Managing HTC workflows with Pegasus

OSG Campus Infrastructures Community Webinar 4/26/13

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Outline

- Overview
  - What is Pegasus?
  - Components of a Pegasus workflow
    - Abstract workflow
    - Replica, transformation and site catalogs
  - Common workflow transformations
  - Debugging and statistics

- Demo
  - Our first workflow
  - Failure / debugging
  - OSG-XSEDE example
  - Task clustering
  - Data management

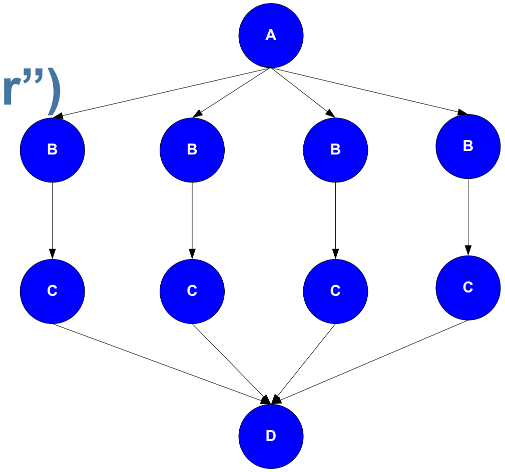
Pegasus Workflow Management System

- NSF funded project and developed since 2001 as a collaboration between USC Information Sciences Institute and the Condor Team at UW Madison

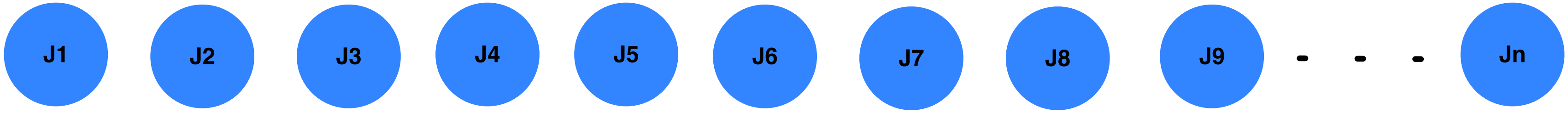
- Builds on top of Condor DAGMan.

- Abstract Workflows - Pegasus input workflow description
  - Workflow “high-level language”
  - Only identifies the computation, devoid of resource descriptions, devoid of data locations

