Workflows using Pegasus

Pegasus Workflow Management System

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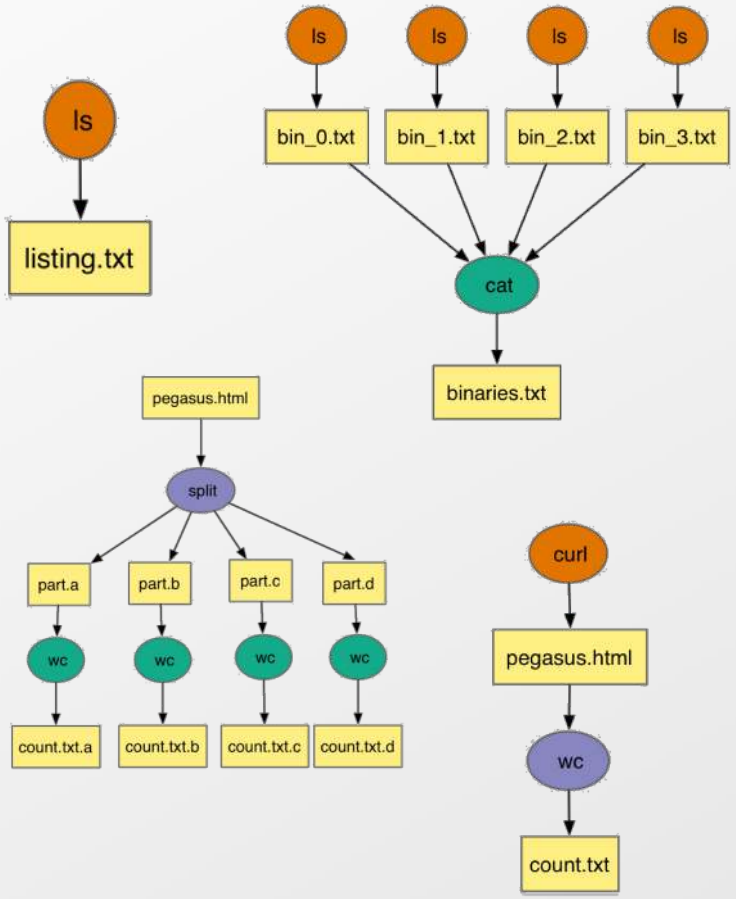
http://pegasus.isi.edu

Compute Pipelines Building Blocks



Compute Pipelines

Allows scientists to connect different codes together and execute their analysis

Pipelines can be very simple (independent or parallel) jobs or complex represented as DAG's

Helps users to automate scale up

However, it is still up-to user to figure out

Data Management

How do you ship in the small/large amounts data required by your pipeline and protocols to use?

How best to leverage different infrastructure setups

OSG has no shared filesystem while XSEDE and your local campus cluster has one!

Debug and Monitor Computations

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

Why Pegasus?

Automates complex, multi-stage processing pipelines

Enables parallel, **distributed computations**

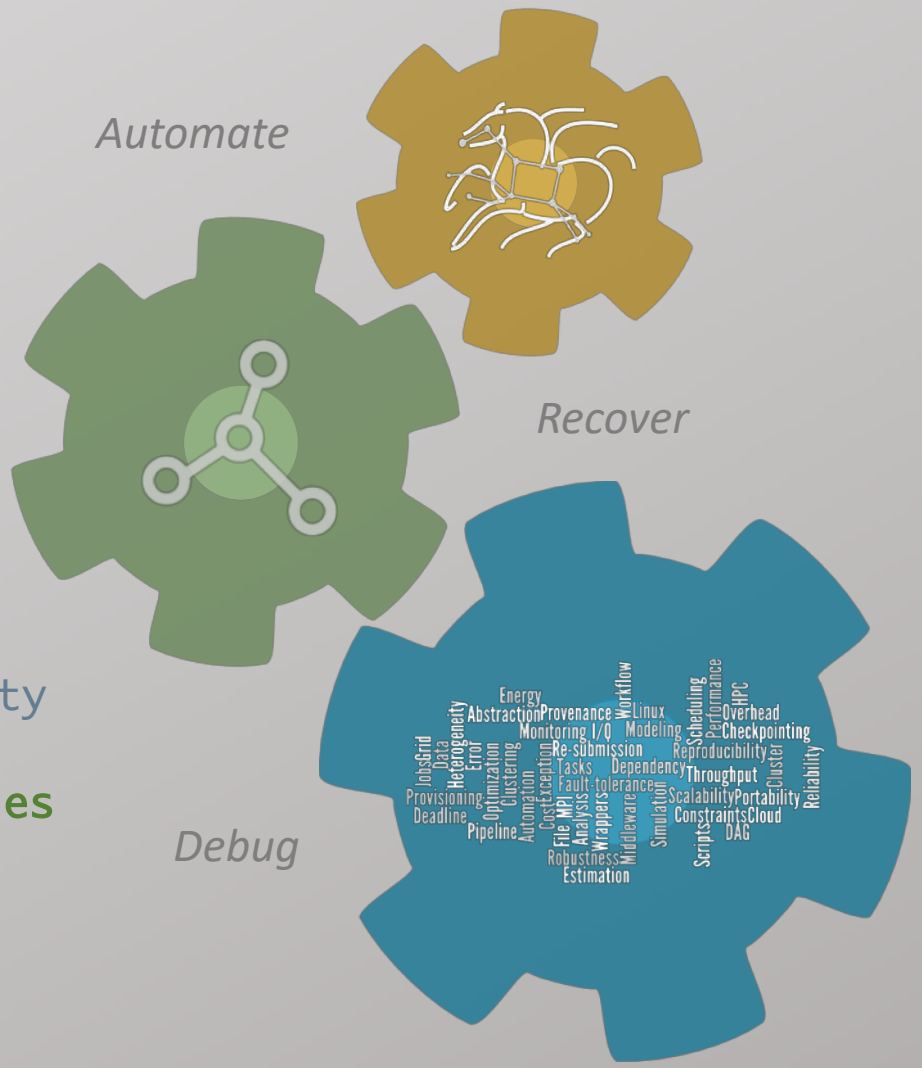
Automatically executes data transfers

Reusable, aids **reproducibility**

Records how data was produced (**provenance**)

Handles **failures** with to provide reliability

Keeps track of data and **files**



HTCondor High Throughput Computing

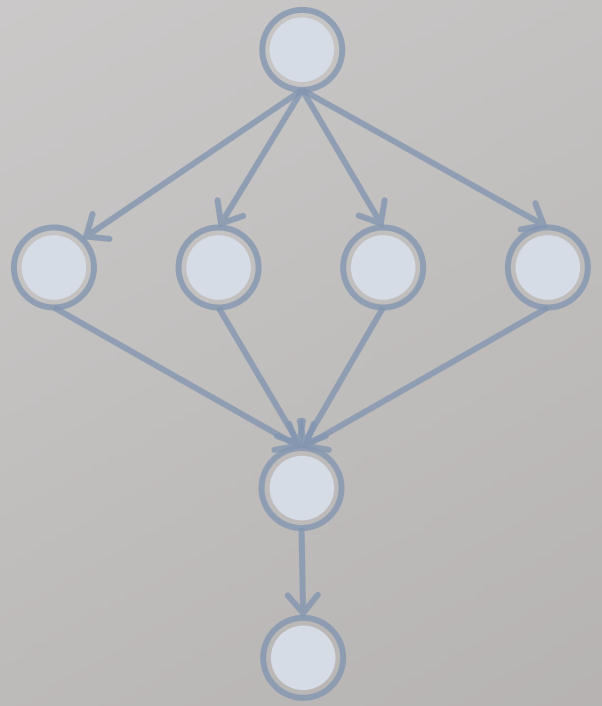
NSF funded project since 2001, with close collaboration with HTCondor team

