Compute Pipelines with Pegasus: An Introduction

Pegasus Workflow Management System

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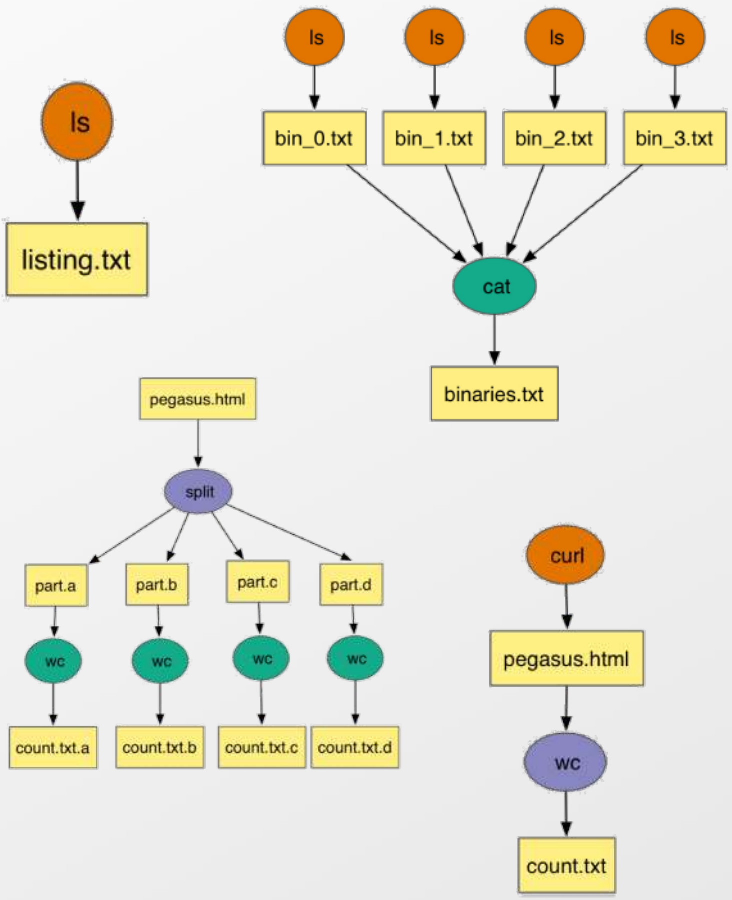
http://pegasus.isi.edu

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**

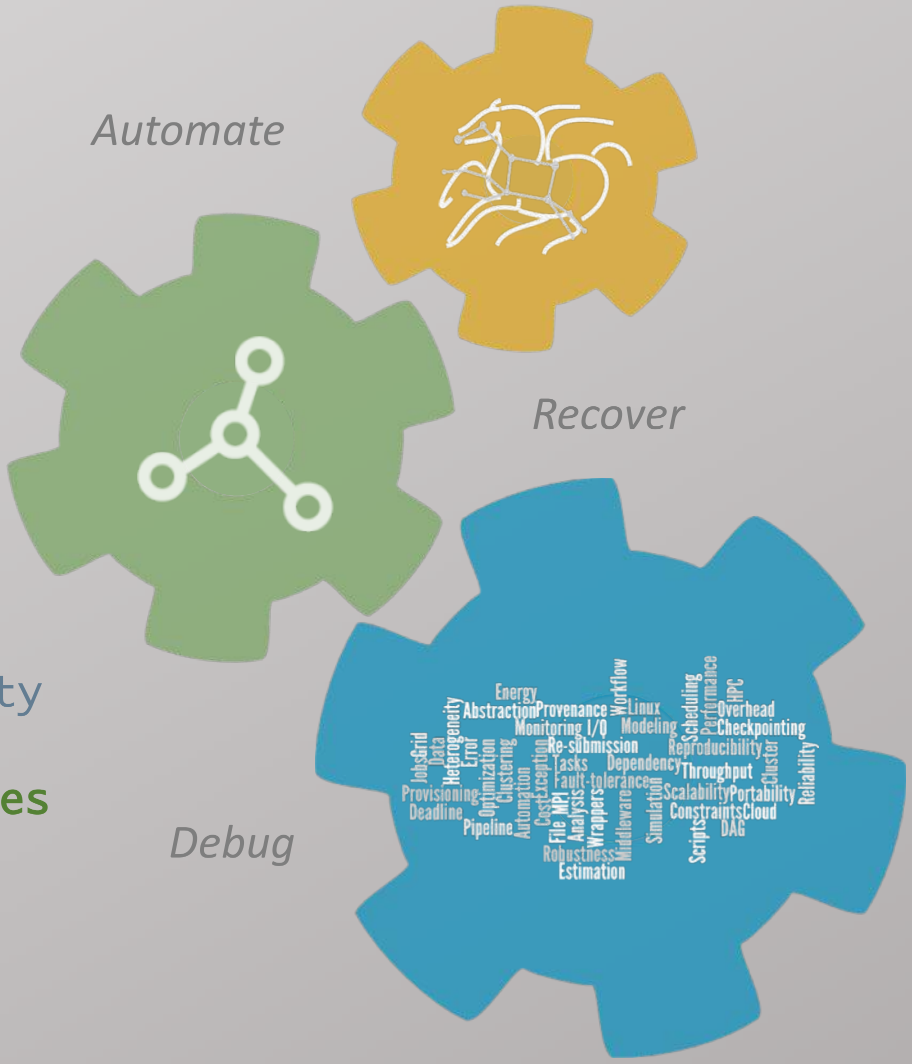
Automatically executes data transfers

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

Some of the successful stories…

Advanced LIGO PyCBC Workflow

Laser Interferometer Gravitational-Wave Observatory
Supported by the National Science Foundation
Operated by Caltech and MIT

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

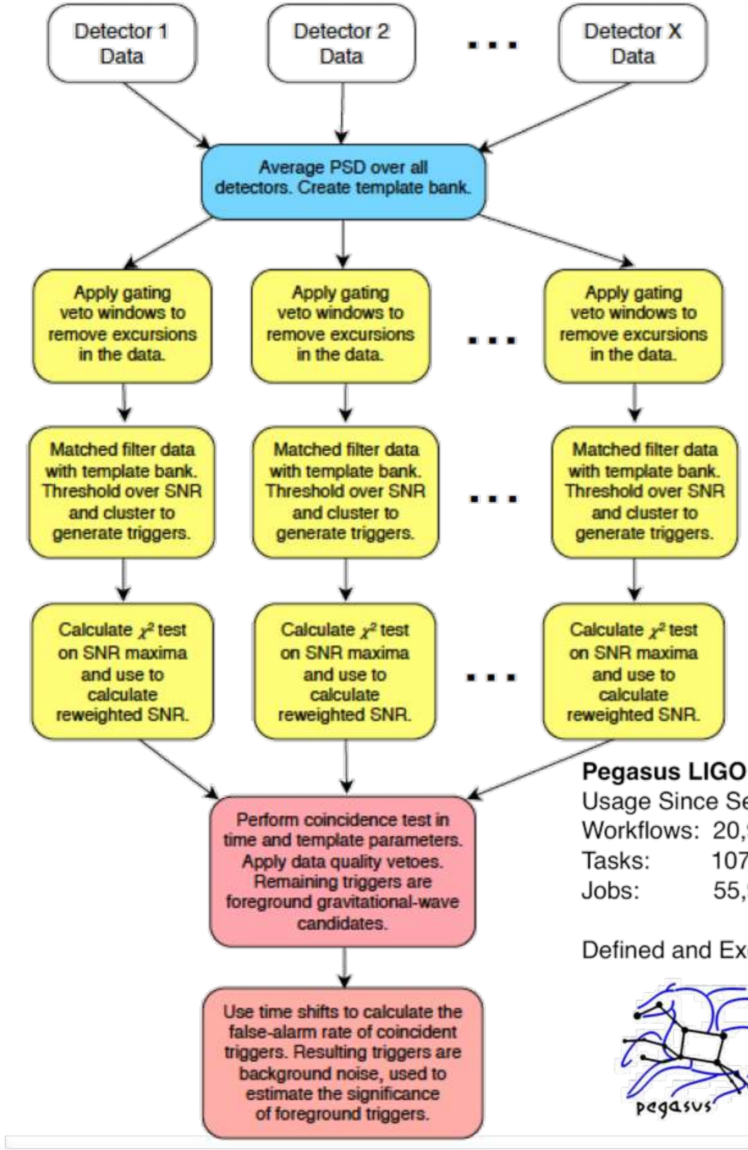
Contains **100's of thousands of jobs** and accesses on order of **terabytes of data**