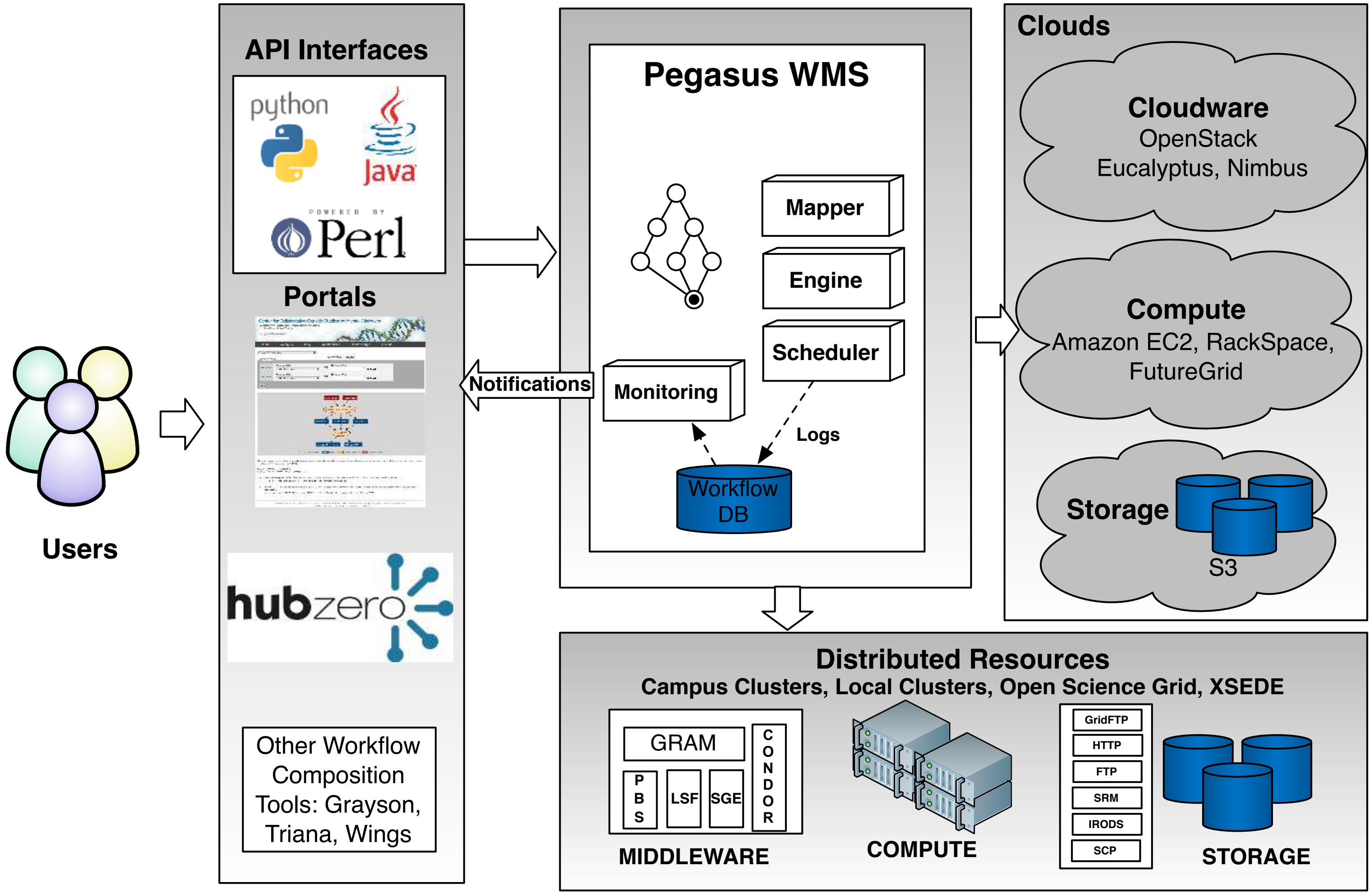
- Pegasus is a workflow planner/mapper (“compiler”)
  - Target is DAGMan DAGs and Condor submit files
  - Transforms the workflow for performance and reliability
  - Automatically locates physical locations for both workflow components and data
  - Collects runtime provenance