Basic concepts…

Key Pegasus Concepts

Pegasus WMS == Pegasus planner (mapper) + DAGMan workflow engine + HTCondor scheduler/broker

- Pegasus maps workflows to infrastructure
- DAGMan manages dependencies and reliability
- HTCondor is used as a broker to interface with different schedulers



Workflows are DAGs

- Nodes: jobs, edges: dependencies
- No while loops, no conditional branches
- Jobs are standalone executables

Planning occurs ahead of execution

Planning converts an abstract workflow into a concrete, executable workflow

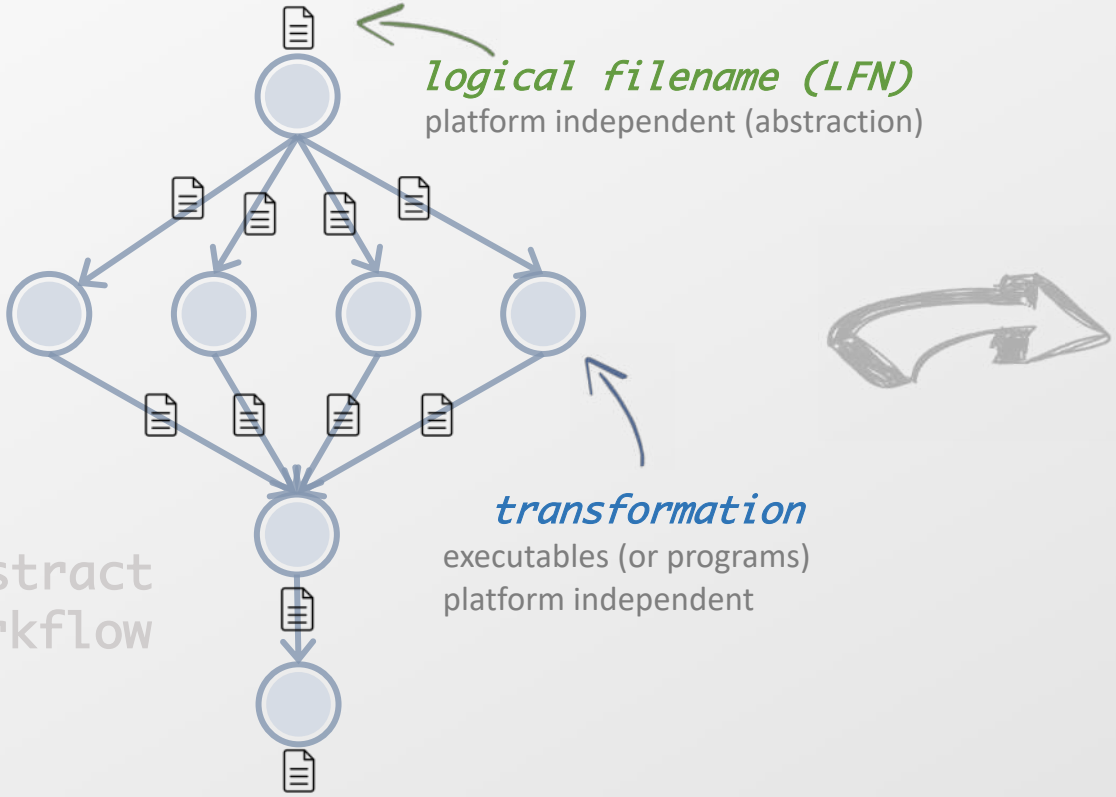
- Planner is like a compiler

DAX

DAG in XML

Portable Description

Users do not worry about
low level execution details



logical filename (LFN)
platform independent (abstraction)

transformation
executables (or programs)
platform independent

abstract workflow

DAG

directed-acyclic graphs

stage-in job
Transfers the workflow input data

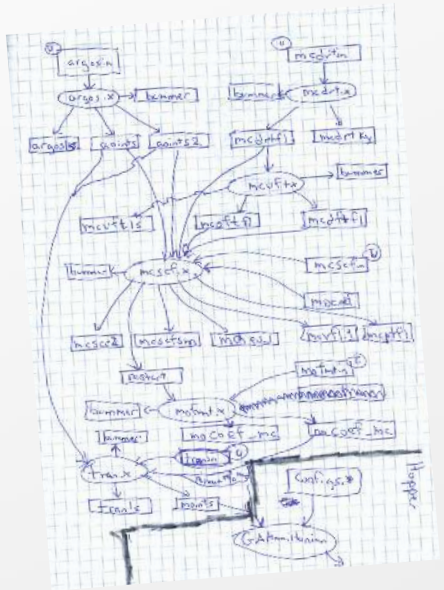
cleanup job
Removes unused data

stage-out job
Transfers the workflow output data

registration job
Registers the workflow output data

executable workflow

Pegasus also provides tools to generate the abstract workflow



```python
#!/usr/bin/env python

from Pegasus.DAX3 import *
import sys
import os

# Create a abstract dag
dax = ADAG("hello_world")

# Add the hello job
hello = Job(namespace="hello_world",
            name="hello", version="1.0")
b = File("f.b")
hello.uses(a, link=Link.INPUT)
hello.uses(b, link=Link.OUTPUT)
dax.addJob(hello)

# Add the world job (depends on the hello job)
world = Job(namespace="hello_world",
            name="world", version="1.0")
c = File("f.c")
world.uses(b, link=Link.INPUT)
world.uses(c, link=Link.OUTPUT)
dax.addJob(world)

# Add control-flow dependencies
dax.addDependency(Dependency(parent=hello,
                             child=world))

# Write the DAX to stdout
dax.writeXML(sys.stdout)
```

