Scientific Workflows with Pegasus

Karan Vahi

Science Automation Technologies Group
USC Information Sciences Institute

Workloads – Simple Workflows.

Workloads or Workflows: Users have same concerns!

- **Data Management**
  - 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?

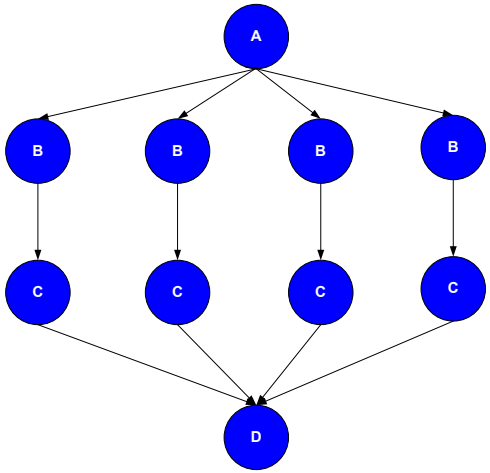
- **Debug and Monitor Workflows**
  - Users need automated tools to go through the log files
  - Need to correlate data across lots of log files
  - Need to know what host a job ran on and how it was invoked

- **Restructure Workflows for Improved Performance**
  - Short running tasks?
  - Data placement?

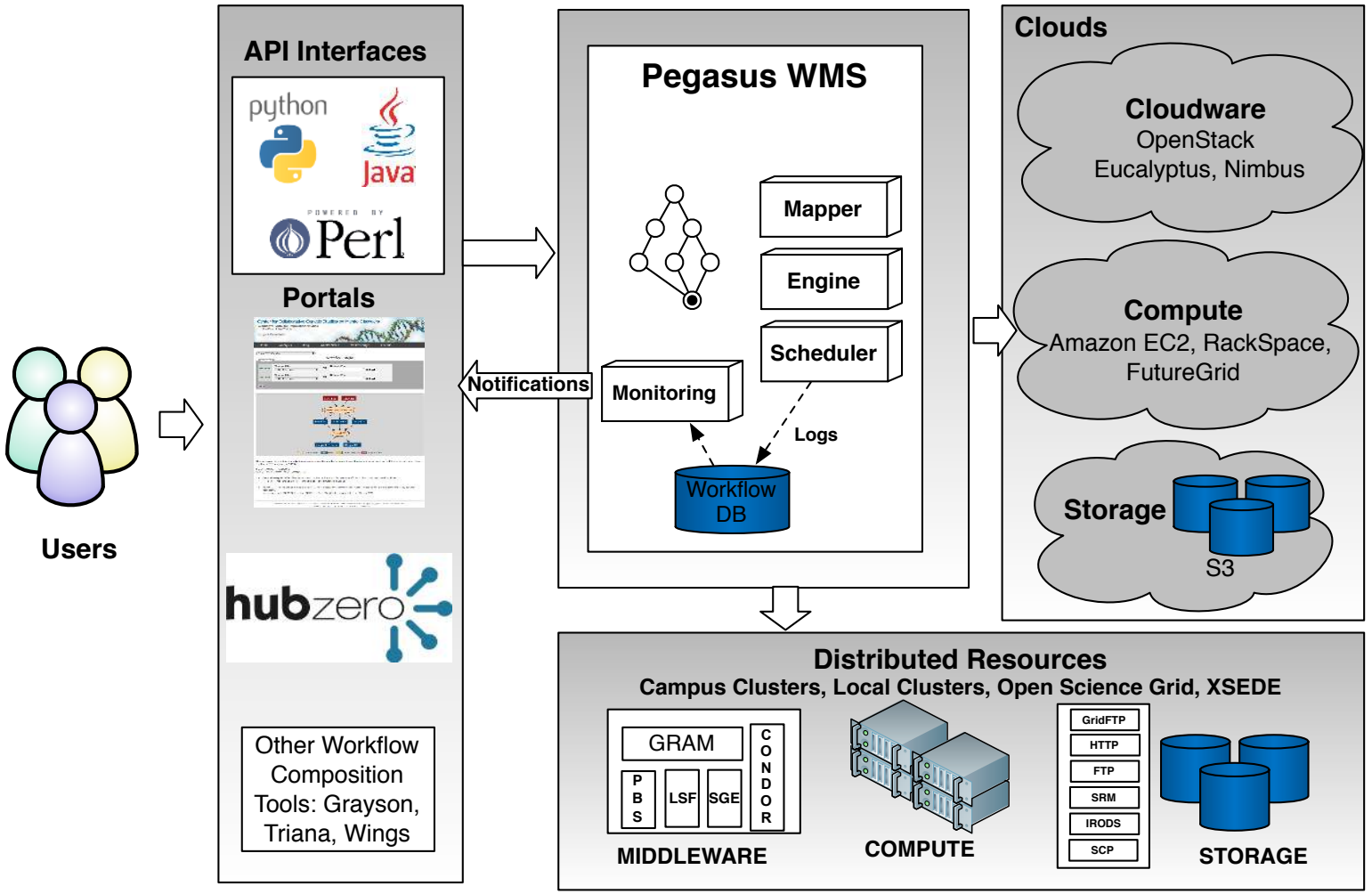
- **Integrate with higher level tools such as HubZero and provisioning infrastructure**
  - such as GlideinWMS, BOSCO