Workflows can be simple



Pegasus WMS



Users

API Interfaces

Portals

Other Workflow Composition Tools: Grayson, Triana, Wings

Notifications

Pegasus WMS

Mapper

Engine

Scheduler

Monitoring

Logs

Workflow DB

Clouds

Cloudware
OpenStack
Eucalyptus, Nimbus

Compute
Amazon EC2, RackSpace, FutureGrid

Storage
S3

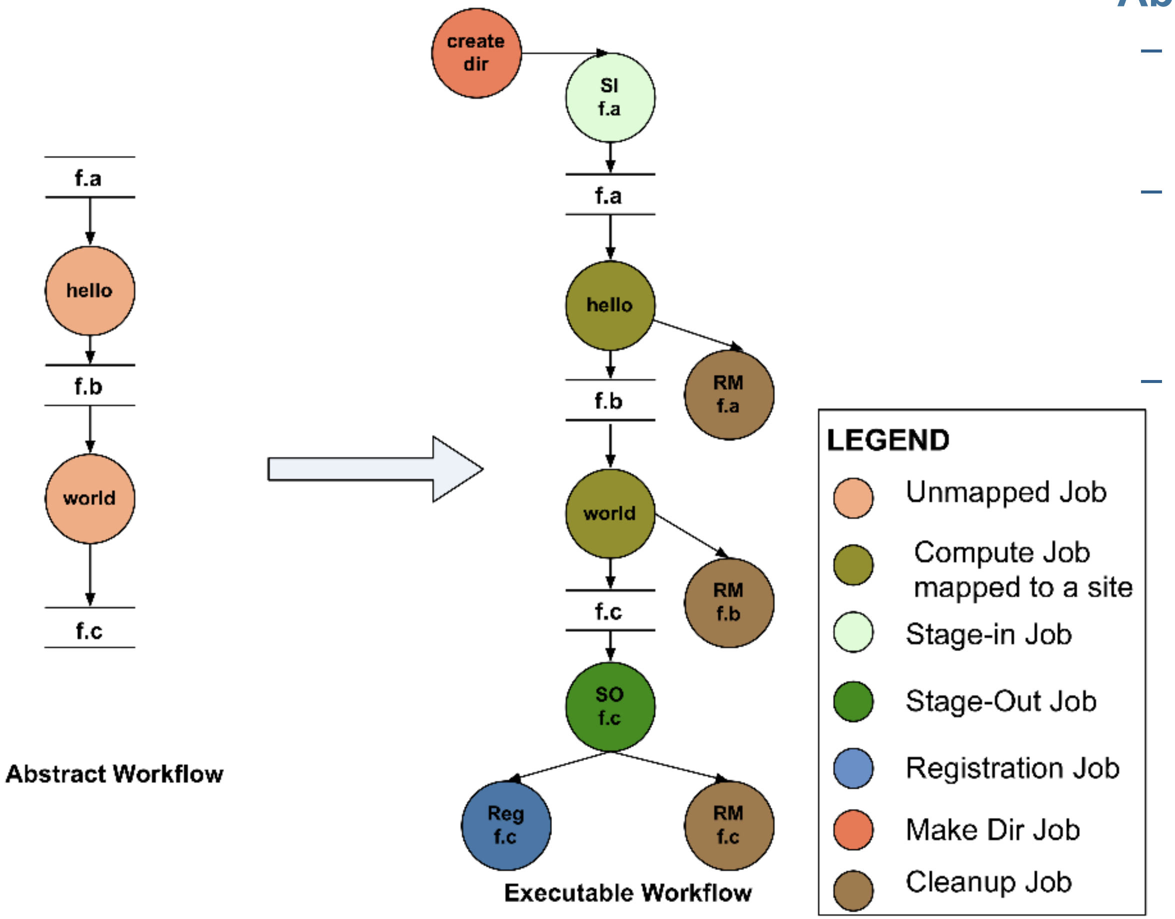
Distributed Resources
Campus Clusters, Local Clusters, Open Science Grid, XSEDE

GRAM
PBS
LSF
SGE
CONDOR
MIDDLEWARE

COMPUTE

GridFTP
HTTP
FTP
SRM
IRODS
SCP
STORAGE

Abstract to Executable Workflow Mapping



Abstract Workflow

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)**

Catalogs

- Site catalog
  - Defines the execution environment and potential data staging resources
  - Simple in the case of Condor pool, but can be more complex when running on grid resources

- Transformation catalog
  - Defines executables used by the workflow
  - Executables can be installed in different locations at different sites

- Replica catalog
  - Locations of existing data products – input files and intermediate files from previous runs