python™

Java

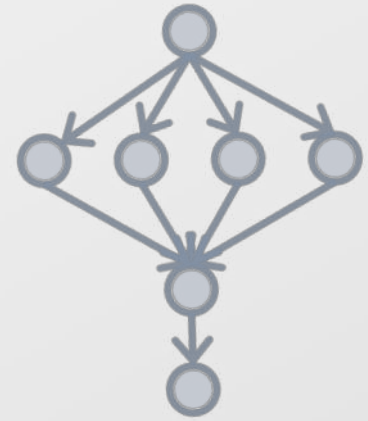
R

perl

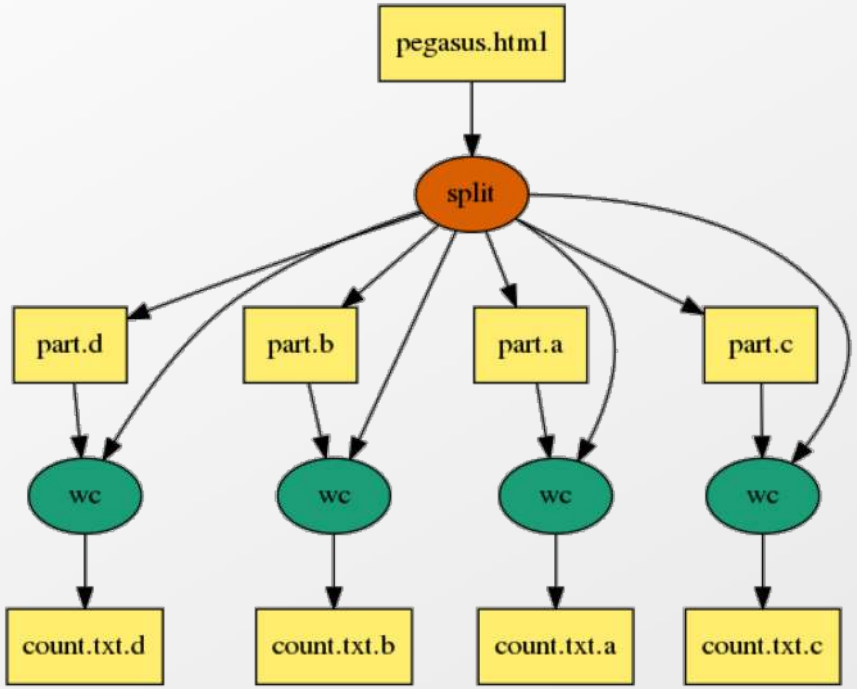
jupyter

```xml
<?xml version="1.0" encoding="UTF-8"?>

<!-- generator: python -->
<adag xmlns="http://pegasus.isi.edu/schema/DAX"
            version="3.4" name="hello_world">

    <!-- describe the jobs making
        up the hello world pipeline -->
    <job id="ID0000001" namespace="hello_world"
                    name="hello" version="1.0">

        <uses name="f.b" link="output"/>
        <uses name="f.a" link="input"/>
    </job>

    <job id="ID0000002" namespace="hello_world"
                    name="world" version="1.0">

        <uses name="f.b" link="input"/>
        <uses name="f.c" link="output"/>
    </job>

    <!-- describe the edges in the DAG -->
    <child ref="ID0000002">
        <parent ref="ID0000001"/>
    </child>
</adag>
```

DAX



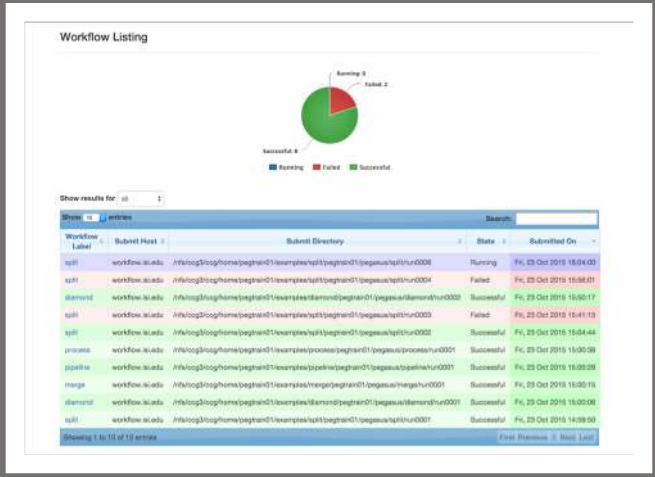
An example
Split Workflow



Visualization Tools:
pegasus-graphviz
pegasus-plots

https://pegasus.isi.edu/documentation/tutorial_submitting_wf.php

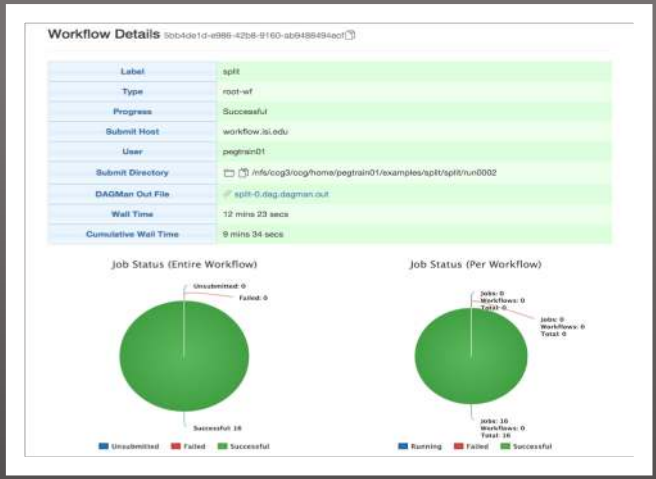
```
#!/usr/bin/env python

import os, pwd, sys, time
from Pegasus.DAX3 import *

# Create an abstract dag
dax = ADAG("split")

webpage = File("pegasus.html")

# the split job that splits the webpage into smaller chunks
split = Job("split")
split.addArguments("-l","100","-a","1",webpage,"part.")
split.uses(webpage, link=Link.INPUT)
# associate the label with the job. all jobs with same label
# are run with PMC when doing job clustering
split.addProfile( Profile("pegasus","label","p1"))
dax.addJob(split)

# we do a parmeter sweep on the first 4 chunks created
for c in "abcd":
    part = File("part.%s" % c)
    split.uses(part, link=Link.OUTPUT, transfer=False, register=False)
    count = File("count.txt.%s" % c)
    wc = Job("wc")
    wc.addProfile( Profile("pegasus","label","p1"))
    wc.addArguments("-l",part)
    wc.setStdout(count)
    wc.uses(part, link=Link.INPUT)
    wc.uses(count, link=Link.OUTPUT, transfer=True, register=True)
    dax.addJob(wc)

    #adding dependency
    dax.depends(wc, split)

f = open("split.dax", "w")
dax.writeXML(f)
f.close()
```



Pegasus dashboard

web interface for monitoring and debugging workflows

Real-time monitoring of workflow executions. It shows the status of the workflows and jobs, job characteristics, statistics and performance metrics. Provenance data is stored into a relational database.



Real-time Monitoring

Reporting

Debugging

Troubleshooting

RESTful API

Pegasus dashboard

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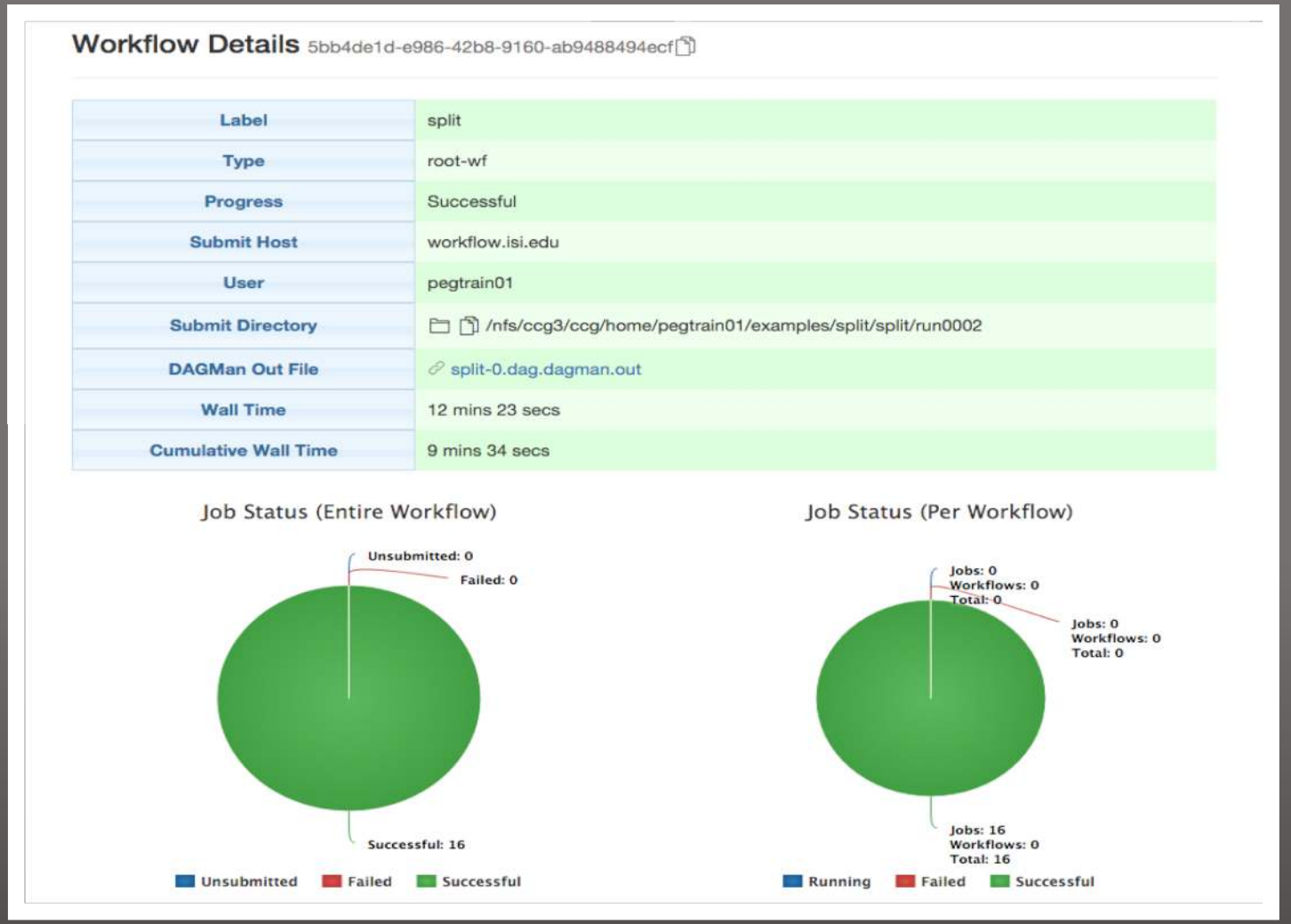