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**



Pegasus LIGO PyCBC Workflow

Usage Since Sept 2015

Workflows: 20,942

Tasks: 107,576,294

Jobs: 55,915,928

Defined and Executed by Pegasus

pegasus

Pegasus

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.*

Benefits to LIGO provided by Pegasus- Expanded Computing Horizons

- No longer limited to a single execution resource
  - Non Pegasus LIGO pipelines can often only run on LIGO clusters
  - Input is replicated out of band , in a rigid directory layout.
  - Rely on the shared filesystem to access data.

- Pegasus made it possible to leverage Non LDG Computing Resources

  - Open Science Grid
    - Dynamic – Best Effort Resource with no shared filesystem available

  - Large NSF Supercomputing Clusters XSEDE
    - No HTCondor
    - Geared for Large MPI jobs, not thousands of single node jobs
    - LIGO tried to setup XSEDE cluster as a LDG site but mismatch in setup.
    - Pegasus enabled LIGO to use XSEDE without changes at LIGO or at XSEDE

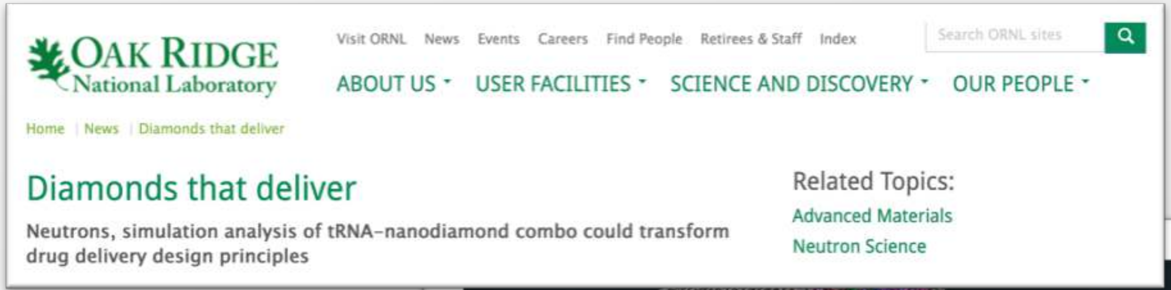
  - VIRGO Resources in Europe
    - Clusters with no shared filesystem and different storage management infrastructure than LDG
    - No HTCondor

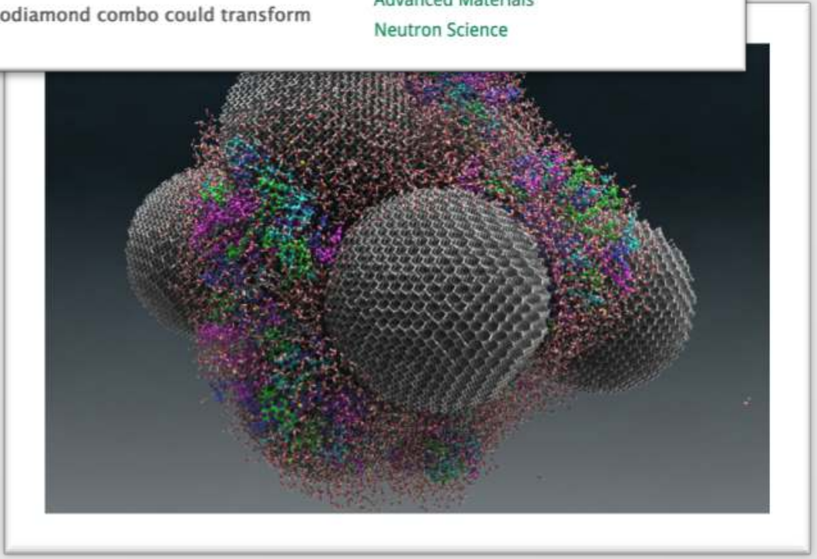
Impact on DOE Science

Enabled cutting-edge domain science (e.g., drug delivery) through collaboration with scientists at the DoE **Spallation Neutron Source (SNS)** facility

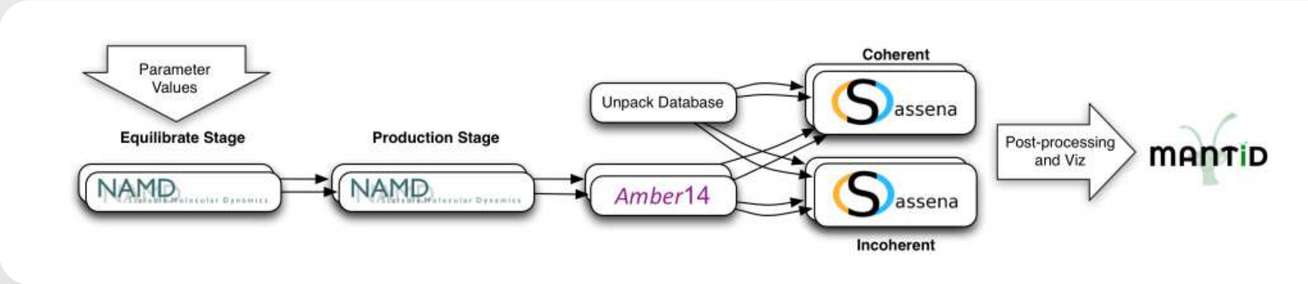
A Pegasus workflow was developed that confirmed that ***nanodiamonds*** can enhance the dynamics of tRNA

- It compared SNS neutron scattering data with MD simulations by calculating the epsilon that best matches experimental data





Water is seen as small red and white molecules on large nanodiamond spheres. The colored tRNA can be seen on the nanodiamond surface. (Image Credit: Michael Mattheson, OLCF, ORNL)



An automated analysis workflow for optimization of force-field parameters using neutron scattering data*. V. E. Lynch, J. M. Borreguero, D. Bhowmik, P. Ganesh, B. G. Sumpter, T. E. Proffen, M. Goswami, Journal of Computational Physics, July 2017.*