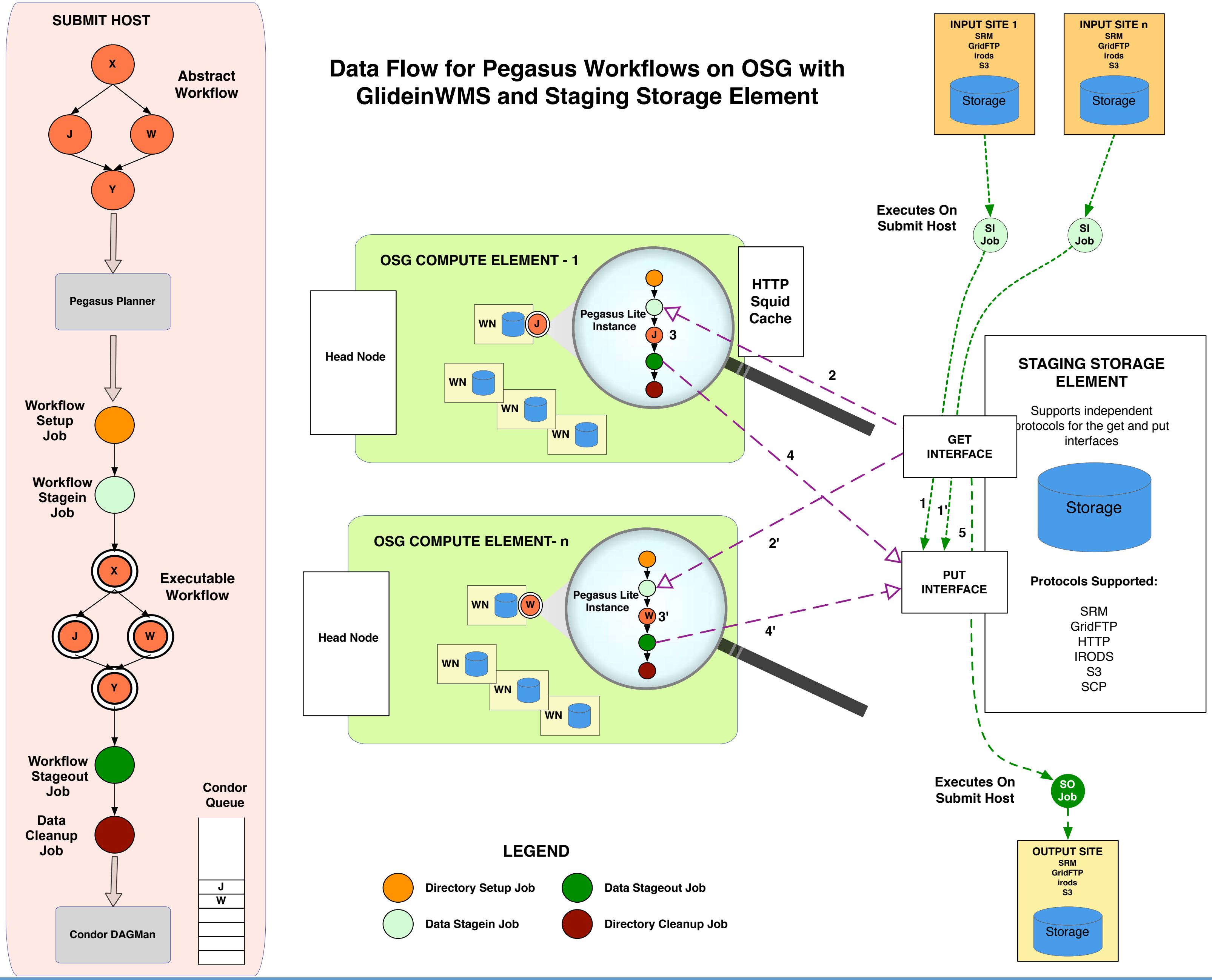
Supported Data Staging Approaches

- NonShared filesystem setup using an existing storage element for staging (typical of OSG and campus Condor pools)
  - Worker nodes don’t share a filesystem.
  - Data is pulled from / pushed to the existing storage element.
  - (Pictured on the next slide)

- Condor IO
  - Worker nodes don’t share a filesystem
  - Data is pulled from / pushed to the submit host via Condor file transfers