>_ command-line…

```
$ pegasus-status pegasus/examples/split/run0001
STAT IN_STATE JOB
Run 00:39 split-0 (/home/pegasus/examples/split/run0001)
Idle 00:03  └─split_ID0000001
Summary: 2 Condor jobs total (I:1 R:1)

UNRDY READY PRE IN_Q POST DONE FAIL %DONE STATE   DAGNAME
 14     0    0    1    0   2    0    11.8 Running *split-0.dag
```

```
$ pegasus-analyzer pegasus/examples/split/run0001
pegasus-analyzer: initializing...

**************************Summary***************************

Total jobs : 7 (100.00%)
# jobs succeeded : 7 (100.00%)
# jobs failed : 0 (0.00%)
# jobs unsubmitted : 0 (0.00%)
```

```
$ pegasus-statistics -s all pegasus/examples/split/run0001
------------------------------------------------------------------------------
Type           Succeeded Failed Incomplete Total Retries Total+Retries
Tasks              5       0        0        5     0         5
Jobs              17       0        0       17     0        17
Sub-Workflows      0       0        0        0     0         0
------------------------------------------------------------------------------

Workflow wall time : 2 mins, 6 secs
Workflow cumulative job wall time : 38 secs
Cumulative job wall time as seen from submit side : 42 secs
Workflow cumulative job badput wall time :
Cumulative job badput wall time as seen from submit side :
```

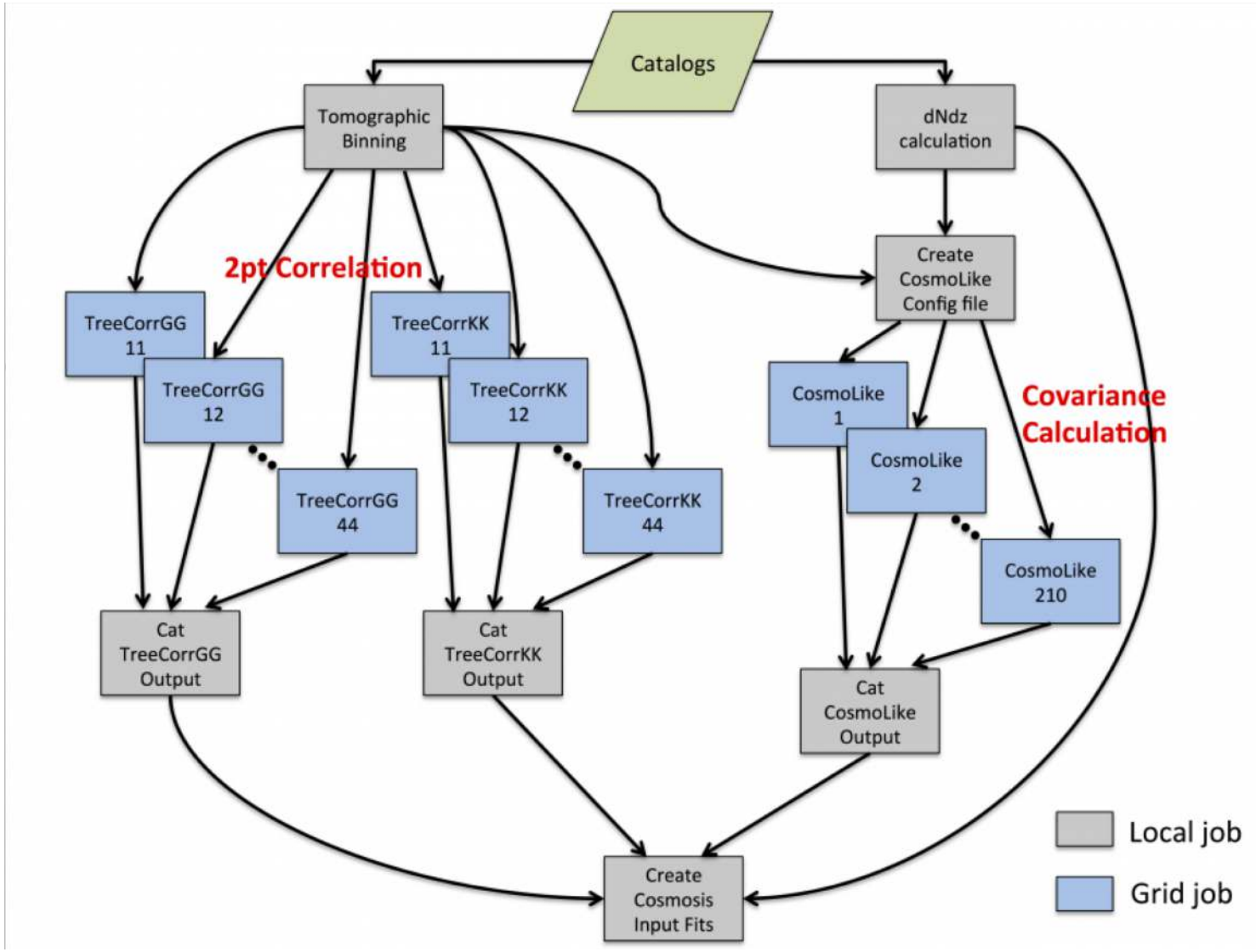
Provenance data can be summarized
pegasus-statistics

