Managing large-scale workflows with Pegasus

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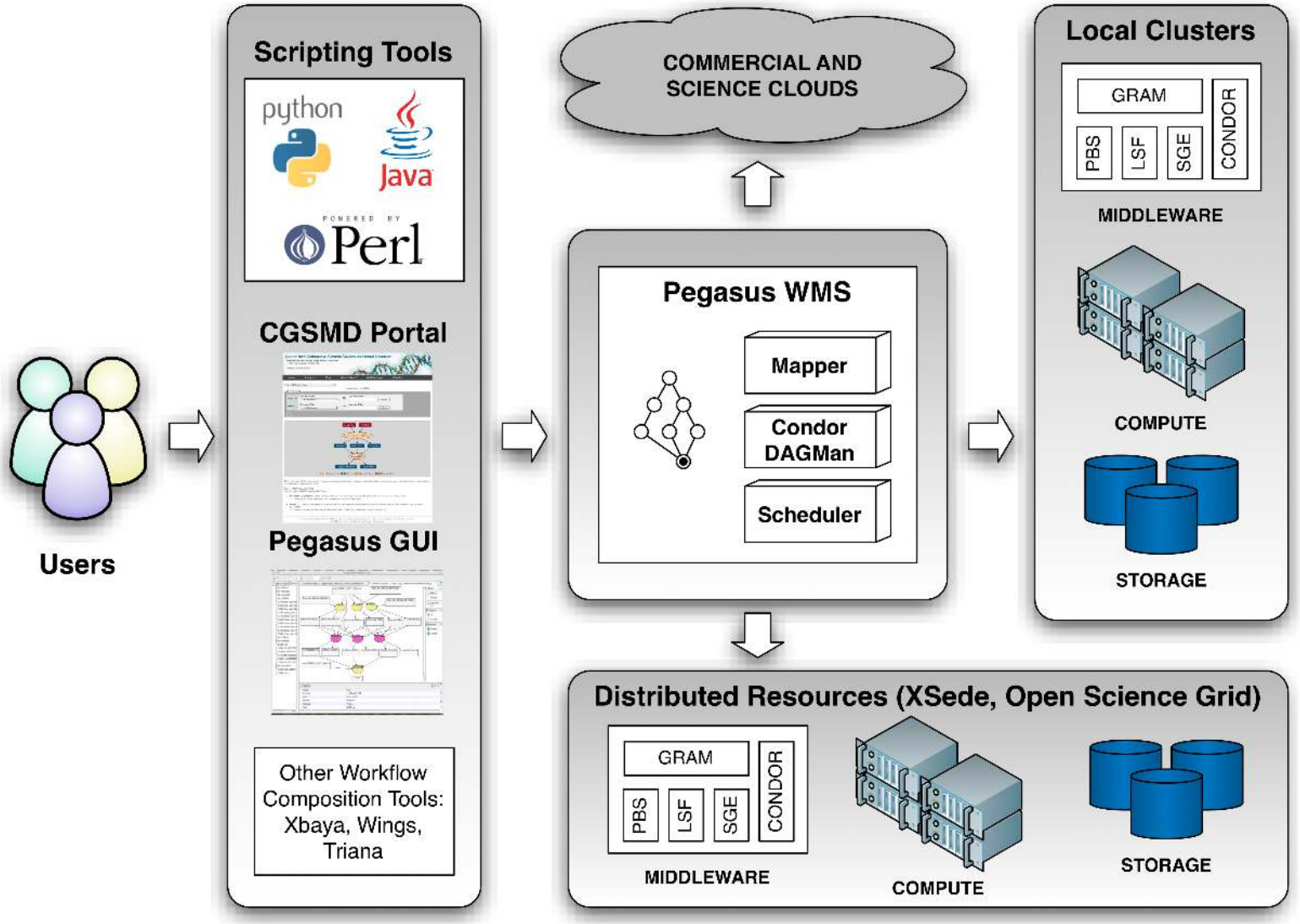
Pegasus Workflow Management System

- Takes in a workflow description and can map and execute it on wide variety of environments
  - Local desktop
  - Local Condor Pool
  - Local Campus Cluster
  - Grid
  - Commercial or Academic Clouds

Pegasus Workflow Management System

- NSF funded Project and developed since 2001
- A collaboration between USC and the Condor Team at UW Madison (includes DAGMan)
- Used by a number of applications in a variety of domains
- Builds on top of Condor DAGMan.
  - Provides reliability—can retry computations from the point of failure
  - Provides scalability—can handle many computations (1- 10^6 tasks)
- Automatically captures provenance information
- Can handle large amounts of data (order of Terabytes)
- Provides workflow monitoring and debugging tools to allow users to debug large workflows

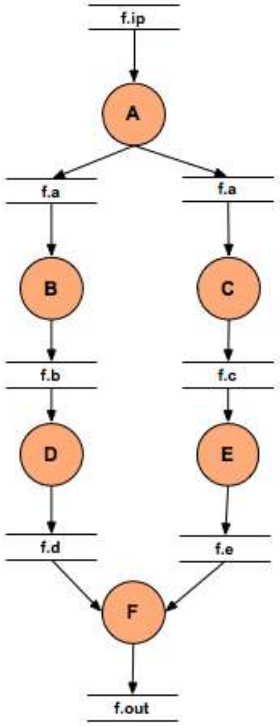
Pegasus WMS


Users
Scripting Tools
python
Java
Perl
CGSMD Portal
Pegasus GUI
Other Workflow Composition Tools: Xbaya, Wings, Triana
COMMERCIAL AND SCIENCE CLOUDS
Pegasus WMS
Mapper
Condor DAGMan
Scheduler
Local Clusters
GRAM
PBS
LSF
SGE
CONDOR
MIDDLEWARE
COMPUTE
STORAGE
Distributed Resources (XSede, Open Science Grid)
GRAM
PBS
LSF
SGE
CONDOR
MIDDLEWARE
COMPUTE
STORAGE