Data Movement In Production Runs

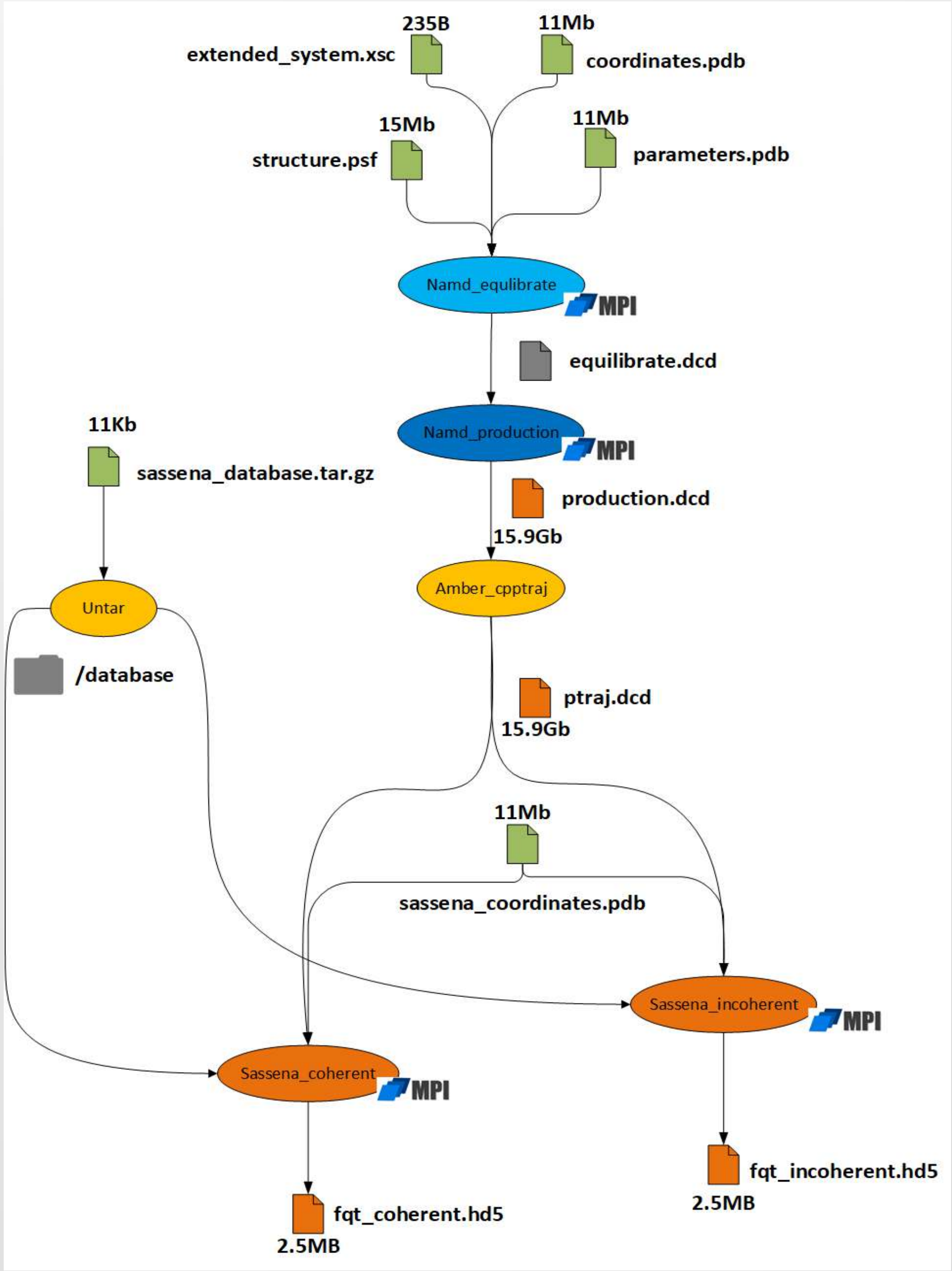
During production runs a single SNS workflow was staging in 48Mb of data (ie. input parameters) and it was generating over 30Gb of data.

Multiple runs, with variable input parameters, conducted on a Cray XE6 at NERSC using 400,000 CPU hours, and generated approximately 3TB of data.