or used for debugging
pegasus-analyzer

Hands-on Demo…

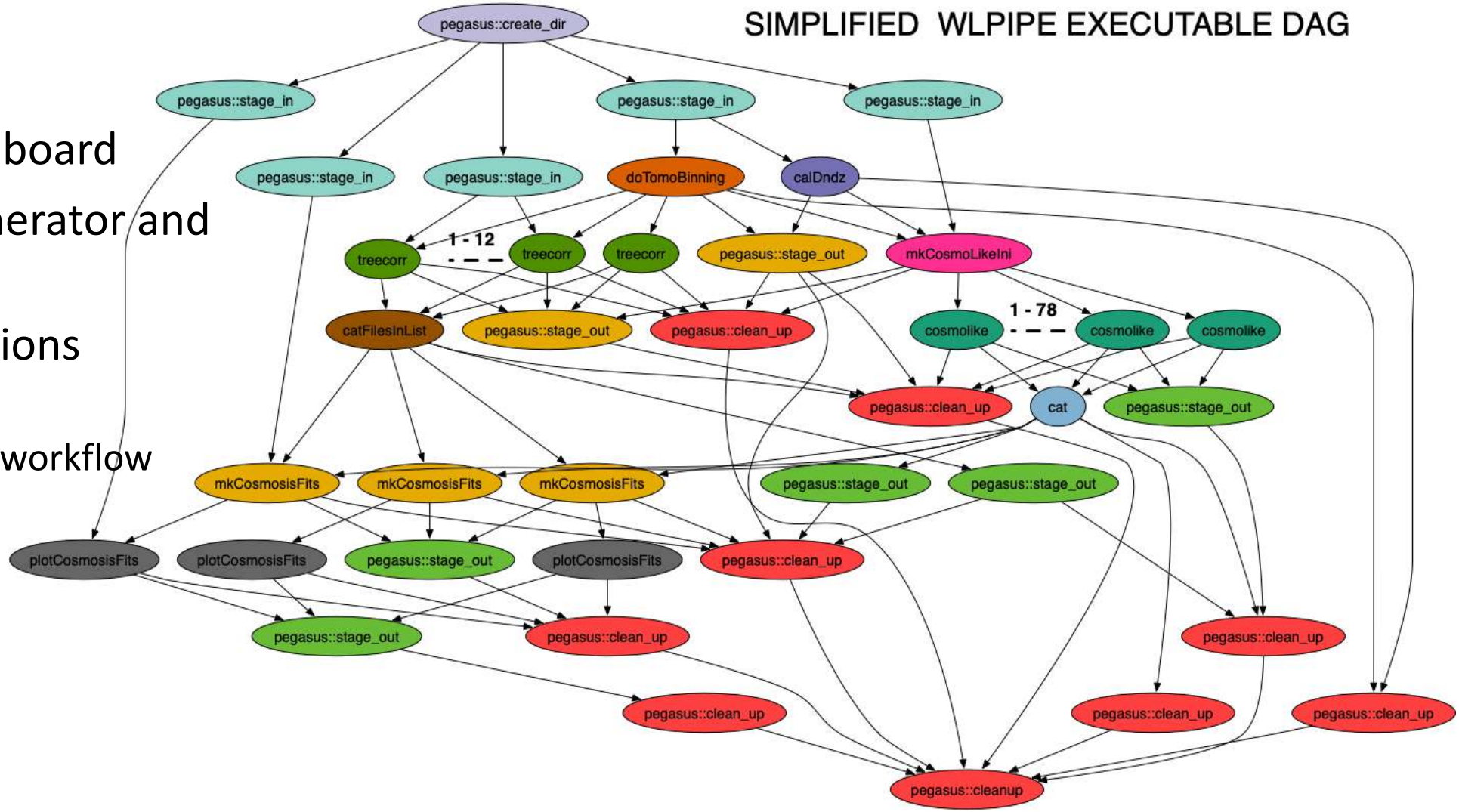
Hands On Demo

- Weak Lensing Pipeline
  - https://github.com/pegasus-isi/pegasus-wlpipe
- An example of a typical gravitational weak lensing analysis. It uses publicly available Science Verification catalogs the Dark Energy Survey (DES-SV).
- The pipeline is run currently at Fermi Grid
- We will run the example version at a cluster at ISI
- Science Codes are bundled into a Singularity Container
- This is an interactive session. Please interrupt at anytime to ask questions.



Outline

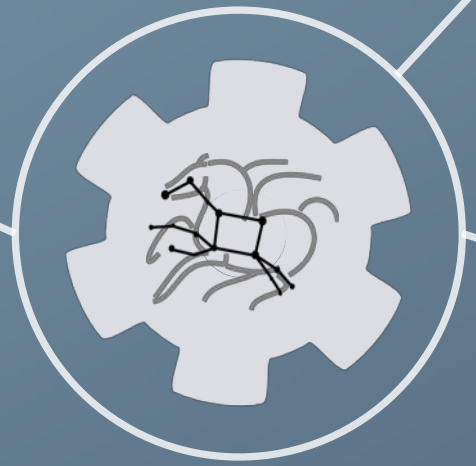
- Submit a workflow
- Go through the dashboard
- Go over the DAX generator and catalogs
- Show debugging options
  - pegasus-analyzer
  - Recover from failed workflow
- pegasus-statistics



So, what information does Pegasus need?

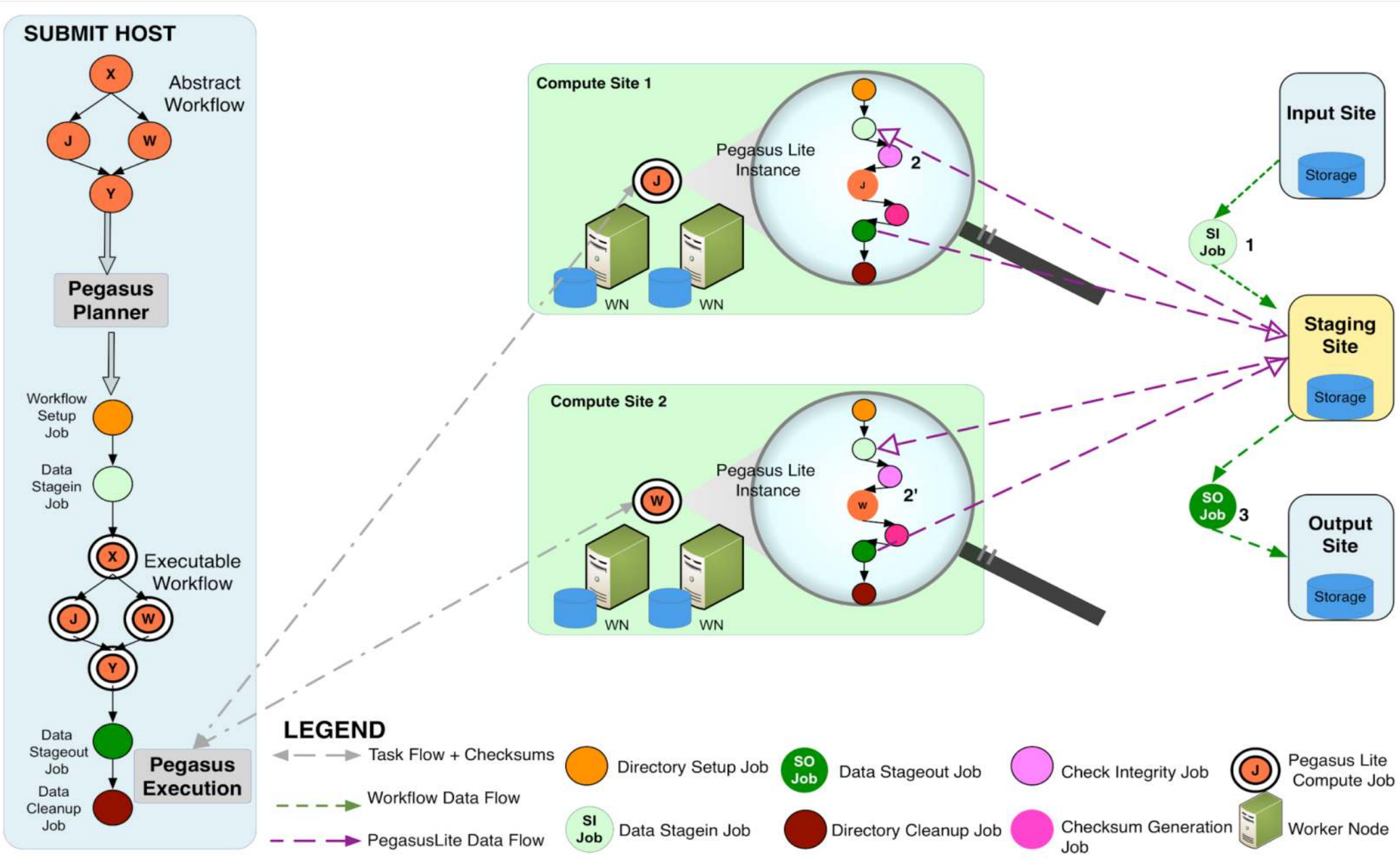
Transformation Catalog
describes all of the executables (called “transformations”) used by the workflow