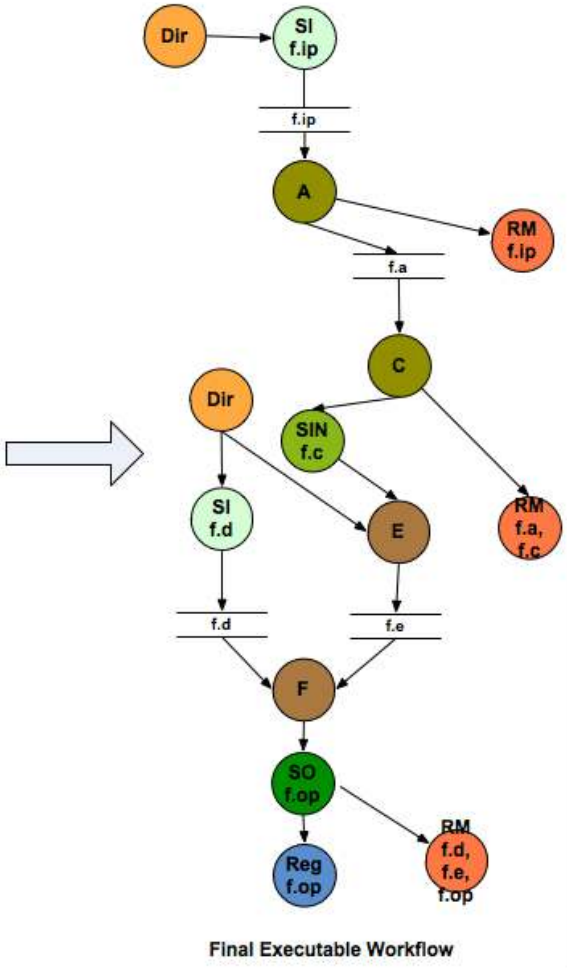
Abstract Workflow (DAX)

- Pegasus Input Workflow description—DAX
  - workflow "high-level language"
  - devoid of resource descriptions
  - devoid of data locations
  - refers to codes as logical transformations
  - refers to data as logical files
- You can use Java, Perl, Python APIs to generate DAXes

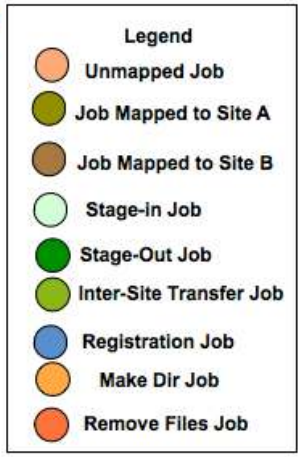
Comparison of DAX and Condor DAG



Abstract Workflow



Final Executable Workflow



- 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)

Issues for Large Scale Workflows

- 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 ?
- Data Management
  - How do you ship in the large amounts data required by the workflows?
- Restructure Workflows for Improved Performance
  - Can have lots of short running jobs
  - Leverage MPI

Workflow Monitoring - Stampede

- Leverage Stampede Monitoring framework with DB backend
  - Separates DB loading infrastructure and log representation
  - Populates data at runtime. A background daemon monitors the logs files and populates information about the workflow to a database
  - Supports SQLite or MySQL
  - Python API to query the framework
  - 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 workflow
  - pegasus-plots
    - Visualization of your workflow execution

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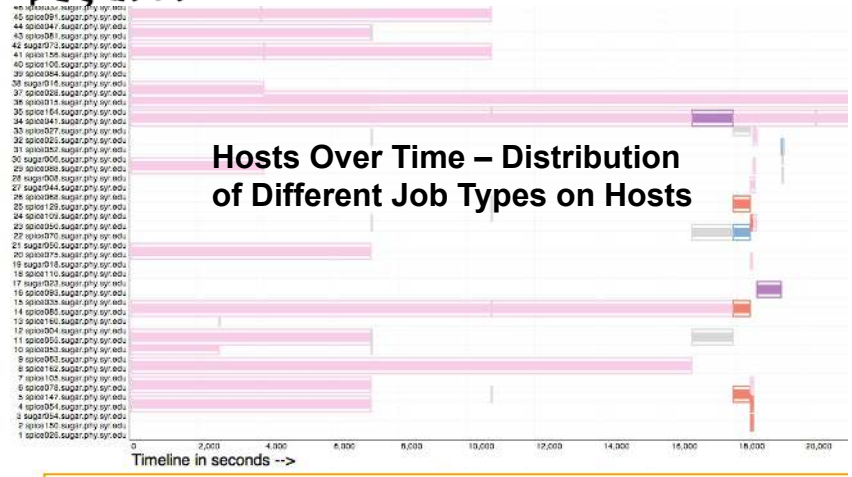
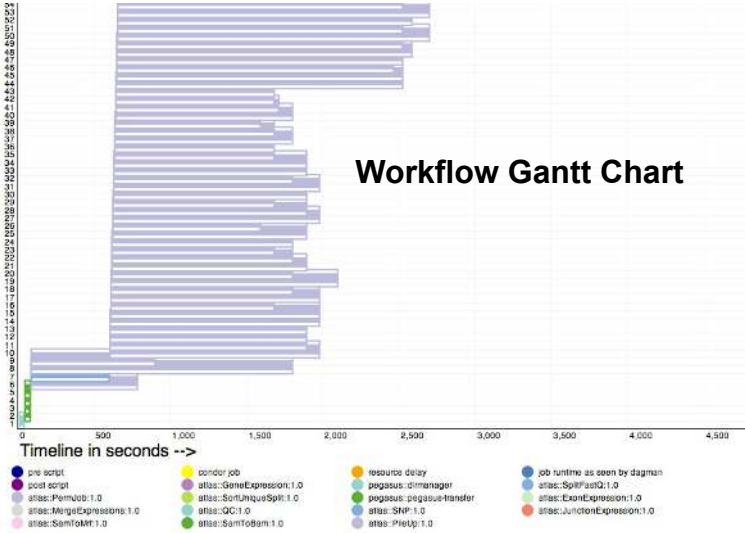
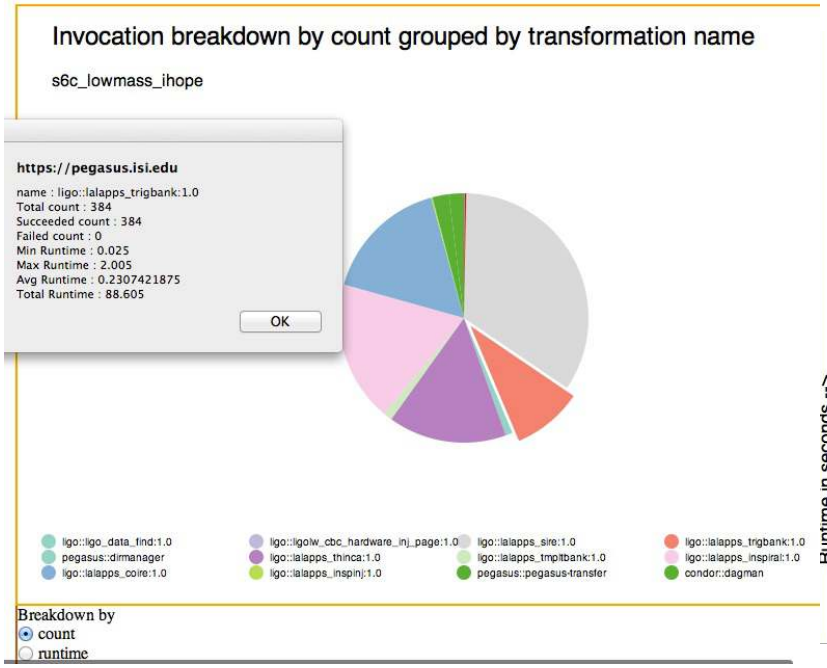
Workflow Monitoring - Stampede