Pegasus Workflow Management System

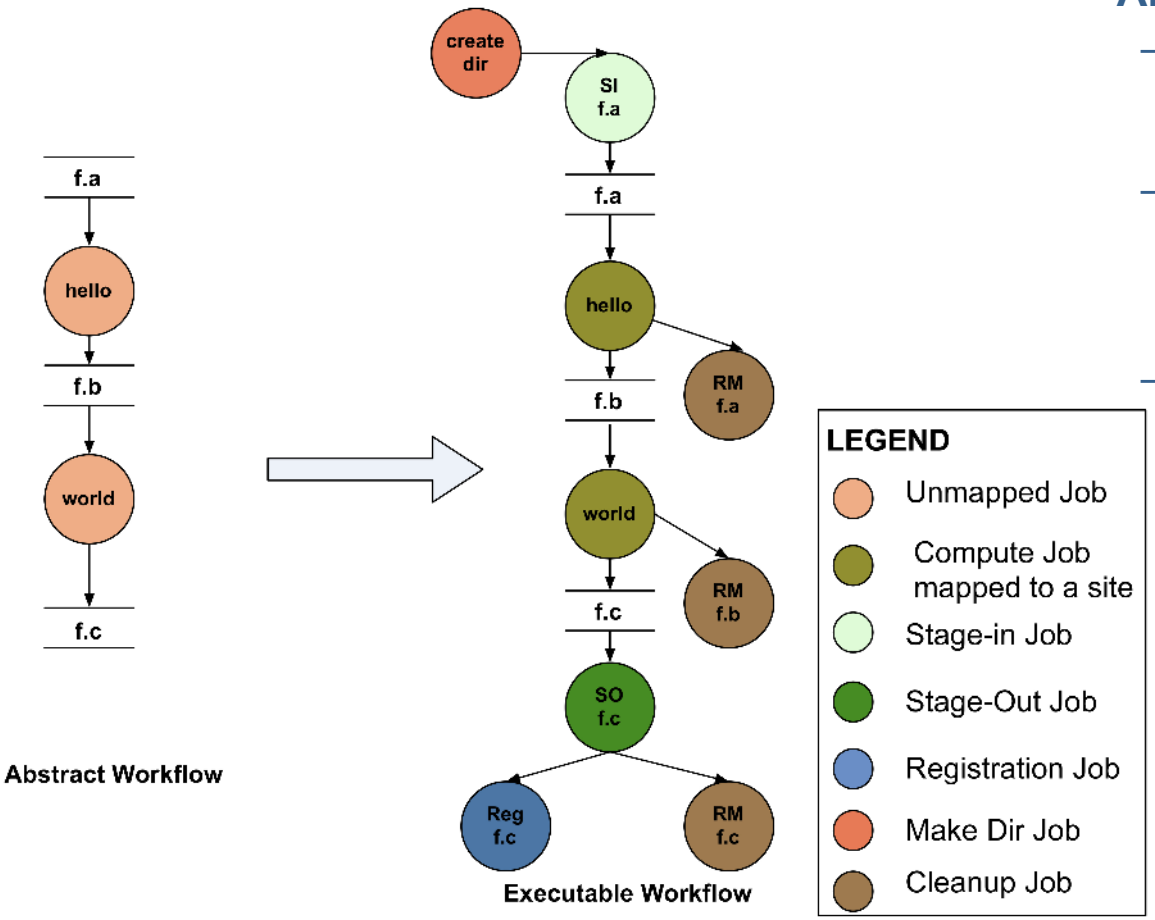
- **NSF funded project since 2001**
  - Developed as a collaboration between USC Information Sciences Institute and the Condor Team at UW Madison
- **Builds on top of Condor DAGMan.**
- **Abstract Workflows - Pegasus input workflow description**
  - Workflow “high-level language”
  - Only identifies the computation, devoid of resource descriptions, devoid of data locations
  - File Aware
- **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