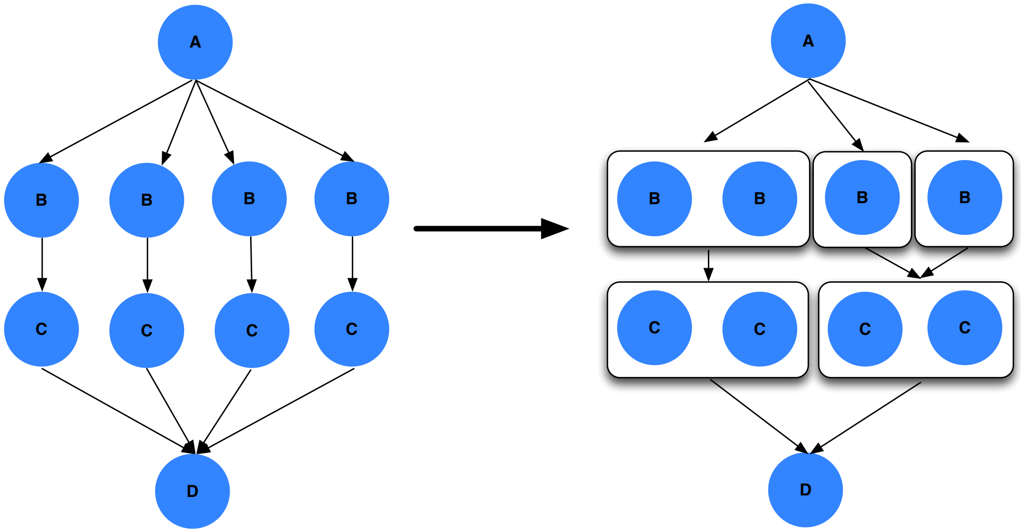
- Shared Filesystem setup (typical of XSEDE and HPC sites)
  - Worker nodes and the head node have a shared filesystem, usually a parallel filesystem with great I/O characteristics
  - Can leverage symlinking against existing datasets

Data Flow for Pegasus Workflows on OSG with GlideinWMS and Staging Storage Element



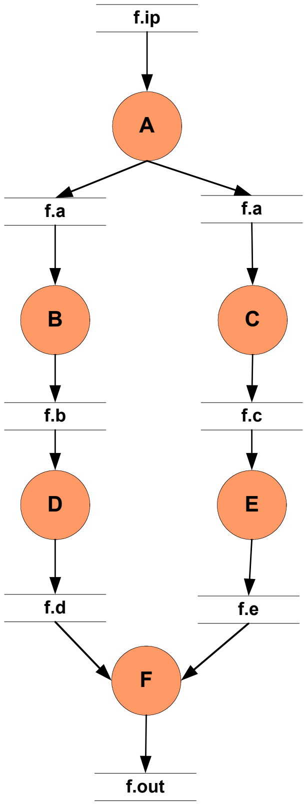
Workflow Restructuring to improve application performance