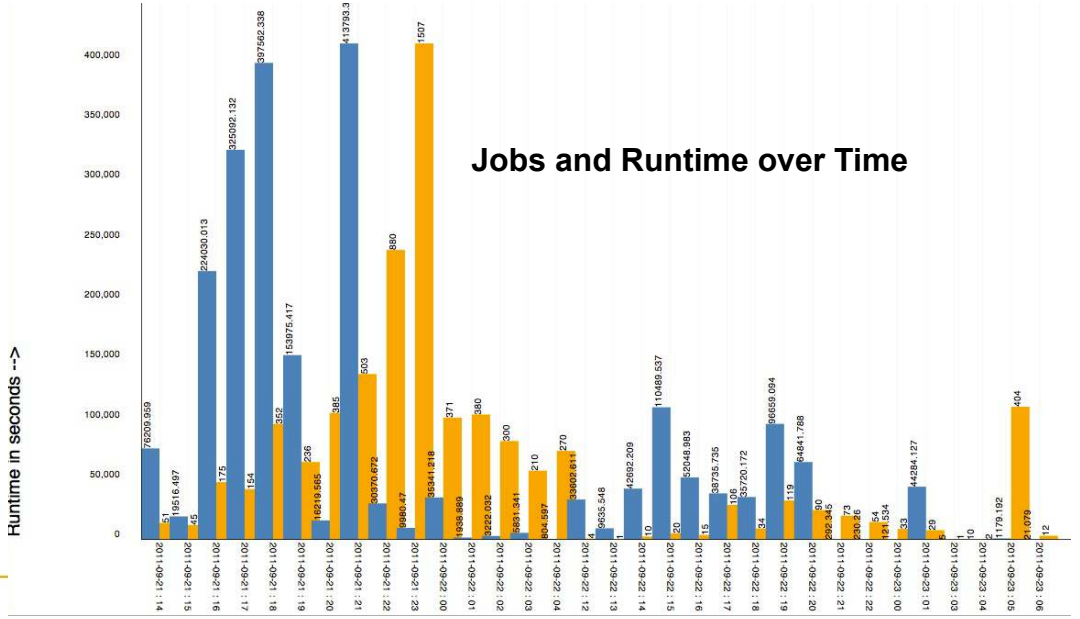


Hosts Over Time – Distribution of Different Job Types on Hosts



Workflow Gantt Chart





Jobs and Runtime over Time

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.

Workflow and Task Notifications

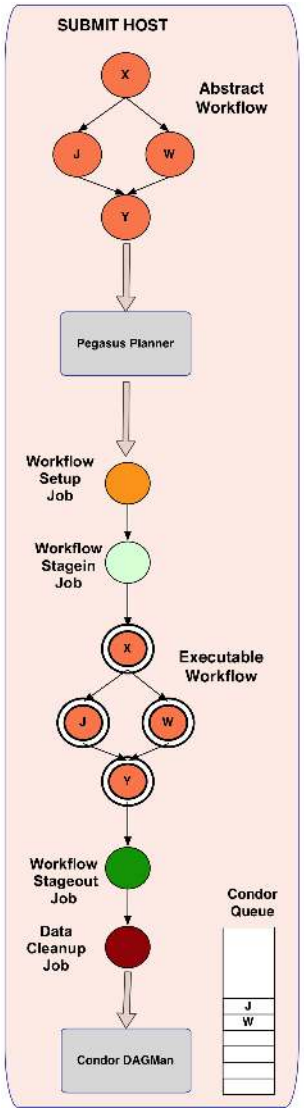
- Users want to be notified at certain points in the workflow or on certain events.