Pegasus WMS

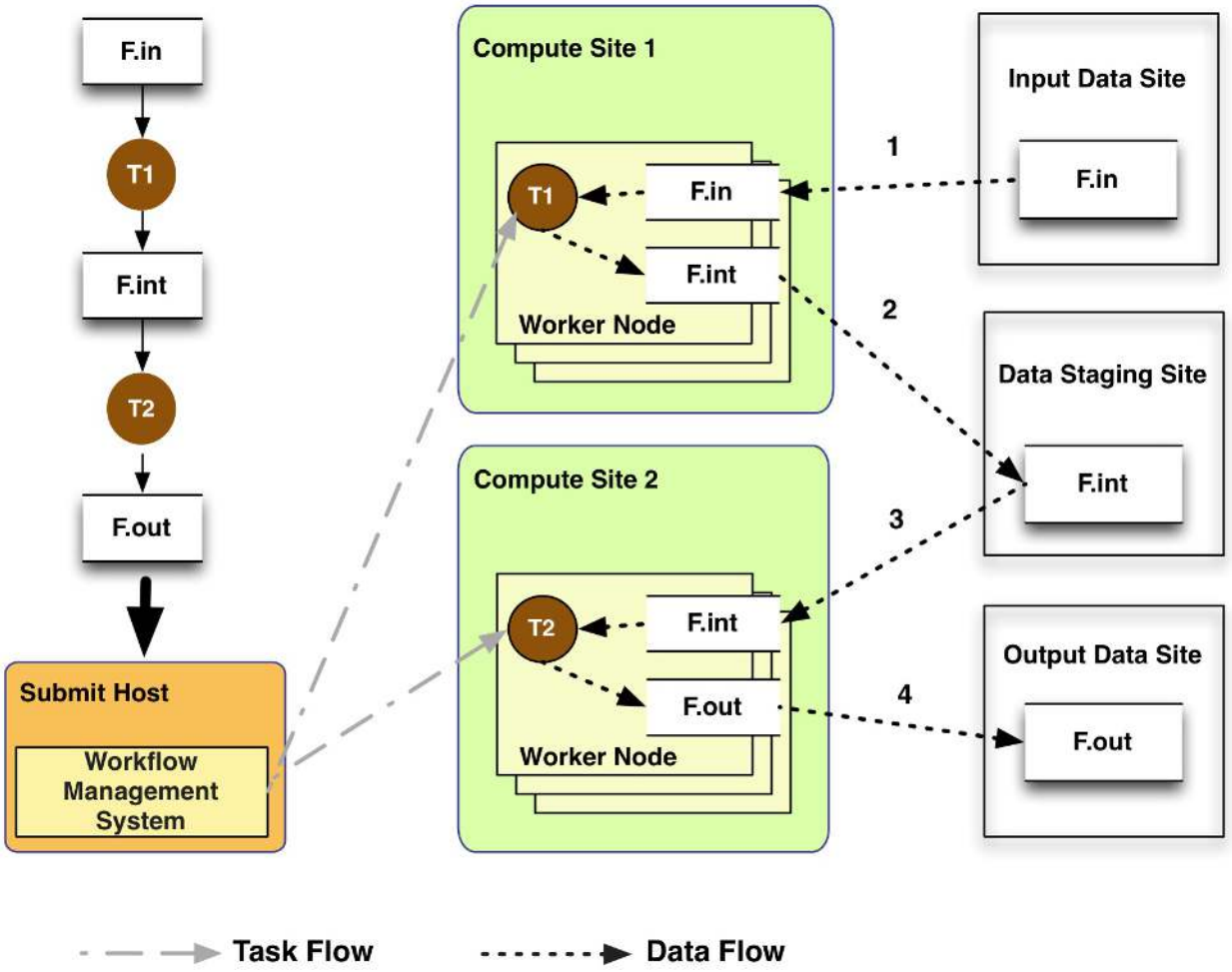

API Interfaces
python
Java
Perl
Portals
hubzero
Other Workflow Composition Tools: Grayson, Triana, Wings
Users
Notifications
Pegasus WMS
Mapper
Engine
Scheduler
Monitoring
Logs
Workflow DB
Clouds
Cloudware
OpenStack
Eucalyptus, Nimbus
Compute
Amazon EC2, RackSpace, FutureGrid
Storage
S3
Distributed Resources
Campus Clusters, Local Clusters, Open Science Grid, XSEDE
GRAM
PBS
LSF
SGE
CONDOR
MIDDLEWARE
COMPUTE
GridFTP
HTTP
FTP
SRM
IRODS
SCP
STORAGE

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)