- 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

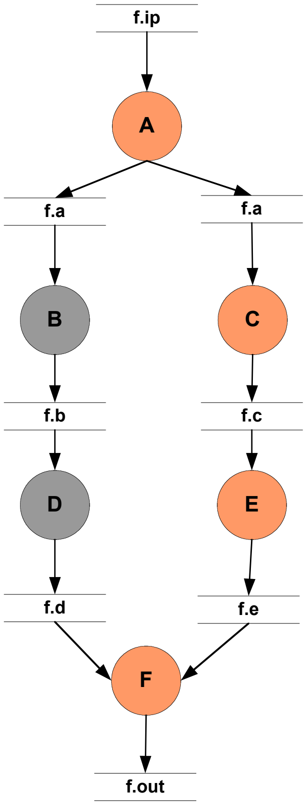


Level-based clustering

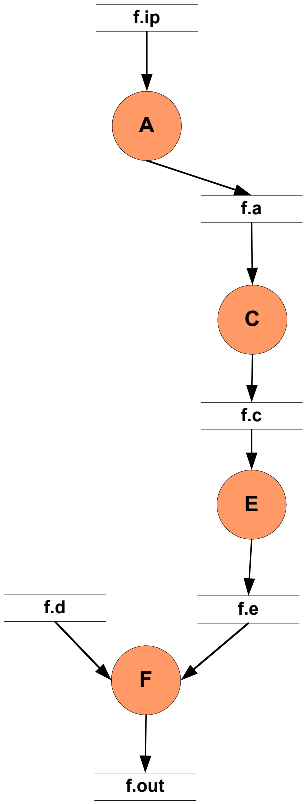
Workflow Reduction (Data Reuse)



Abstract Workflow



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



Delete Job D and Job B

Workflow Monitoring - Stampede

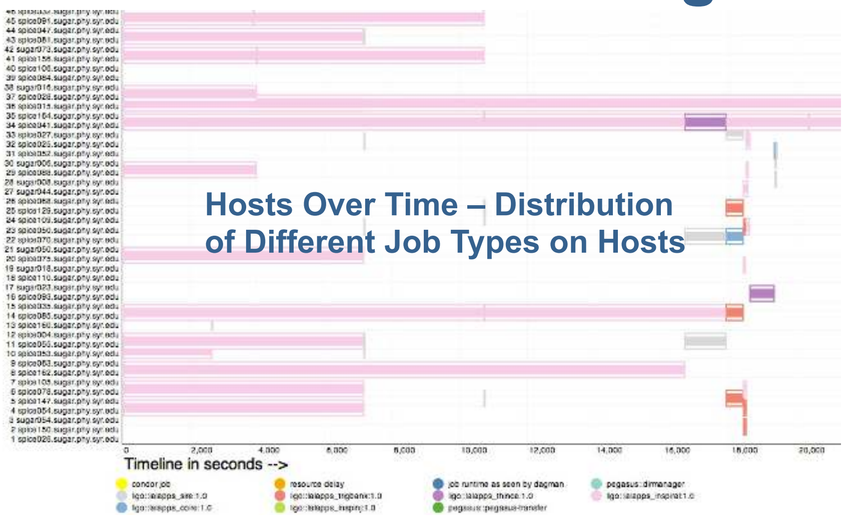
- Leverage Stampede Monitoring framework with DB backend
  - Populates data at runtime. A background daemon monitors the logs files and populates information about the workflow to a database
  - Stores workflow structure, and runtime stats for each task.

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

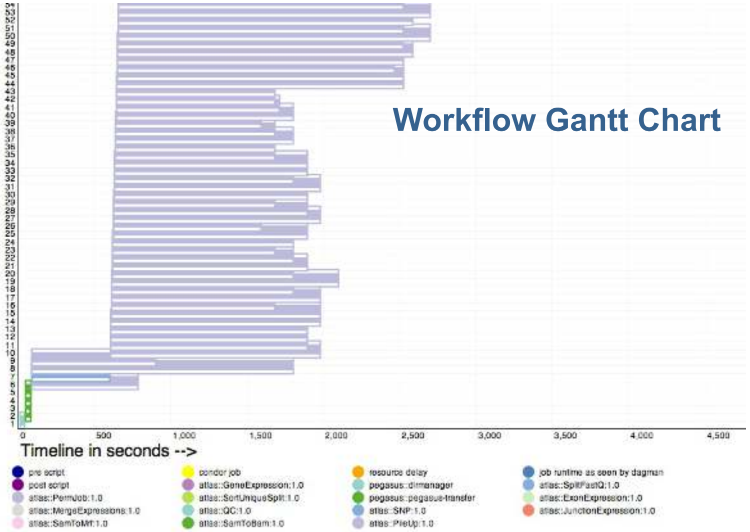
```
------------------------------------------------------------------------------
Type           Succeeded Failed  Incomplete  Total     Retries   Total+Retries
Tasks          135002    0       0           135002    0         135002
Jobs           4529      0       0           4529      0         4529
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)
```