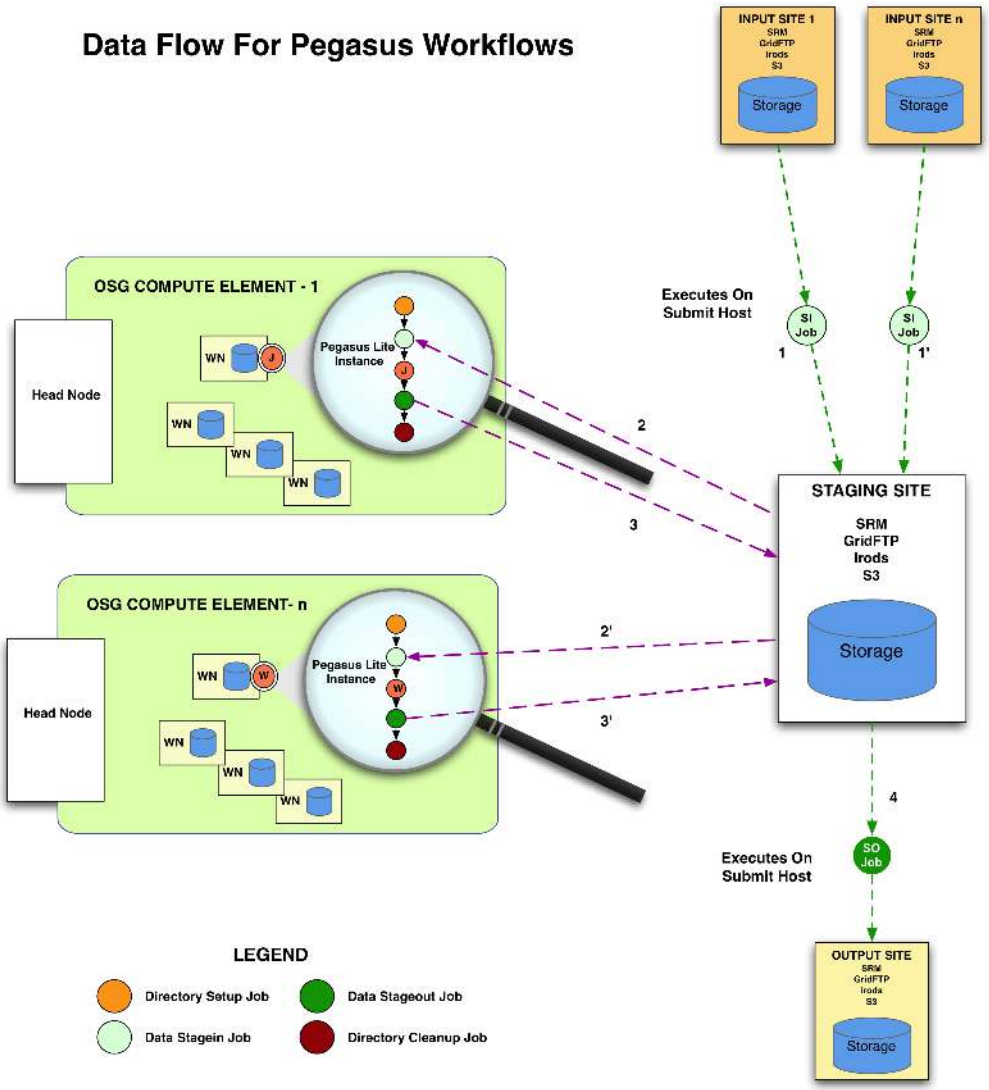
- Support for adding Notification to Workflow and Tasks
  - Event based callouts
    - On Start, On End, On Failure, On Success
  - Provided with email and jabber notification scripts
  - Can run any user provided script as notification.
  - Defined in the DAX.

Supported Data Staging Configurations

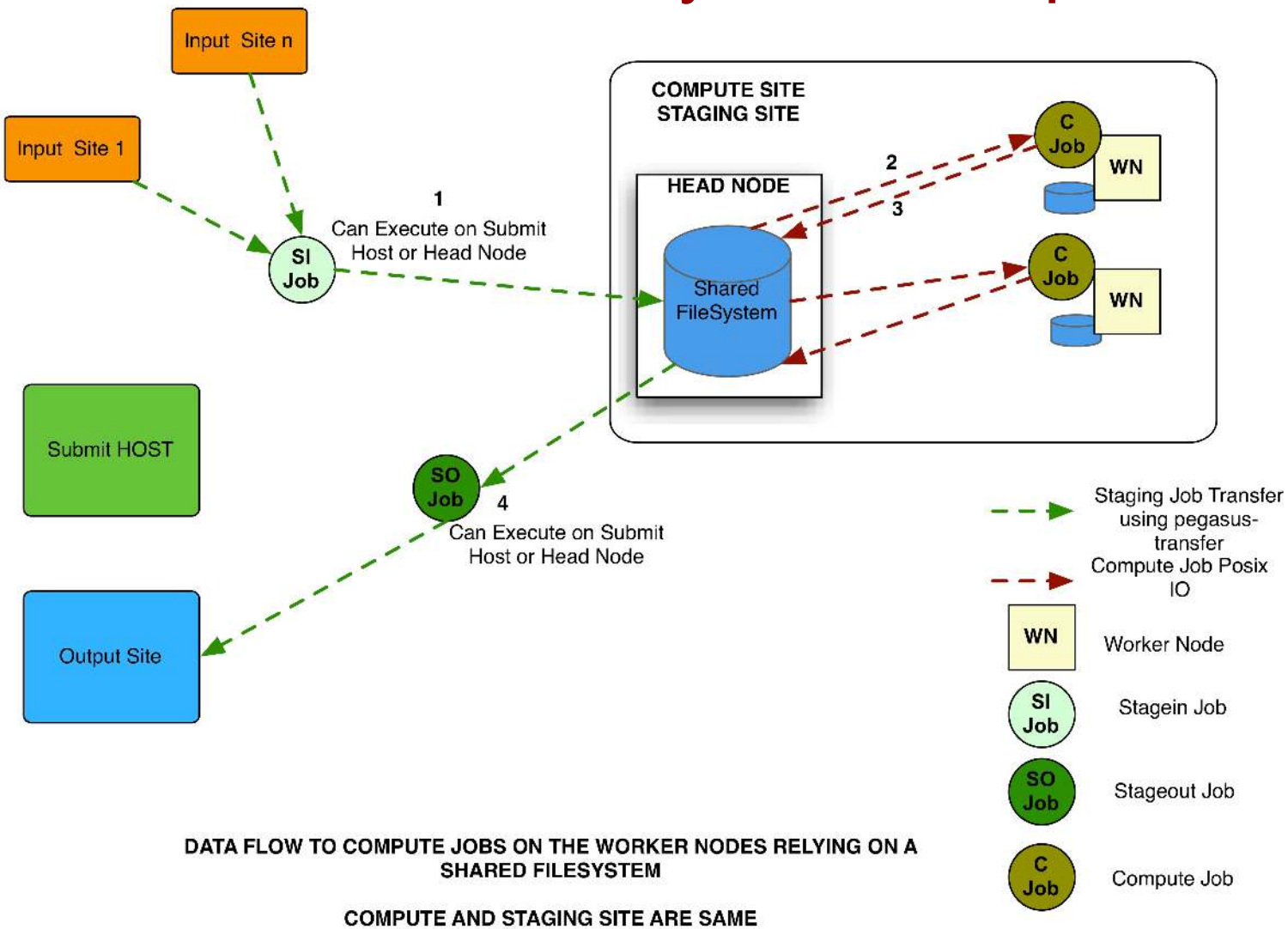
- Three General Configurations Supported
  - Shared Filesystem setup (Typical of Xsede sites)
    - Worker nodes and the Head Node have a shared filesystem.
    - Can leverage symlinking against existing datasets
  - NonShared Filesystem setup with a staging site (Typical of OSG or Campus Condor Pools)
    - Worker Nodes don't share a filesystem.
    - Data is pulled from an external staging site.
  - Condor IO
    - Worker Nodes don't share a filesystem
    - Data is pulled from the submit host.