General Workflow Execution Model



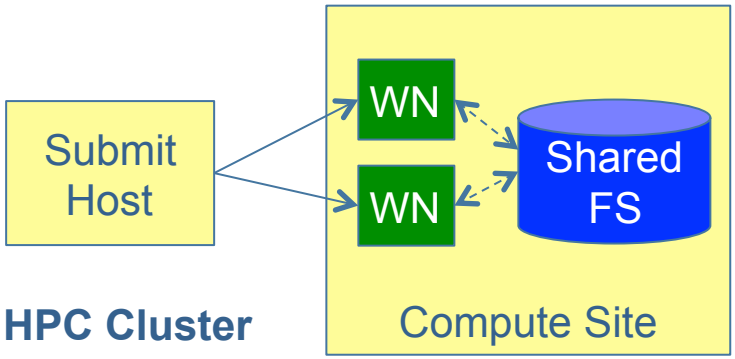
- Most of the tasks in scientific workflow applications require POSIX file semantics
  - Each task in the workflow opens one or more input files
  - Read or write a portion of it and then close the file.

- 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

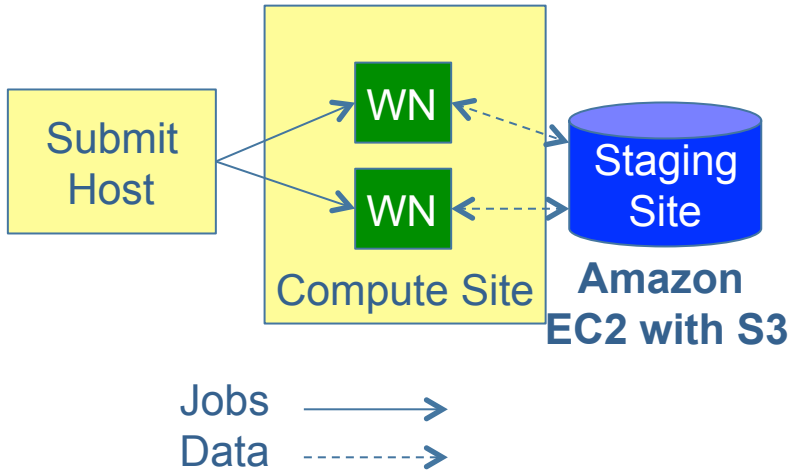
Shared Filesystem setup (typical of XSEDE and HPC sites)

- 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)

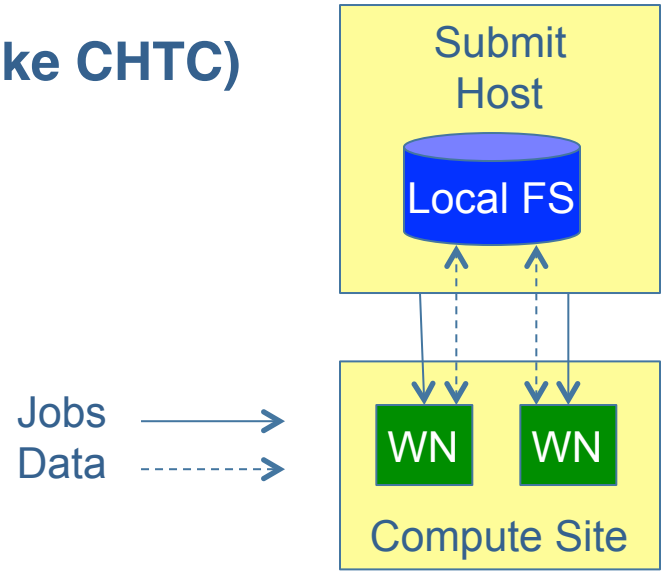
- Worker nodes don't share a filesystem.
- Data is pulled from / pushed to the existing storage element.
- A separate staging site such as S3.



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.