Green files: Input data staged in the execution site by Pegasus

Red files: Output data staged out of the execution by Pegasus

Gray files: Temporary data



Key Pegasus Concepts

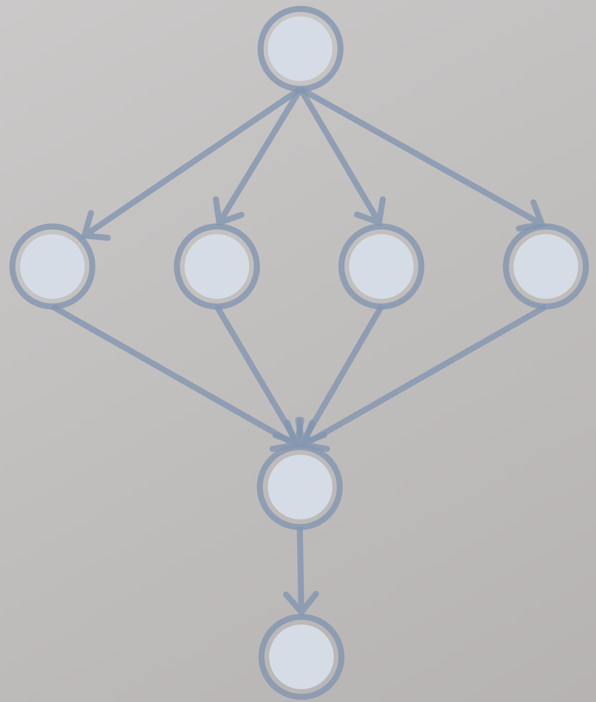
HTCondor High Throughput Computing

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



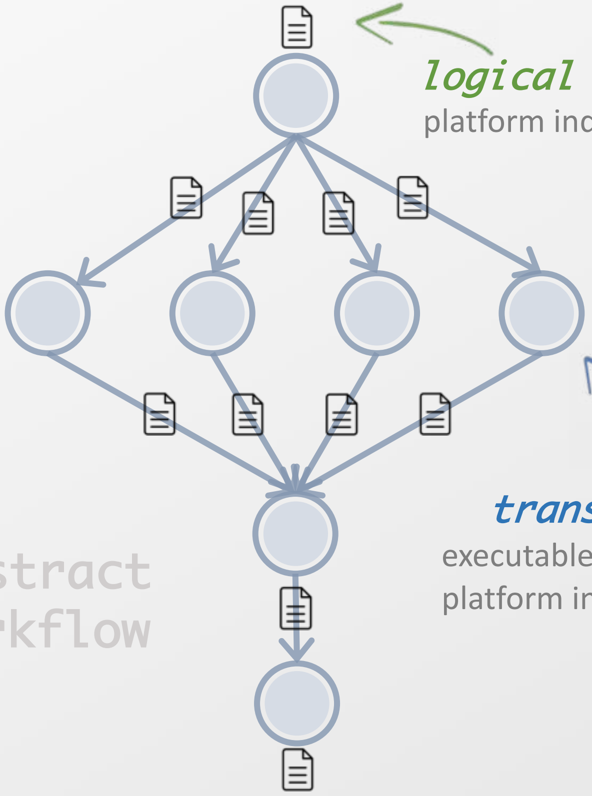
Planning occurs ahead of execution

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

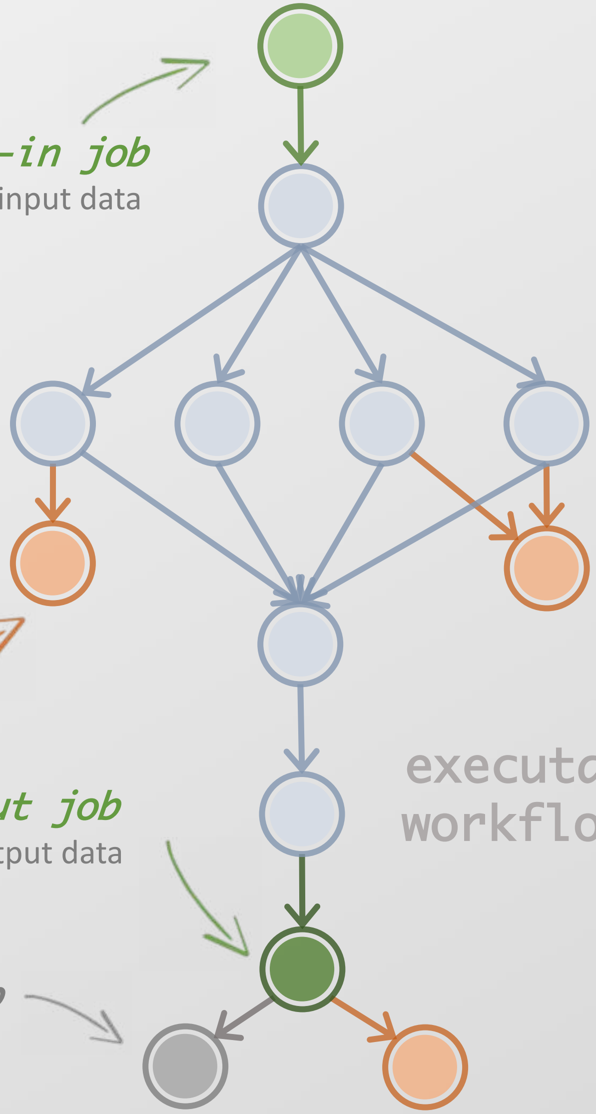


logical filename (LFN)
platform independent (abstraction)

transformation
executables (or programs)
platform independent

abstract workflow

DAG
directed-acyclic graphs



stage-in job
Transfers the workflow input data

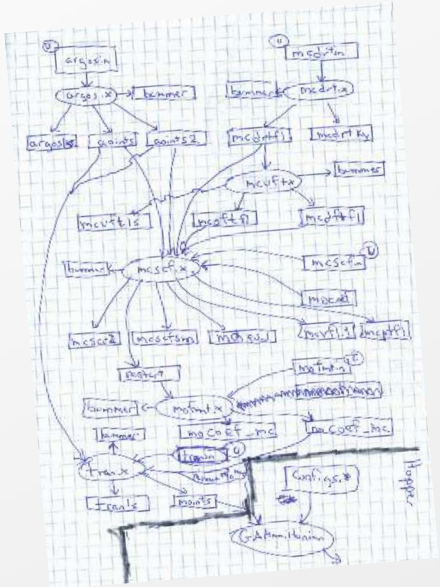
cleanup job
Removes unused data

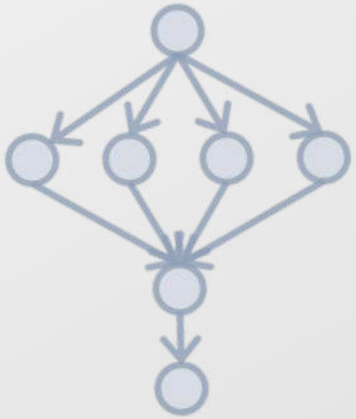
stage-out job
Transfers the workflow output data

