What Does Pegasus provide an Application - I

- **All the great features that DAGMan has**
  - Scalability / hierarchal workflows
  - Retries in case of failure.
- **Portability / Reuse**
  - User created workflows can easily be mapped to and run in different environments without alteration.
- **Performance**
  - The Pegasus mapper can reorder, group, and prioritize tasks in order to increase the overall workflow performance.

Summary –
What Does Pegasus provide an Application - II

- **Provenance**
  - Provenance data is collected in a database, and the data can be summaries with tools such as pegasus-statistics, pegasus-plots, or directly with SQL queries.

- **Reliability and Debugging Tools**
  - Jobs and data transfers are automatically retried in case of failures. Debugging tools such as pegasus-analyzer helps the user to debug the workflow in case of non-recoverable failures.

- **Data Management**
  - Pegasus handles replica selection, data transfers and output registrations in data catalogs. These tasks are added to a workflow as auxiliary jobs by the Pegasus planner.

Relevant Links

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

- **Tutorial and documentation: http://pegasus.isi.edu/wms/docs/latest/**

- **Support: pegasus-users@isi.edu**
  pegasus-support@isi.edu

Acknowledgements

Pegasus Team, Condor Team, funding agencies, NSF, NIH, and everybody who uses Pegasus.