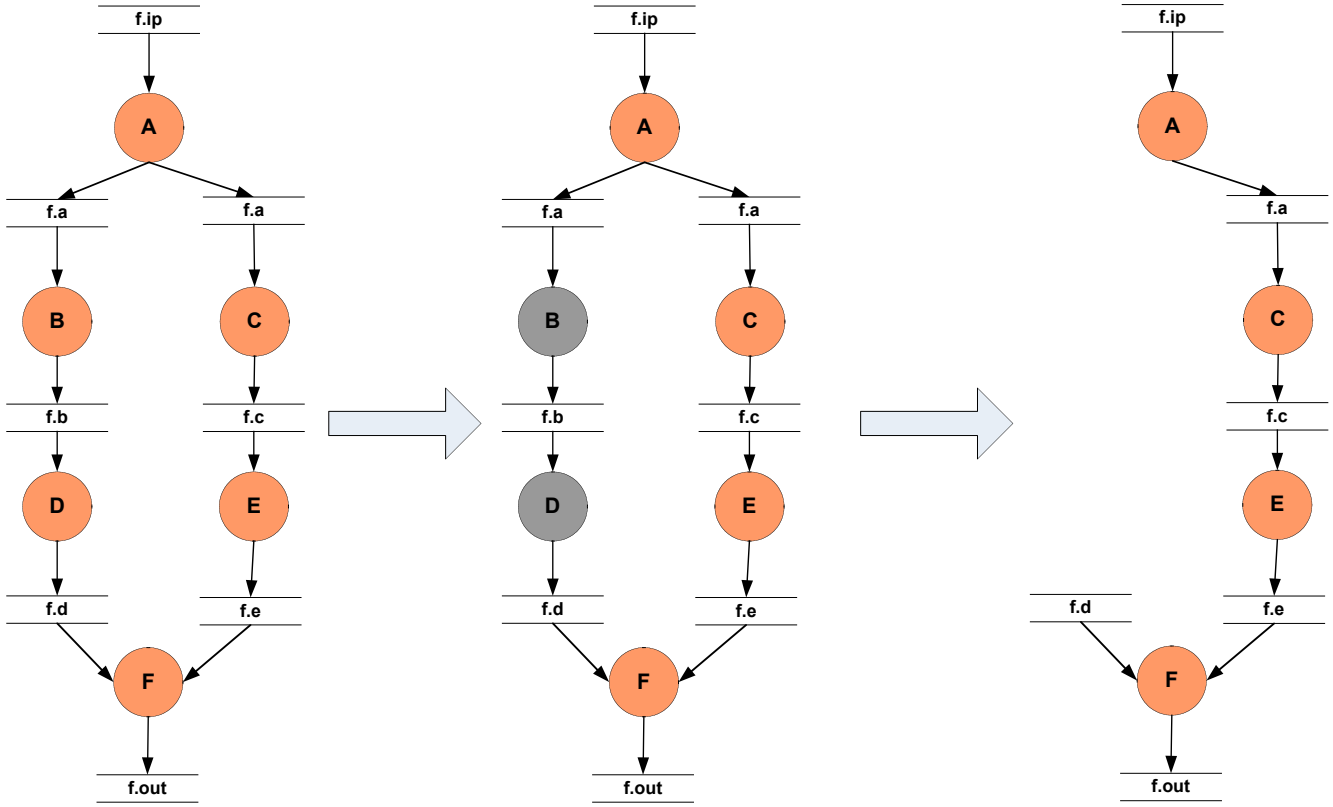


Supported Transfer Protocols

- HTTP
- SCP
- GridFTP
- IRODS
- S3
- Condor File IO
- File Copy

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

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

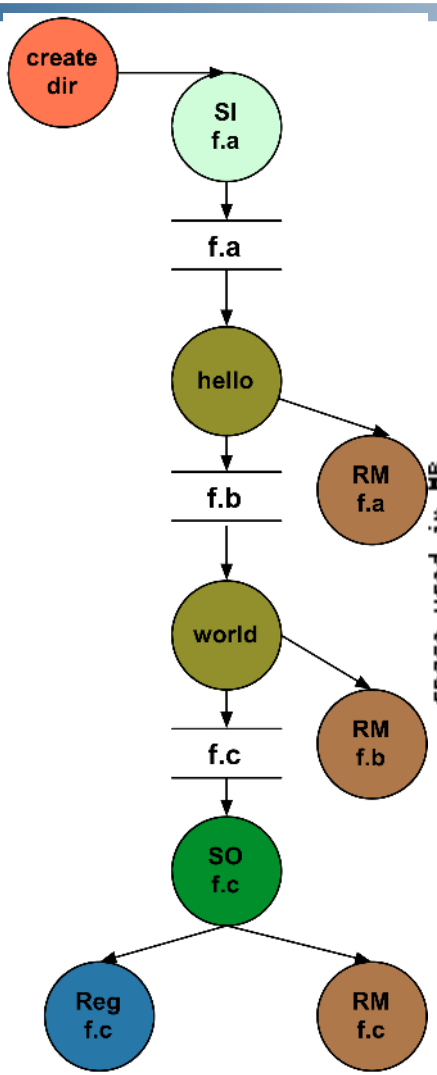
Useful when you have done a part of computation and then realize the need to change the structure. Re-plan instead of submitting rescue DAG!