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

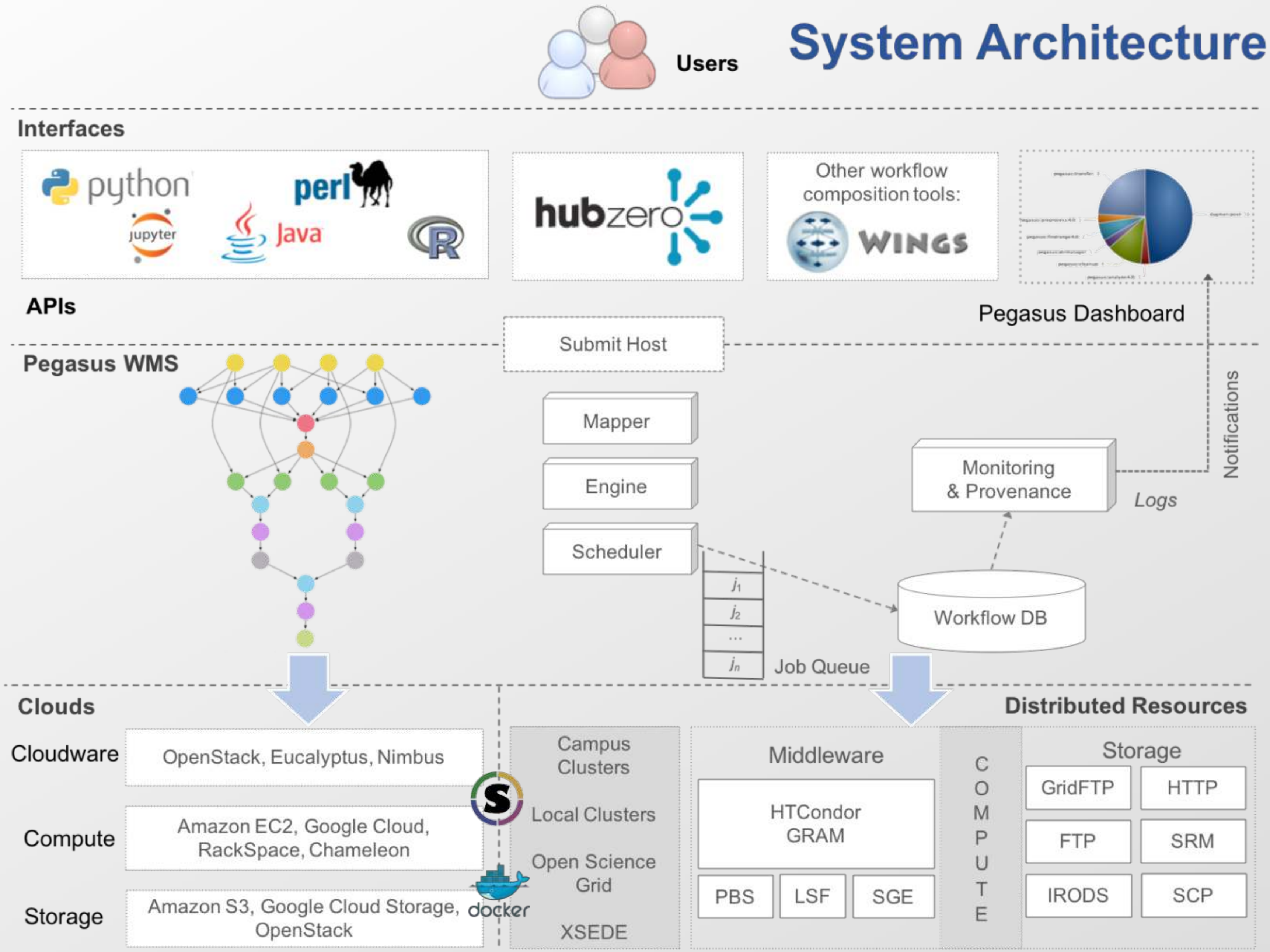
jupyter

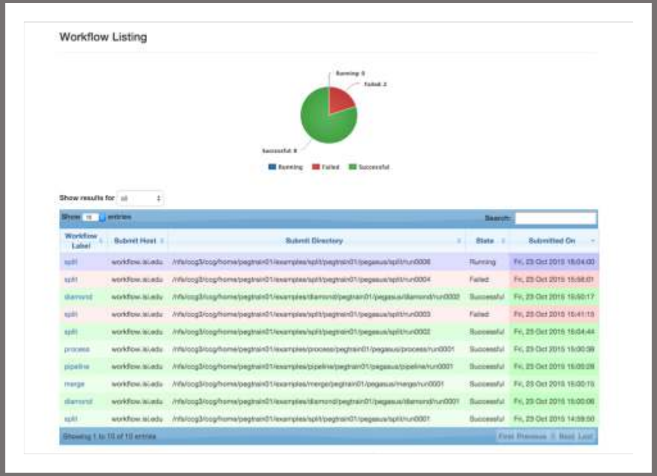
```xml
<?xml version="1.0" encoding="UTF-8"?>

<!-- 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

DAG in XML

System Architecture





Pegasus dashboard

web interface for monitoring and debugging workflows

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

Real-time Monitoring

Reporting

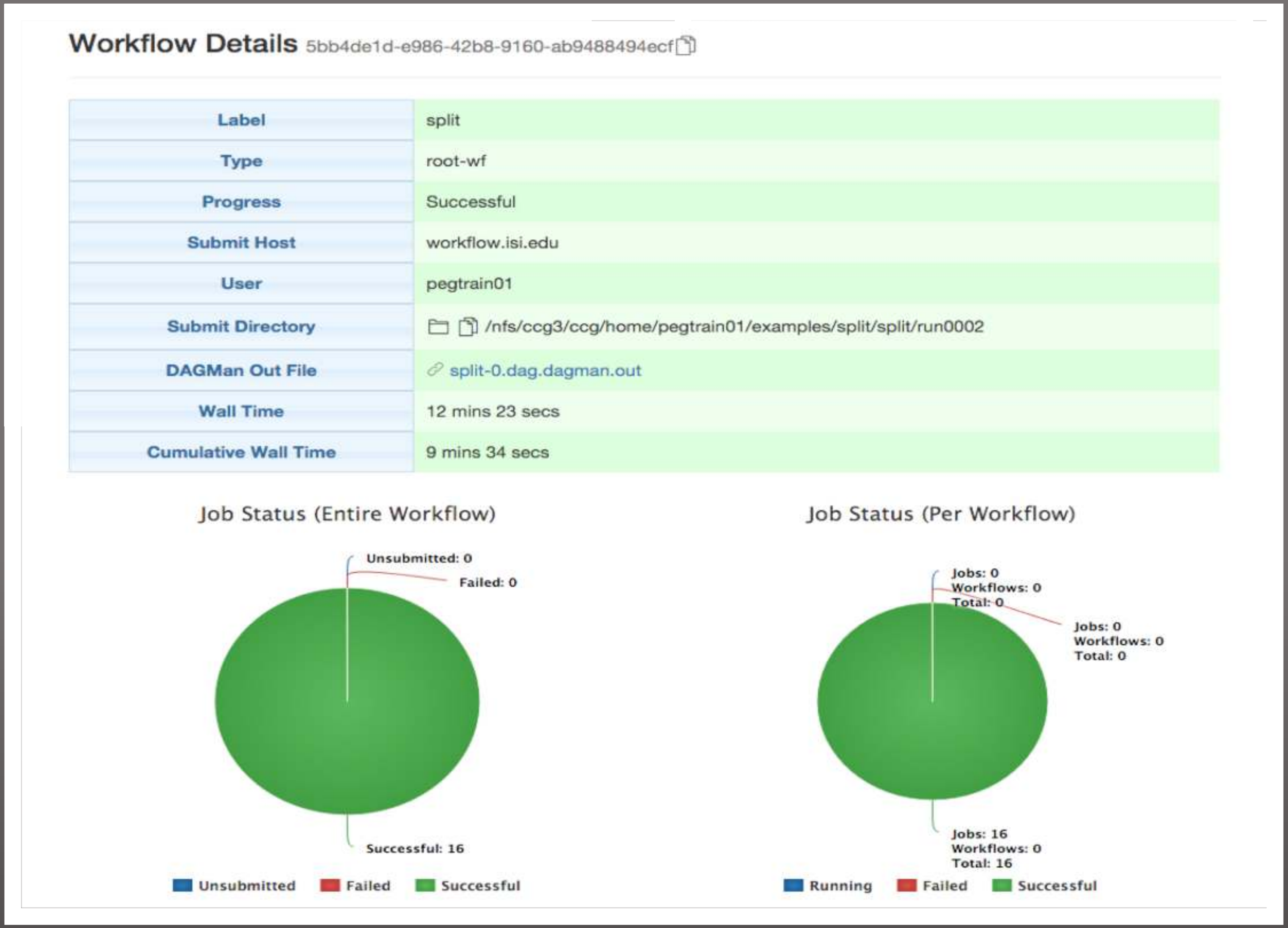
Debugging

Troubleshooting

RESTful API

Pegasus dashboard

web interface for monitoring and debugging workflows



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

>_ 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%)
```