Site Catalog
describes the sites where the workflow jobs are to be executed



Replica Catalog
describes all of the input data stored on external servers

Distributed Execution



Job Submissions

Local

Submit Machine
Personal HTCondor

*Local Campus Cluster accessible via Submit Machine **
HTCondor via Glite

Remote

*BOSCO + SSH***
Each node in executable workflow submitted via SSH connection to remote cluster

*BOSCO based Glideins***
SSH based submission of Glideins

PyGlidein
ICE Cube Glidein service

OSG using glideinWMS

CREAMCE
Uses CondorG

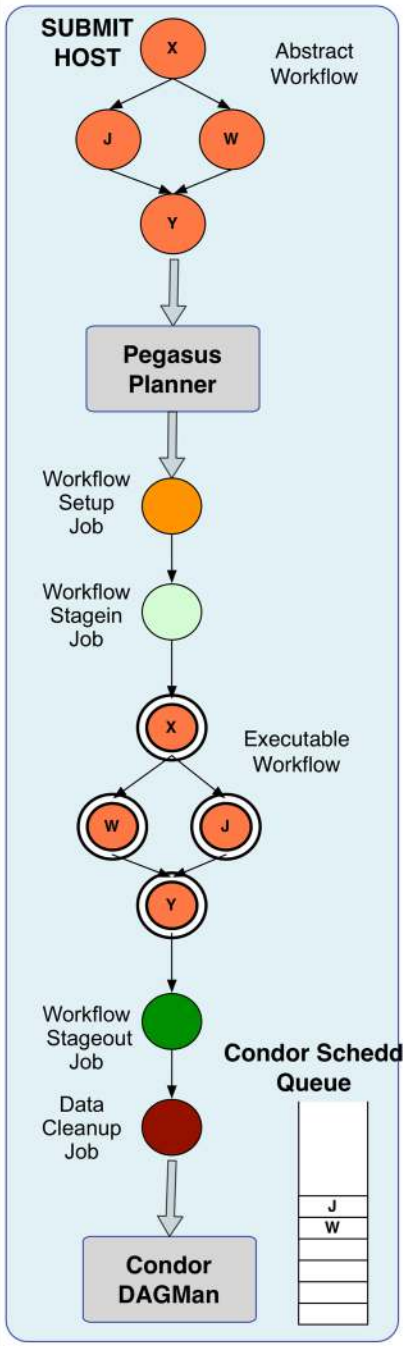
Globus GRAM
Uses CondorG

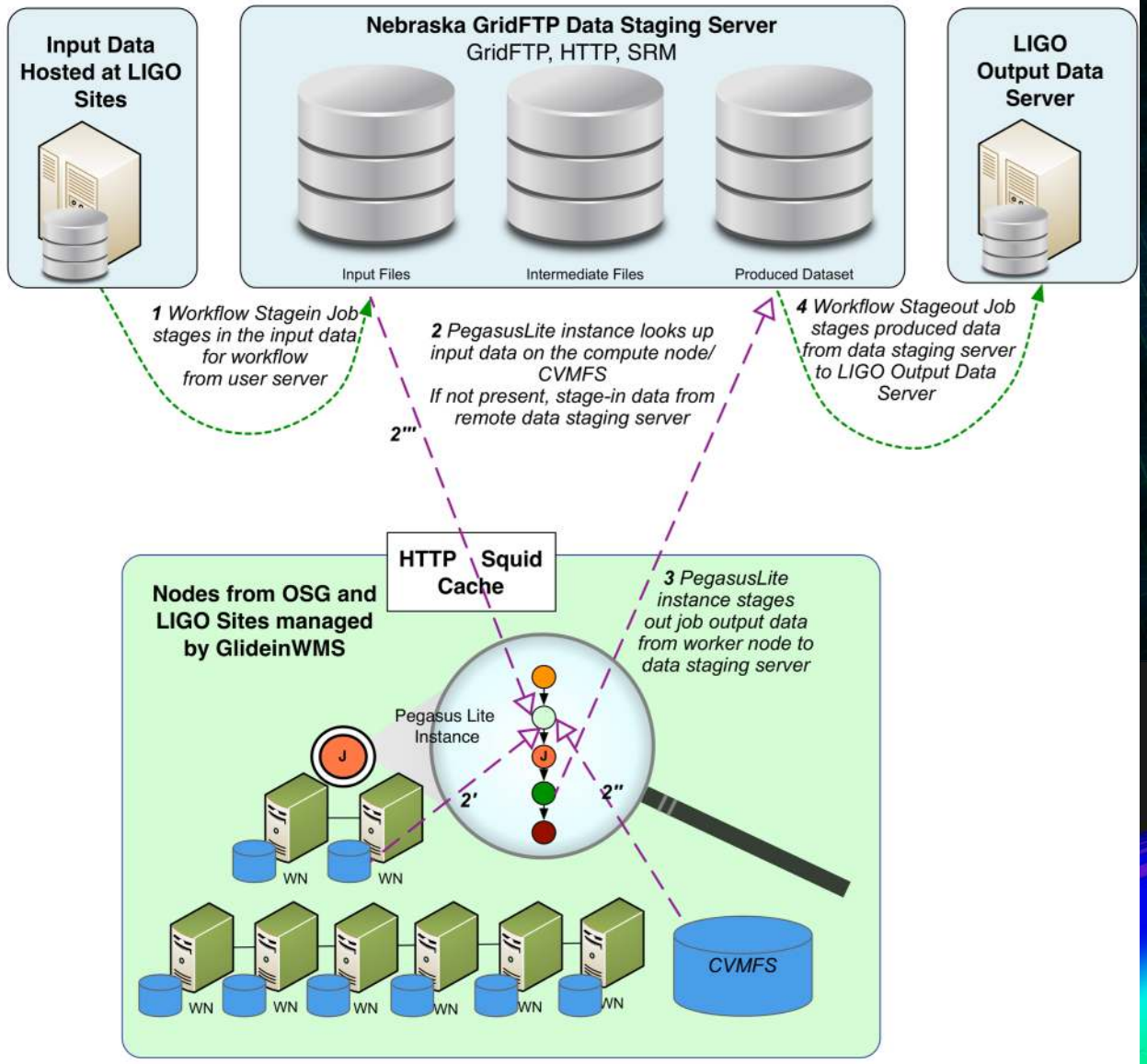
** Both Glite and BOSCO build on HTCondor BLAHP Support.
Supported schedulers