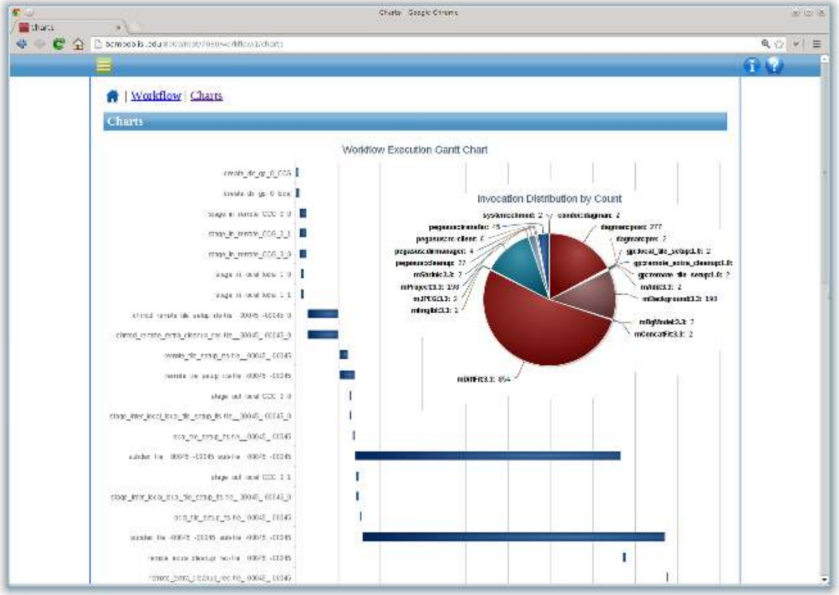
Workflow Monitoring - Stampede

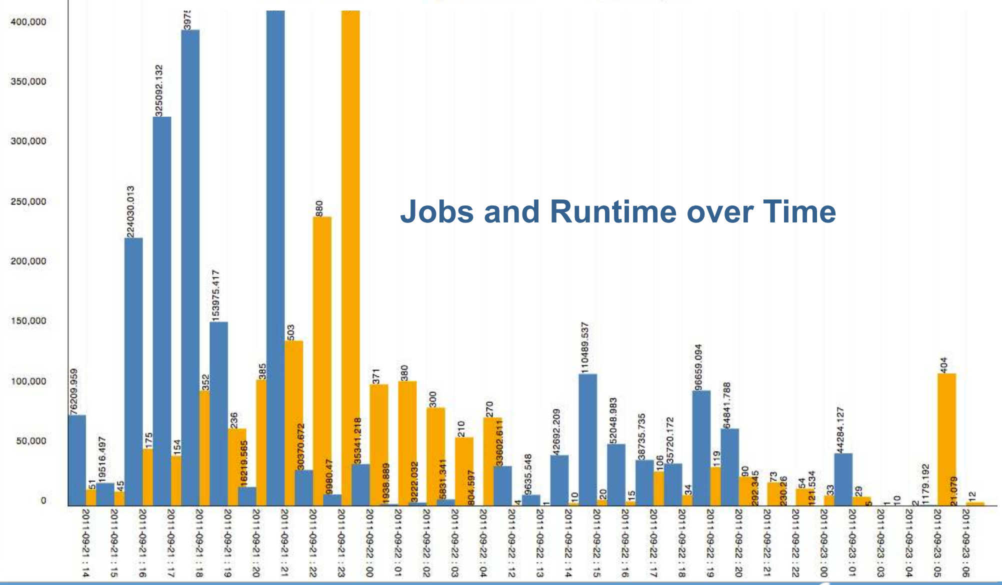


Hosts Over Time – Distribution of Different Job Types on Hosts



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.

Relevant Links

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

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