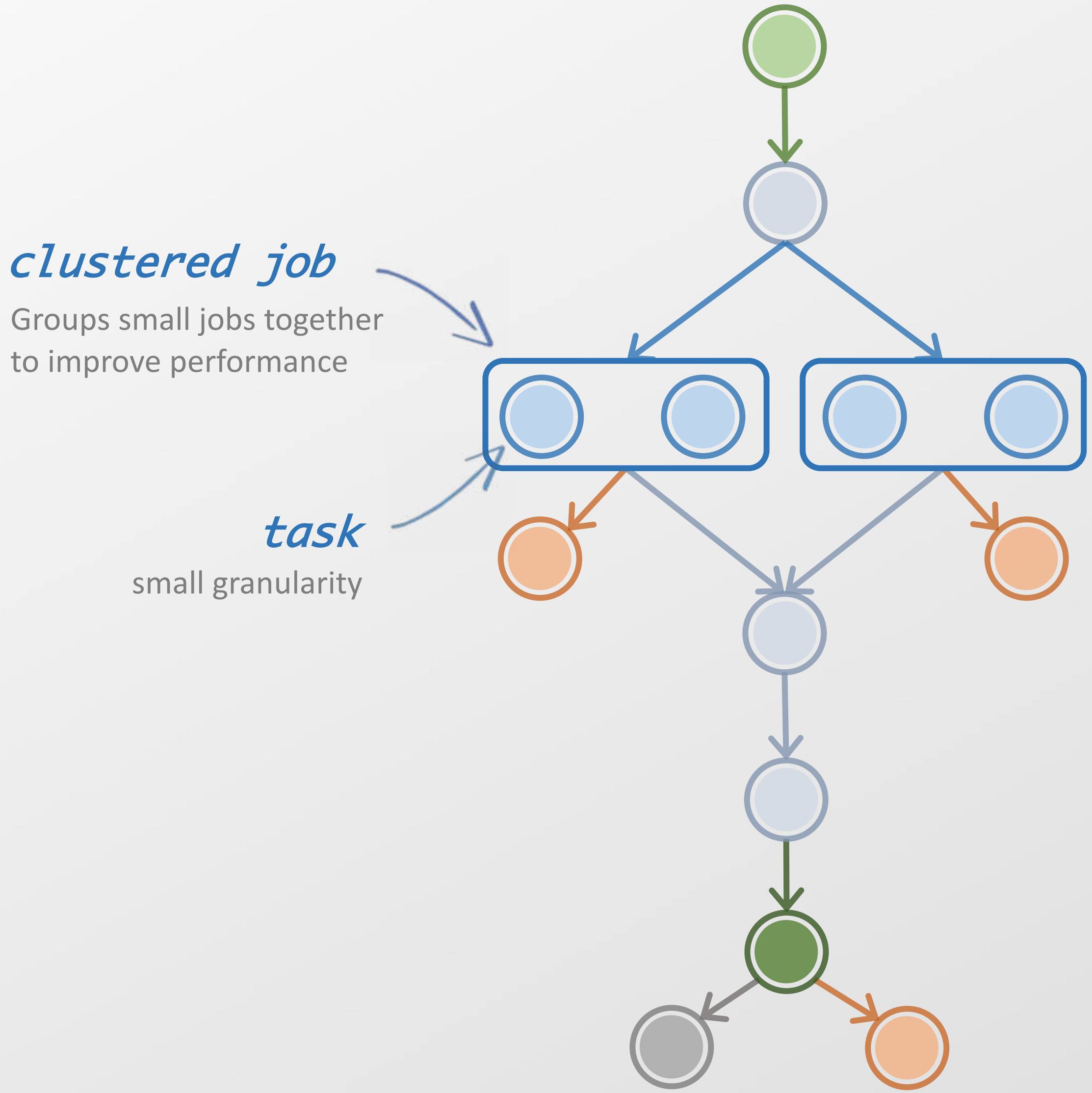
```
$ pegasus-statistics -s all pegasus/examples/split/run0001
------------------------------------------------------------------------------
Type           Succeeded Failed Incomplete Total Retries Total+Retries
Tasks              5        0         0        5     0          5
Jobs              17 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

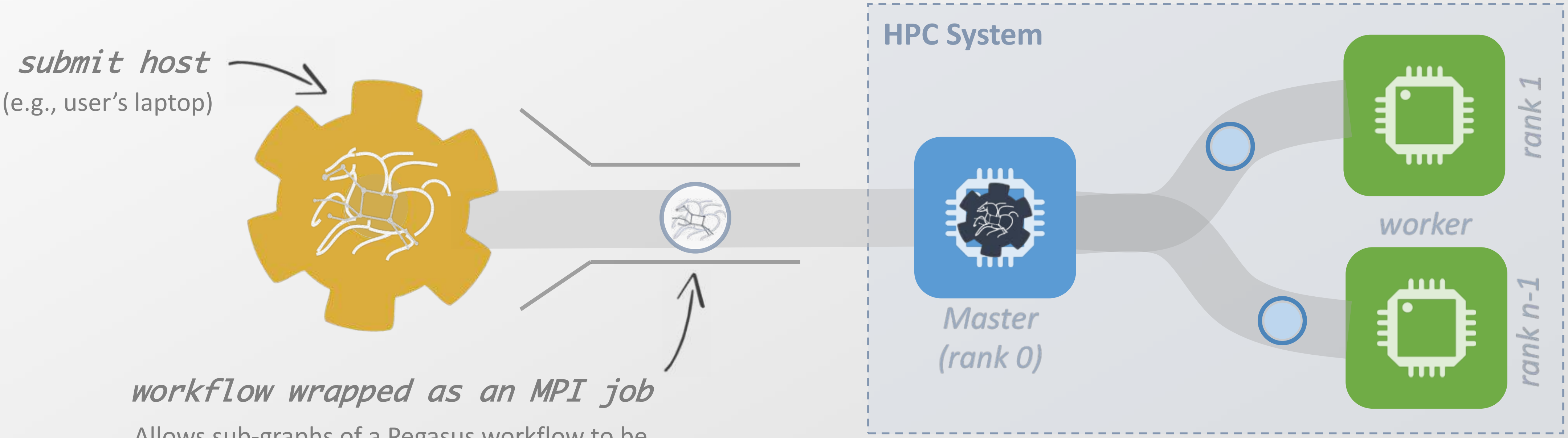
or used for debugging
pegasus-analyzer

Performance, why not improve it?

workflow restructuring
workflow reduction
hierarchical workflows
pegasus-mpi-cluster



Running fine-grained workflows on HPC systems…

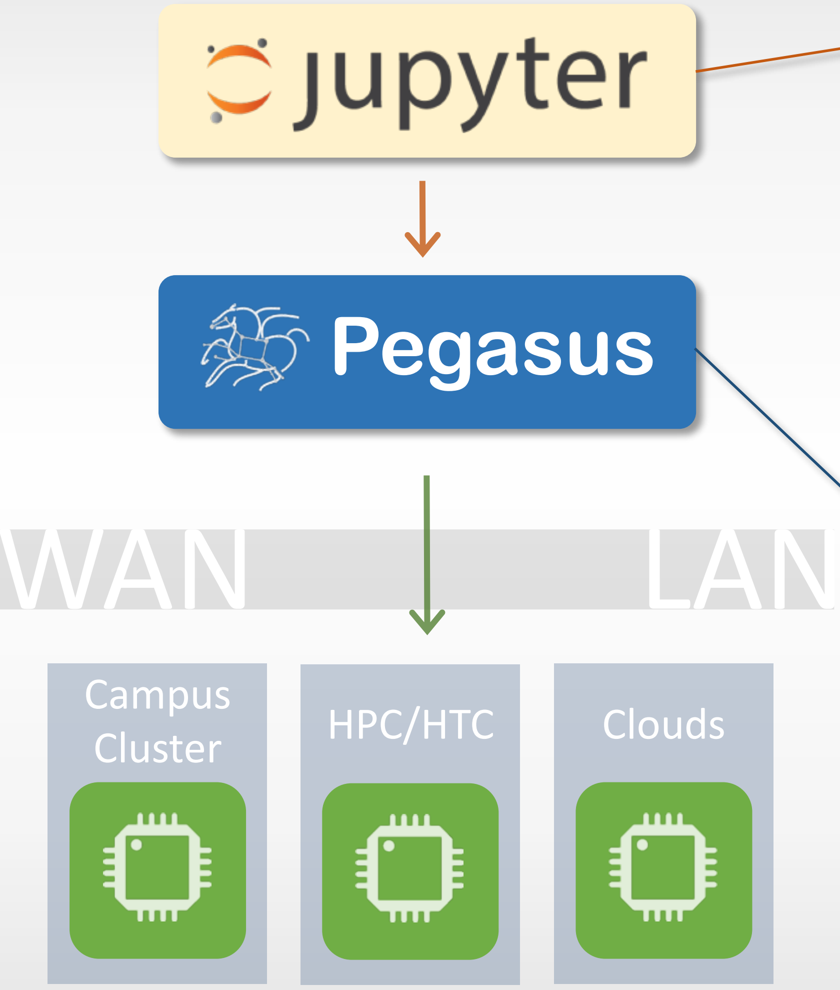


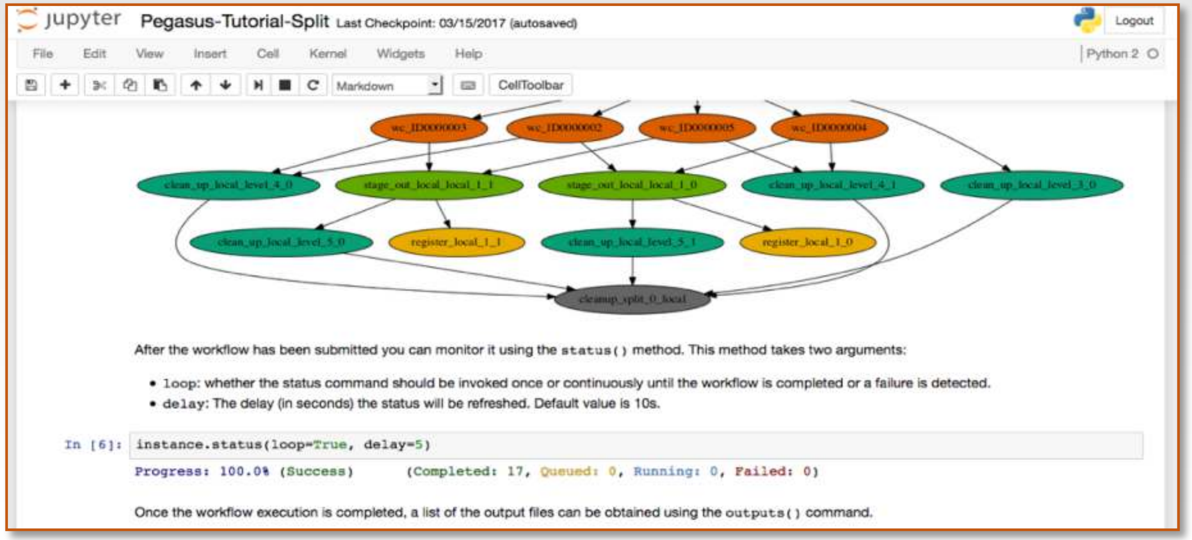
Allows sub-graphs of a Pegasus workflow to be submitted as monolithic jobs to remote resources

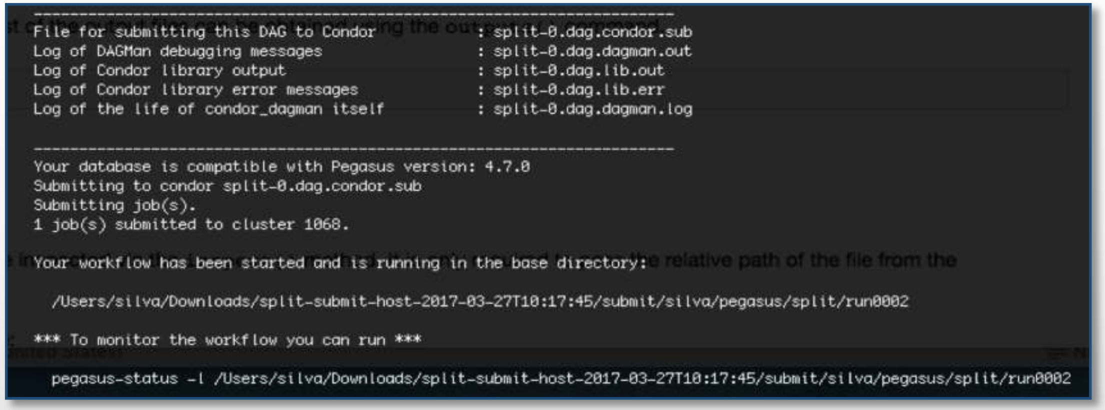
Pegasus Container Support

- Support for
  - Docker
  - Singularity – Widely supported on OSG
- Users can refer to containers in the Transformation Catalog with their executable preinstalled.
- Users can refer to a container they want to use. However, they let Pegasus stage their executable to the node.
  - Useful if you want to use a site recommended/standard container image.
  - Users are using generic image with executable staging.
- Future Plans
  - Users can specify an image buildfile for their jobs.
  - *Pegasus will build the Docker image as separate jobs in the executable workflow, export them at tar file and ship them around* (planned for 4.8.X)

Running Pegasus workflows with Jupyter







Pegasus-Jupyter Python API