Data Flow For Pegasus Workflows



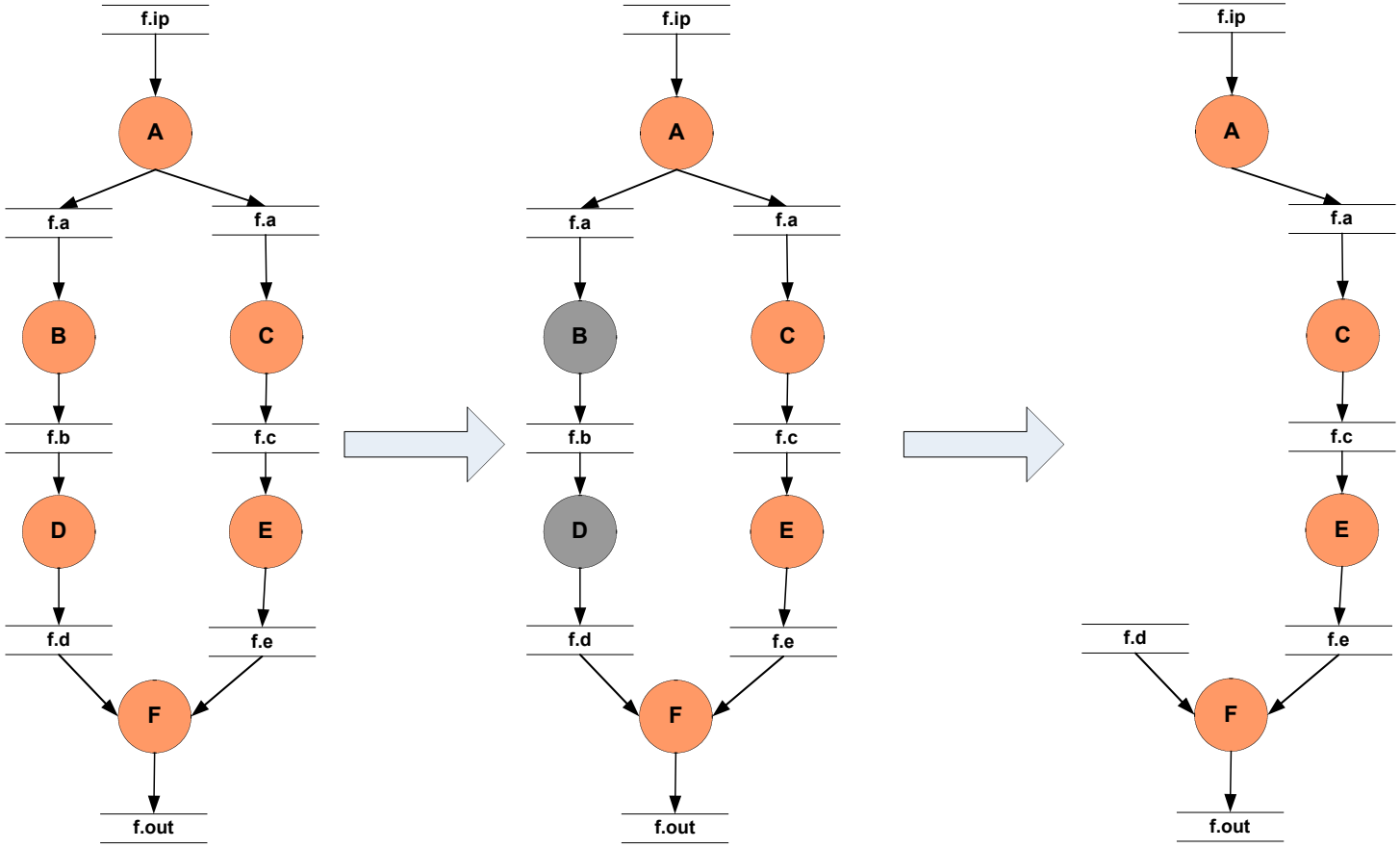


Shared Filesystem Setup



Tip: Set pegasus.data.configuration = sharedfs

WF Reduction (Data Reuse)