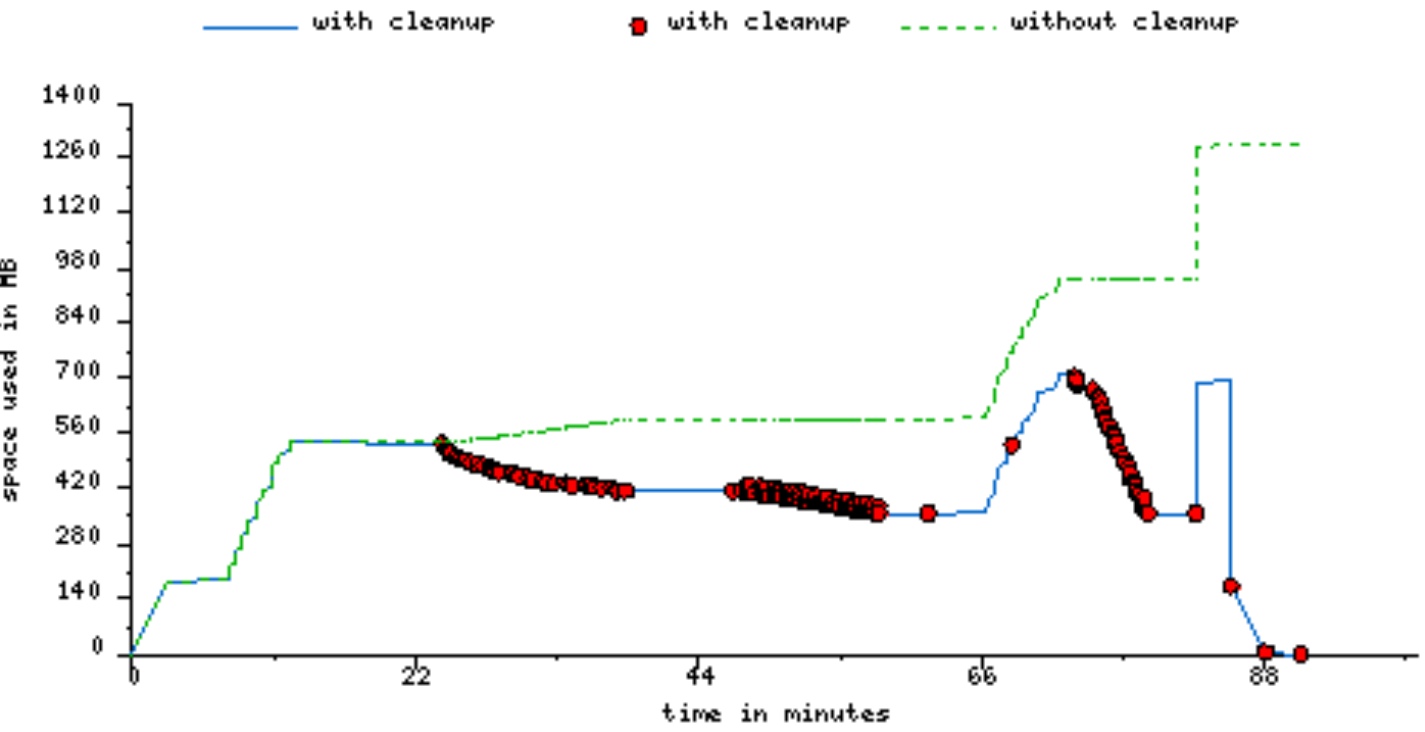
File cleanup

- **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)
  - **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**

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

File cleanup (cont)

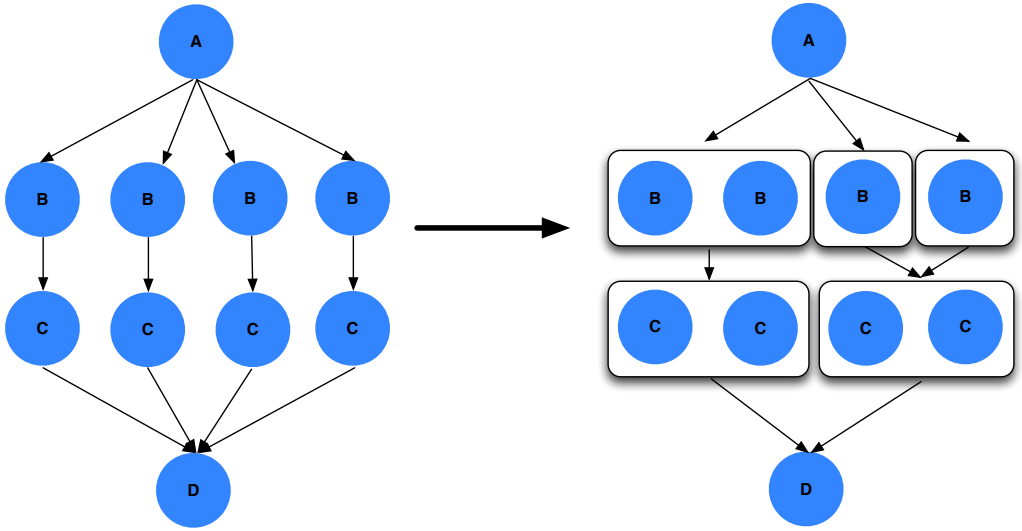




Montage 1 degree workflow run with cleanup

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



Level-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
  - Beta version released in 4.2
  - 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.