```
from Pegasus.jupyter.instance import *
```

importing the API

```
instance = Instance(dax)
```

creating an instance of the DAX

```
instance.run(site='condorpool')
```

running a workflow

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

# 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)
```

using the Pegasus DAX3 API to write a workflow

```
instance.status(loop=True, delay=5)
```

monitoring a workflow execution

```
Progress: 100.0% (Success)      (Completed: 17, Queued: 0, Running: 0, Failed: 0)
```

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

Pegasus: Data Management for Scientific Workflows

Pegasus Workflow Management System

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DAG in XML

DAG
directed-acyclic graphs

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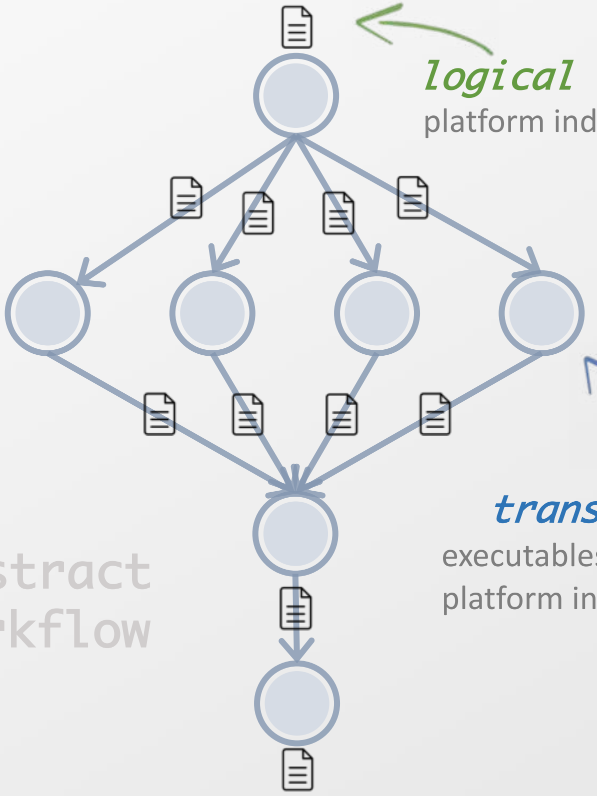

logical filename (LFN)
platform independent (abstraction)