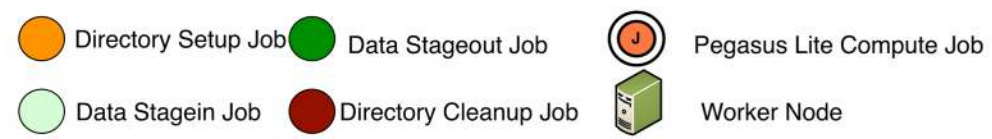
PBS SGE SLURM MOAB

Some of the successful stories…

Data Flow for LIGO Pegasus Workflows in OSG



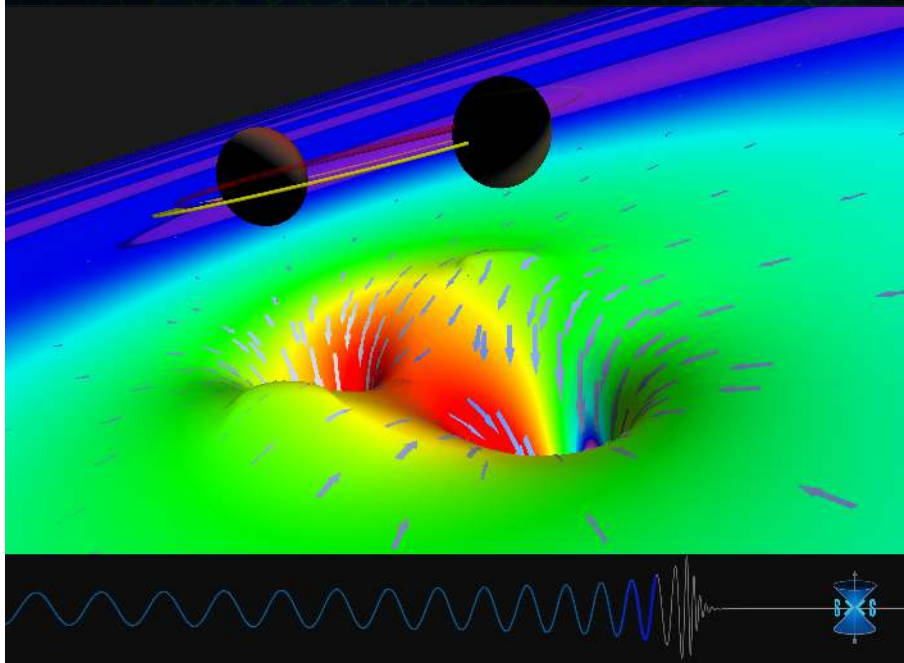




Advanced LIGO – Laser Interferometer Gravitational Wave Observatory

60,000 compute tasks
Input Data: 5000 files (10GB total)
Output Data: 60,000 files (60GB total)

executed on LIGO Data Grid, Open Science Grid and XSEDE



Advanced LIGO PyCBC Workflow

One of the main pipelines to measure the statistical significance of data needed for discovery

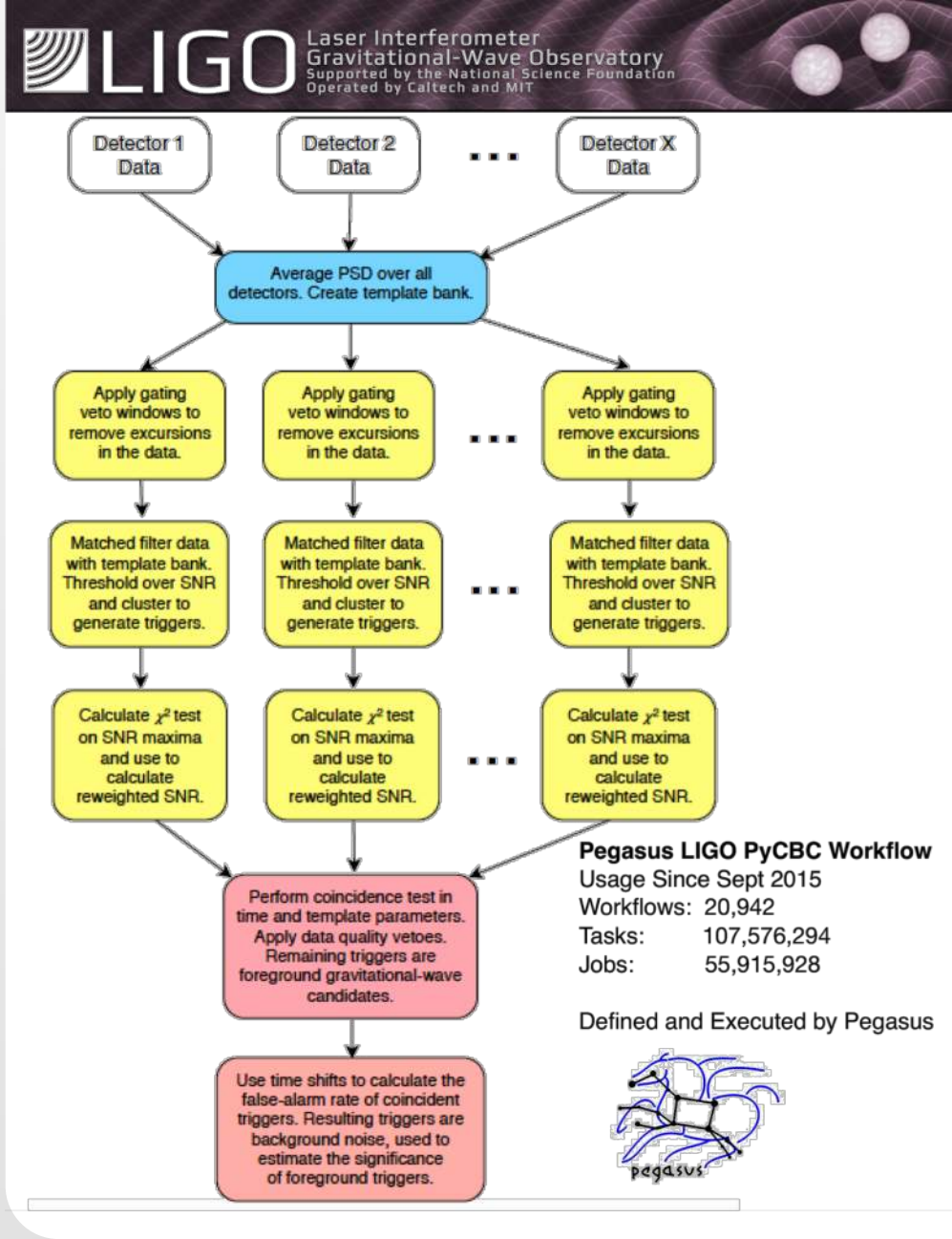
Contains **100's of thousands of jobs** and accesses on order of **terabytes of data**

Uses data from multiple detectors

For the detection, the pipeline was executed on Syracuse and Albert Einstein Institute Hannover

A single run of the binary black hole + binary neutron star search through the O1 data (about 3 calendar months of data with 50% duty cycle) requires a **workflow** with **194,364 jobs**

Generating the final O1 results with all the review required for the first discovery took about **20 million core hours**