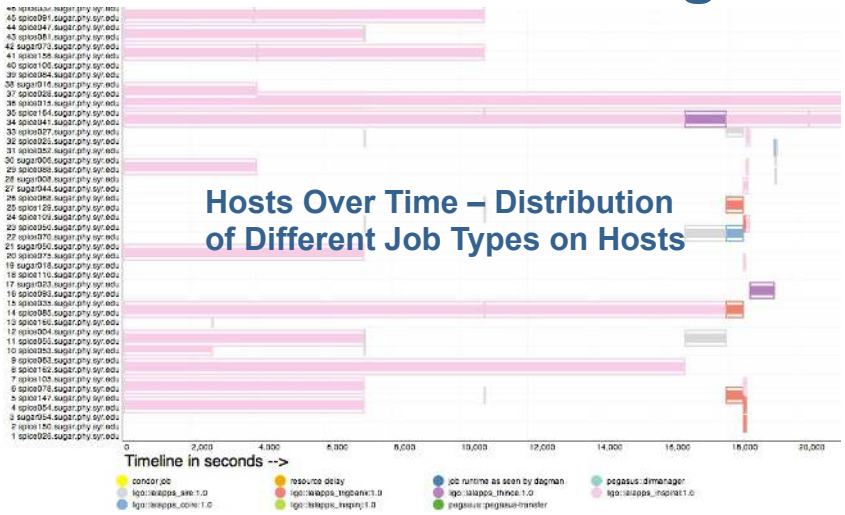
Workflow Monitoring Dashboard: pegasus-dashboard

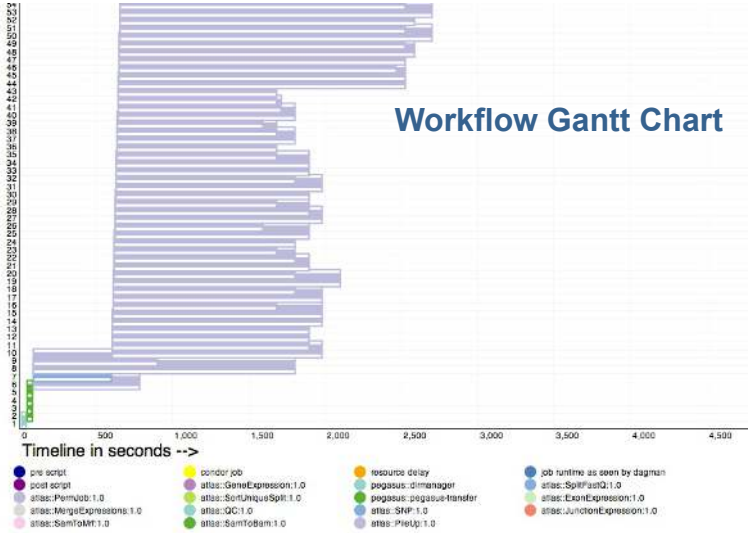
- **Job Page**
  - Lists information captured in kickstart record for the job.
  - Will show the various retries of the job

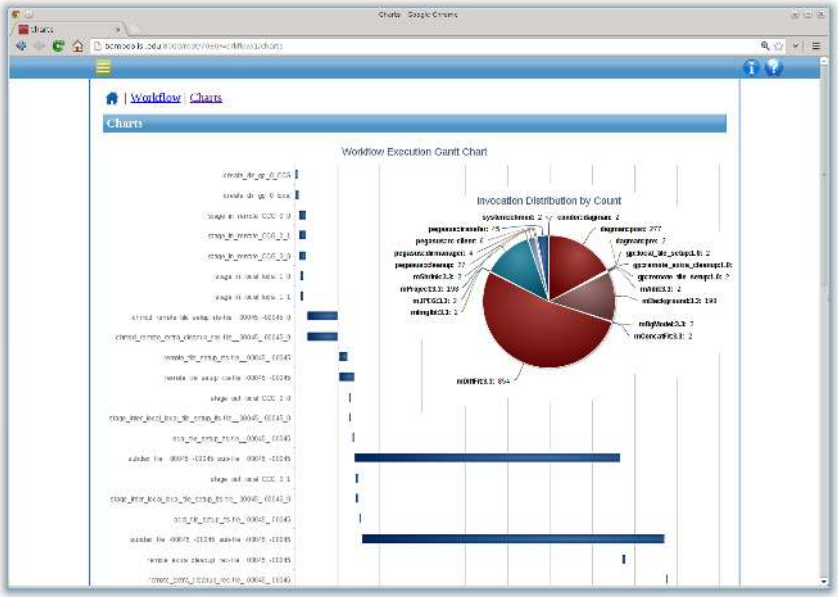
- **Statistics Page for the Workflow**
  - Generates Statistics for the workflow, similar to pegasus-statistics command line tool