Abstract Workflow

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

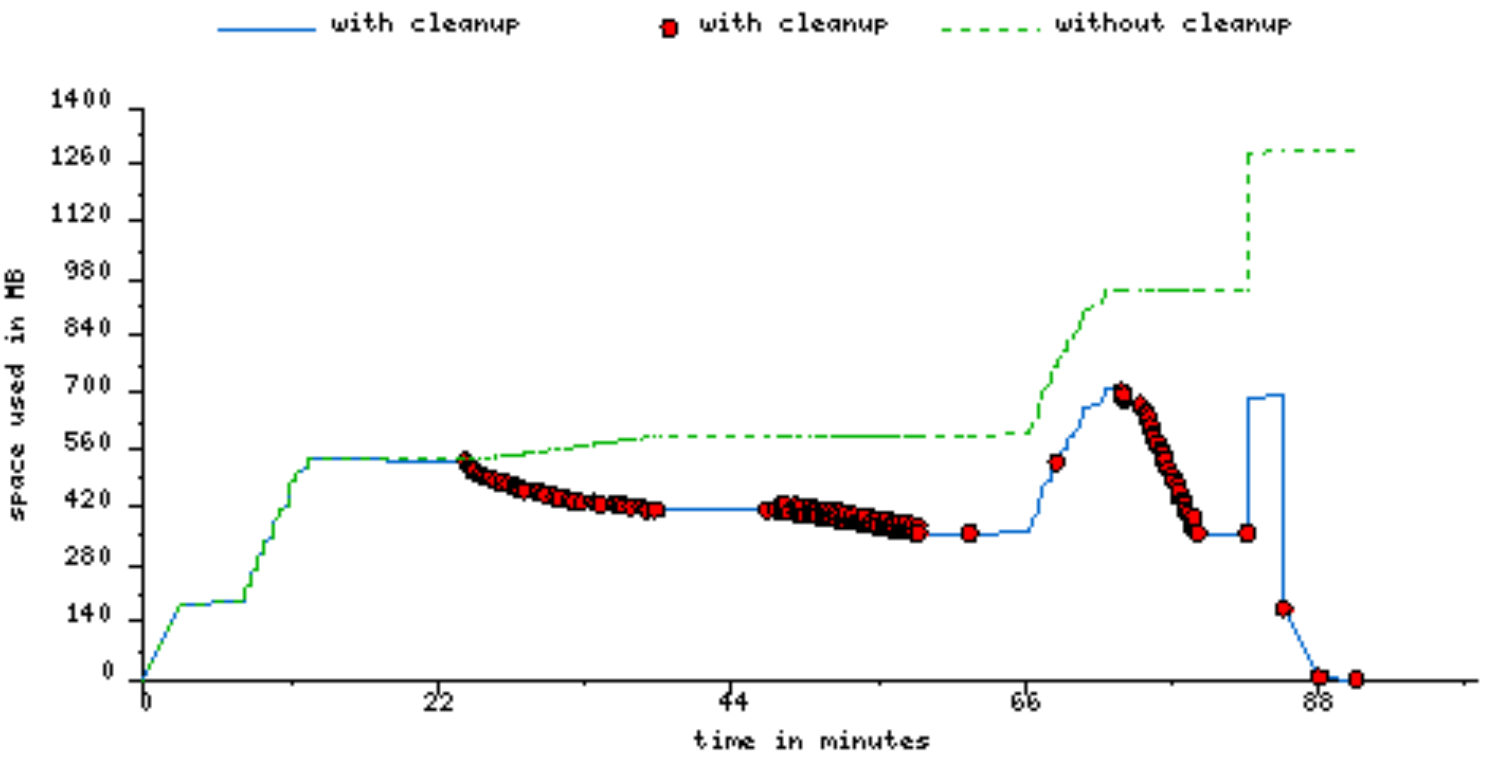
Delete Job D and Job B

Users can use this to move their computations to a different cluster in case of failure

File cleanup

- Problem: Running out of space on shared scratch
  - In OSG scratch space is limited to 30Gb for all users
- Why does it occur
  - Workflows 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
    - Does not work as the scratch may get filled much before during execution
  - Interleave cleanup automatically during workflow execution.
    - Requires an analysis of the workflow to determine, when a file is no longer required

Storage Improvement for Montage Workflows



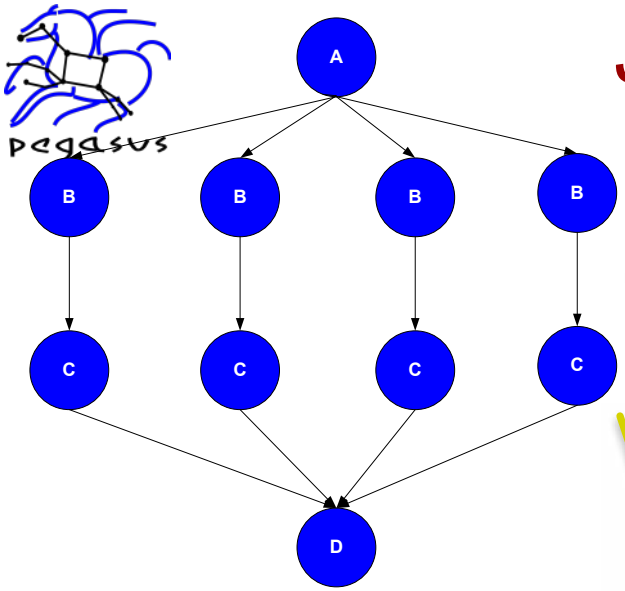
Montage 1 degree workflow run with cleanup on OSG-PSU

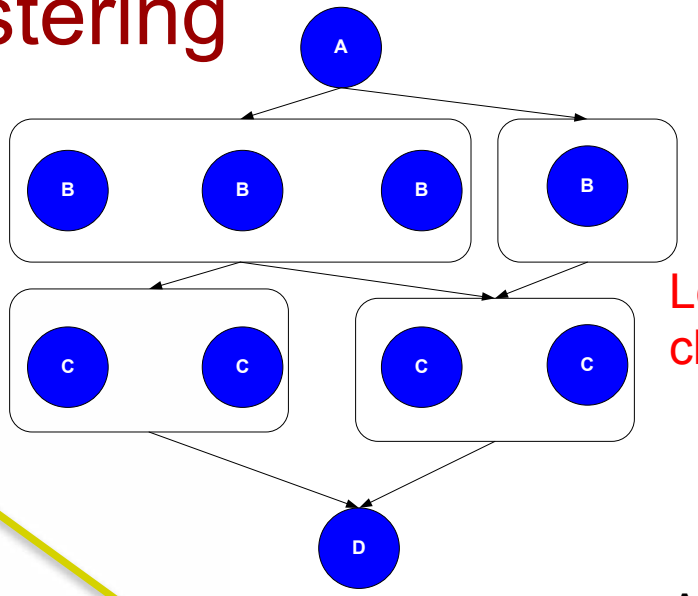
Workflow Restructuring to improve Application Performance