PyCBC Papers: An improved pipeline to search for gravitational waves from compact binary coalescence. *Samantha Usman, Duncan Brown et al.*
The PyCBC search for gravitational waves from compact binary coalescence, *Samantha Usman et al* (https://arxiv.org/abs/1508.02357)
PyCBC Detection GW150914: First results from the search for binary black hole coalescence with Advanced LIGO. *B. P. Abbott et al.*

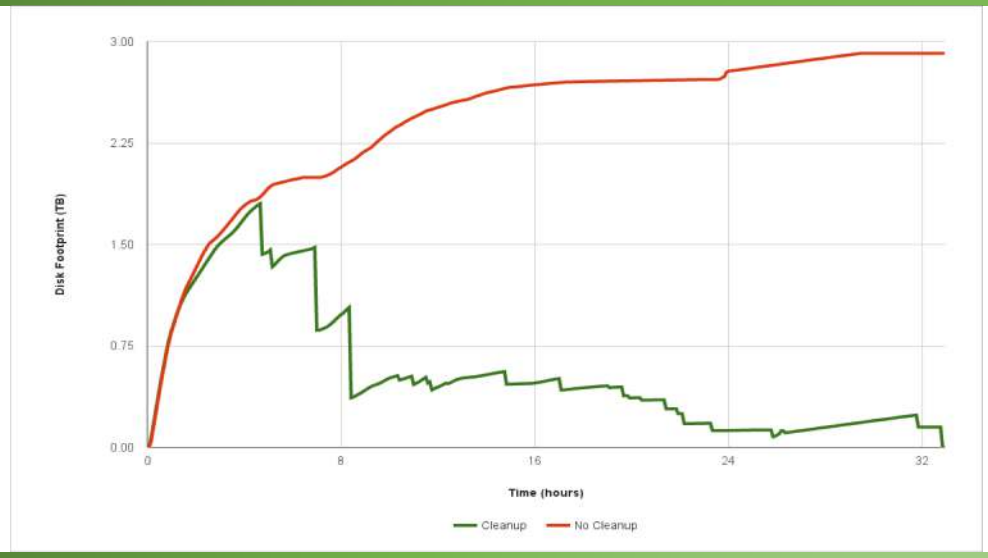
Soybean Workflow

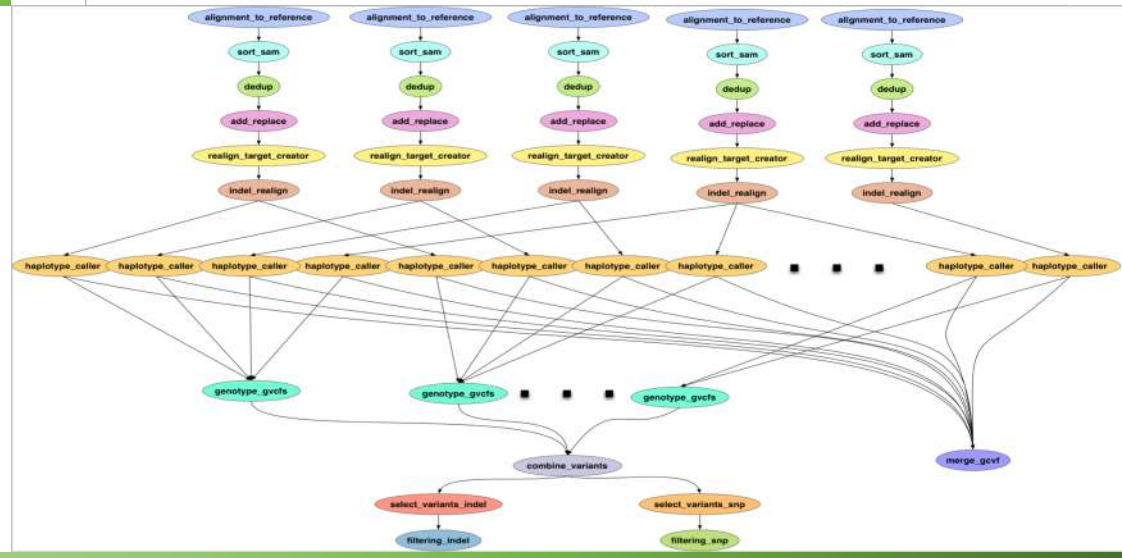
TACC Wrangler as Execution Environment

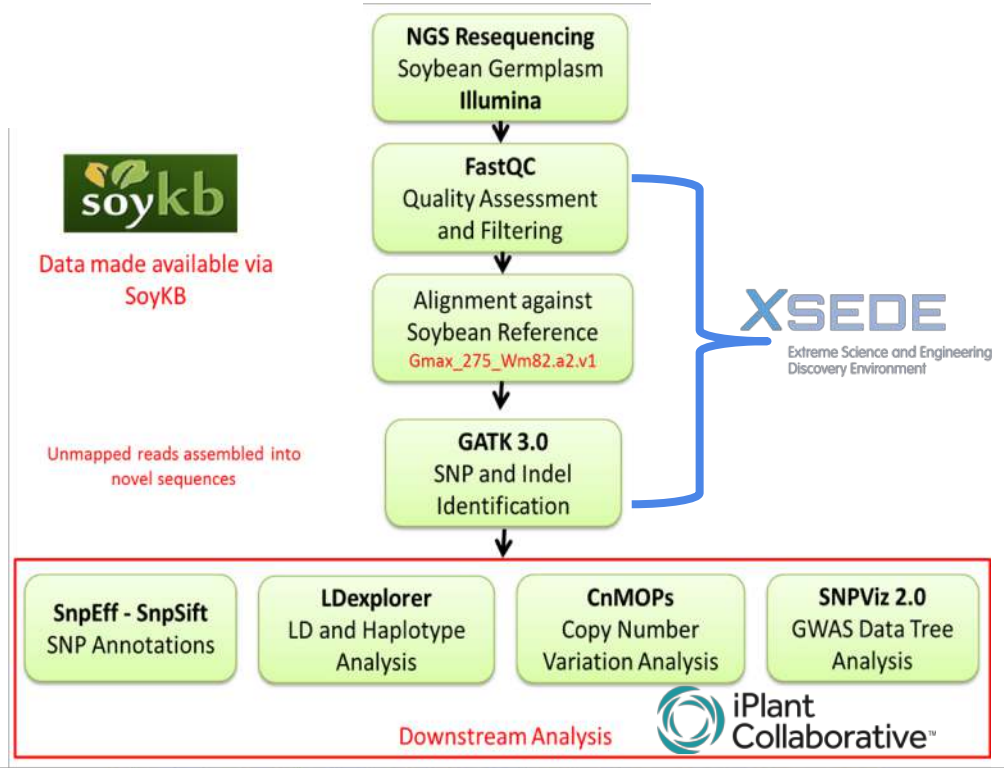
Flash Based Shared Storage

Switched to glideins (pilot jobs) - Brings in remote compute nodes and joins them to the HTCondor pool on the submit host - Workflow runs at a finer granularity

Works well on Wrangler due to more cores and memory per node (48 cores, 128 GB RAM)







Pegasus est. 2001

Automate, recover, and debug scientific computations.

Get Started

Pegasus Website

http://pegasus.isi.edu

Users Mailing List

pegasus-users@isi.edu

Pegasus Online Office Hours

https://pegasus.isi.edu/blog/online-pegasus-office-hours/

Bi-monthly basis on second Friday of the month, where we address user questions and also apprise the community of new developments

Support

pegasus-support@isi.edu

Pegasus

Workflow Management System

USC University of Southern California

Information Sciences Institute

https://pegasus.isi.edu/jobs

We're Hiring!