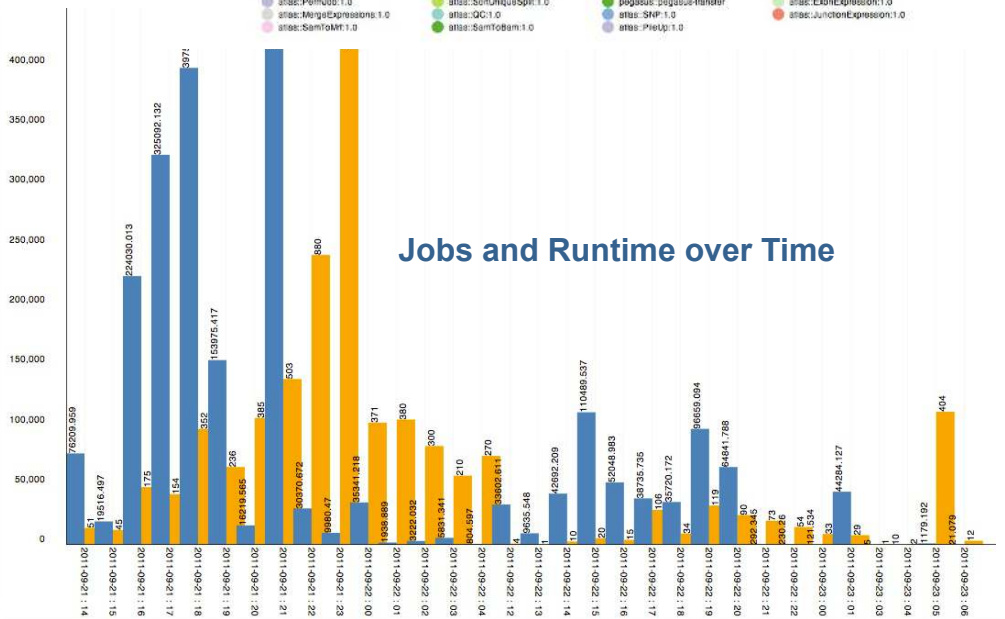
- **Charts Page For the Workflow**
  - Workflow Gantt Chart
  - Job Distribution by Count/Time
  - Time Chart by Job/Invocation

Workflow Monitoring Dashboard – pegasus-dashboard









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

Metrics Collection

- **Why?**
  - A requirement of being funded as part of the NSF SI2 Program
  - Reporting ON by default. Can be turned off.

- **What do we collect?**
  - Anonymous planner metrics
    - Duration of the planner
    - Start and end time
    - Exitcode
    - Breakdown of tasks and jobs in the workflow
  - We leave a copy of the metrics file in the submit directory for the users

- **Capturing Errors**
  - In addition to capturing usage data, the planner also reports back **fatal errors**
  - Using it to drive usability improvements for Pegasus

- http://pegasus.isi.edu/wms/docs/latest/funding_citing_usage.php#usage_statistics

Show results for the last year Update Showing 2013-04-25 14:19:58 to 2014-04-25 14:19:58

Metametrics

Number of raw objects	231,761
Number of invalid objects	8
Number of processed objects	231,753

Planner Metrics

Workflows Planned	224,279
Tasks Planned	1,321,249,267
Jobs Planned	62,510,152
Errors Reported	4,551

Top Planner Domains

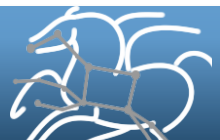
Domain	Workflows	Tasks	Jobs
us-west-2.compute.amazonaws.com	37,288	36,023,295	3,868,573
isi.edu	37,238	184,951,338	16,841,265
mps.mpg.de	36,106	1,012,466	1,290,070
grid.iu.edu	27,464	500,294,080	14,859,482
usc.edu	27,075	552,593,558	6,153,451

Top Planner Hosts

Host	Workflows	Tasks	Jobs
cartman.isi.edu	30,461	181,965,576	13,736,116
osg-xsede.grid.iu.edu	27,464	500,294,080	14,859,482
shock.usc.edu	26,979	552,502,104	6,109,904
condor.nanohub.org	23,554	48,926	146,562
seismo3.mps.mpg.de	23,080	666,402	844,427

Download Metrics

Number of downloads	1,009



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.