- 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 minutes to execute

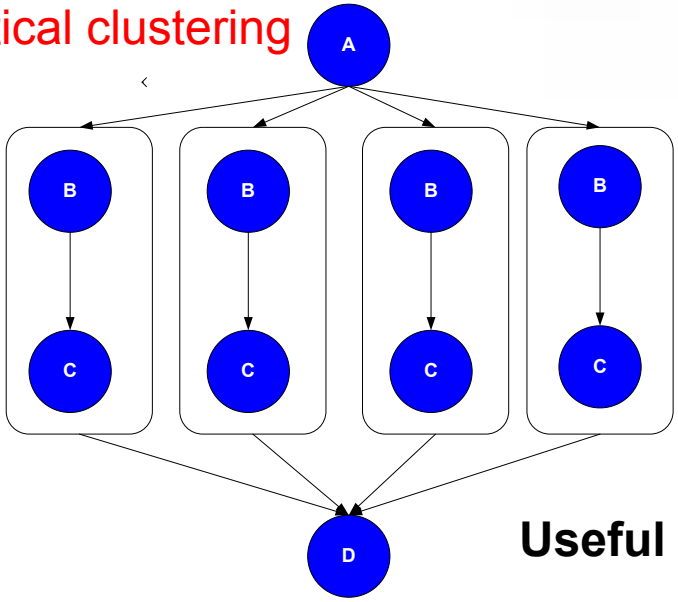
Job Clustering



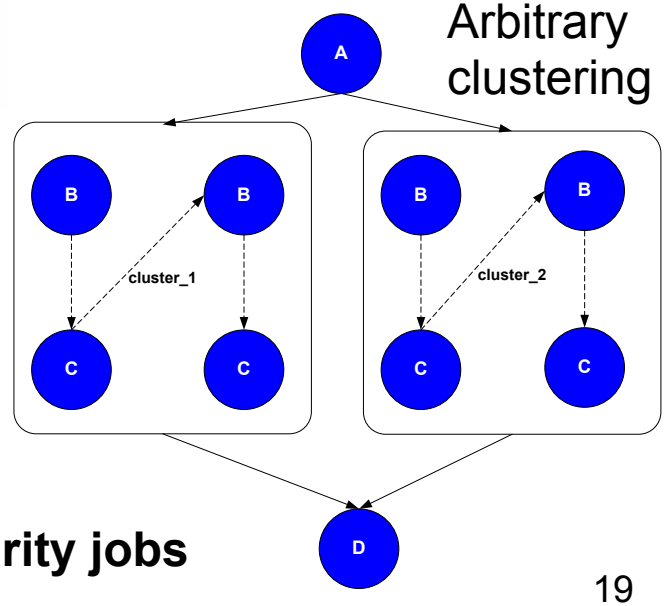


Level-based clustering

Vertical clustering



Arbitrary clustering

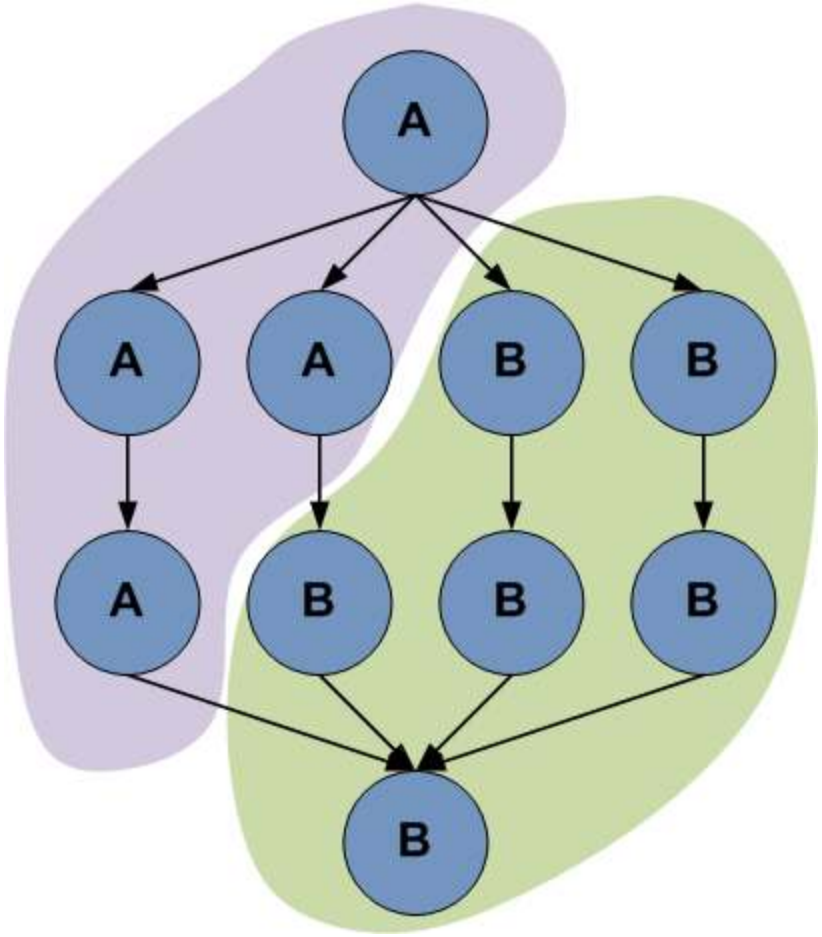


Useful for small granularity jobs

Previous solution : Glideins

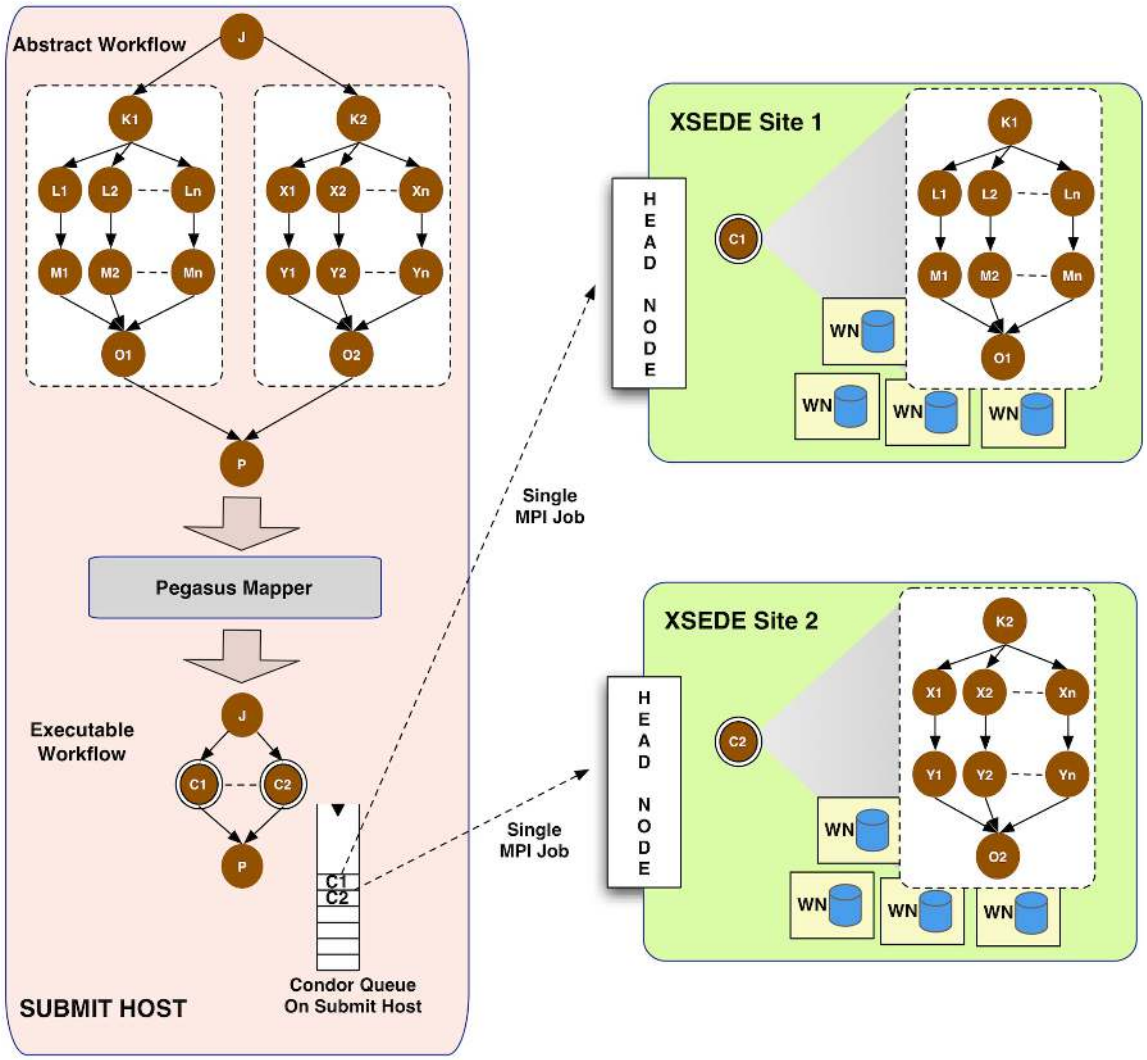
- Pegasus clusters the jobs in a workflow and runs these jobs on a dynamic Condor pool
  - Pool is grown by submitting condor_startd daemons to remote cluster
- Works great on "regular" clusters
  - XSEDE: Ranger, …
  - OSG
- Not so great on some newer Cray/IBM/… architectures
  - Problem 1: no/limited networking on compute nodes
  - Problem 2: queuing system optimized for large jobs

pegasus-mpi-cluster



- Planner creates subgraph based on user assigned labels
- Subgraph is expressed as DAG (simplified Condor DAGMan format)
- Submitted to remote resource (usually GRAM and CondorG)
- Executed with MPI master/ worker DAG engine

Large Workflows on Xsede using PMC



Summary – What Does Pegasus provide an Application - I

- **All the great features that DAGMan has!**
  - Scalability - Hierarchal Workflows. Pegasus runs workflows ranging from few computational tasks upto 1 million
  - Retries in case of failure.
- **Portability / Reuse**
  - User created workflows can easily be 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.
- **Data Management**
  - Pegasus handles replica selection, data transfers and output registrations in data catalogs. These tasks are added to a workflow as auxilliary jobs by the Pegasus planner.
- **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.
- **Error Recovery**
  - Reuse existing output products to prune the workflow and move computation to another site.

Some Applications using Pegasus

- **Astronomy**
  - Montage , Galactic Plane, Periodograms
- **Bio Informatics**
  - Brain Span, RNA Seq, SIPHT, Epigenomics, Seqware
- **Earthquake Science**
  - Cybershake, Broadband from Southern California Earthquake Center
- **Physics**
  - LIGO

Complete Listing: *http://pegasus.isi.edu/applications*

Relevant Links

- Pegasus WMS: http://pegasus.isi.edu/wms
- Tutorial and VM : http://pegasus.isi.edu/tutorial/
- Ask not what you can do for Pegasus, but what Pegasus can do for you : pegasus@isi.edu

Acknowledgements

- Pegasus Team, Condor Team, all the Scientists that use Pegasus, Funding Agencies NSF, NIH..