transformation
executables (or programs)
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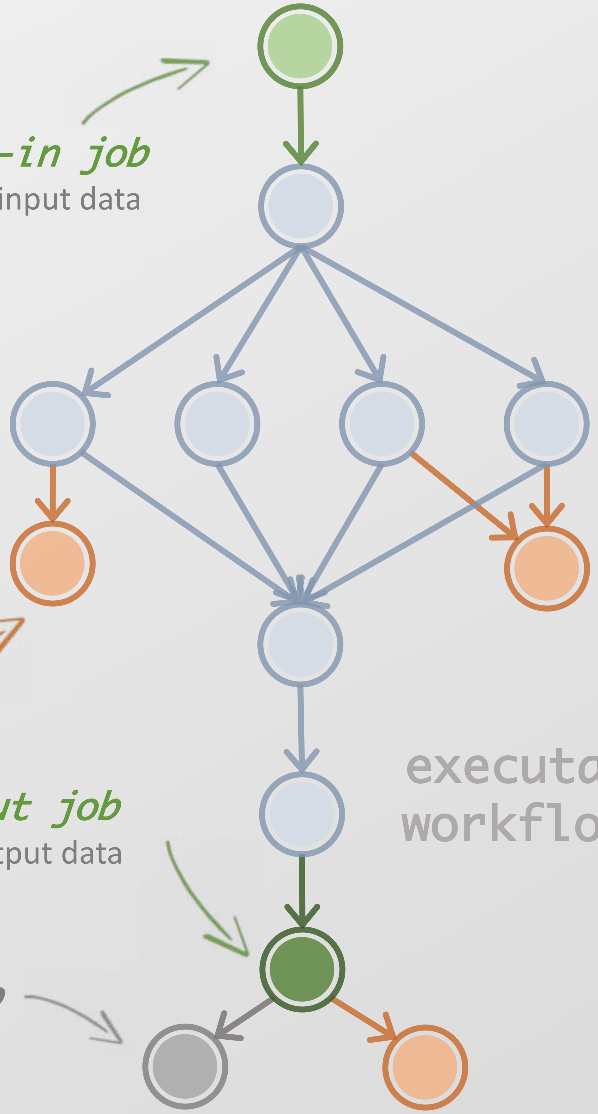
abstract workflow



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

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

How does Pegasus decide where to execute?

site description
describes the compute resources

scratch
tells where temporary data is stored

storage
tells where output data is stored

profiles
key-pair values associated per job level

```
<!-- The local site contains information about the submit host -->
<!-- The arch and os keywords are used to match binaries in the -->
<!-- transformation catalog -->
<site handle="local" arch="x86_64" os="LINUX">

  <!-- These are the paths on the submit host were Pegasus stores data -->
  <!-- Scratch is where temporary files go -->
  <directory type="shared-scratch" path="/home/tutorial/run">
    <file-server operation="all" url="file:///home/tutorial/run"/>
  </directory>

  <!-- Storage is where pegasus stores output files -->
  <directory type="local-storage" path="/home/tutorial/outputs">
    <file-server operation="all" url="file:///home/tutorial/outputs"/>
  </directory>

  <!-- This profile tells Pegasus where to find the user's private key -->
  <!-- for SCP transfers -->
  <profile namespace="env" key="SSH_PRIVATE_KEY">
     /home/tutorial/.ssh/id_rsa
  </profile>

</site>
```

What if data is not local to the submit host?


```
# This is the replica catalog. It lists information about each of the
# input files used by the workflow. You can use this to specify locations to
input files present on external servers.

# The format is:
# LFN PFN site="SITE"

f.a   file:///home/tutorial/examples/diamond/input/f.a   site="local"
```

logical filename

abstract data name

physical filename

data physical location on site
different transfer protocols can be used (e.g., scp, http, ftp, gridFTP, etc.)

site name

in which site the file is available

Replica catalog
multiple sources

pegasus.conf

```
# Add Replica selection options so that it will try URLs first, then
# XrootD for OSG, then gridftp, then anything else
pegasus.selector.replica=Regex
pegasus.selector.replica.regex.rank.1=file:///cvmfs/.*
pegasus.selector.replica.regex.rank.2=file://.*
pegasus.selector.replica.regex.rank.3=root://.*
pegasus.selector.replica.regex.rank.4=gridftp://.*
pegasus.selector.replica.regex.rank.5=.\*
```

rc.data

```
# This is the replica catalog. It lists information about each of the
# input files used by the workflow. You can use this to specify locations
# to input files present on external servers.

# The format is:
# LFN PFN site="SITE"

f.a   file:///cvmfs/oasis.opensciencegrid.org/diamond/input/f.a   site="cvmfs"
f.a   file:///local-storage/diamond/input/f.a   site="prestaged"
f.a   gridftp://storage.mysite/edu/examples/diamond/input/f.a   site="storage"
```

pegasus-transfer

Pegasus' internal data transfer tool with support for a number of different protocols

Directory creation, file removal

If protocol supports, used for cleanup

Two stage transfers

e.g., GridFTP to S3 = GridFTP to local file, local file to S3

Parallel transfers

Automatic retries

Credential management

Uses the appropriate credential for each site and each protocol (even 3rd party transfers)

- HTTP
- SCP
- GridFTP
- Globus
- Online
- iRods
- Amazon S3
- Google
- Storage
- SRM
- FDT
- stashcp
- cp
- ln -s

Data Staging Configurations

HTCondor I/O (HTCondor pools, OSG, …)

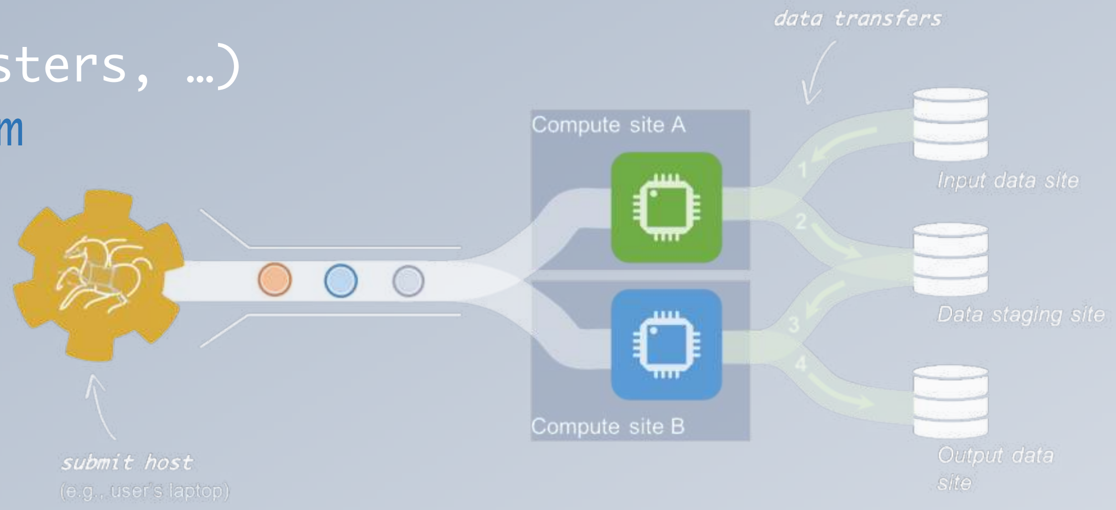
- Worker nodes do not share a file system
- Data is pulled from / pushed to the submit host via HTCondor file transfers
- Staging site is the submit host

Non-shared File System (clouds, OSG, …)

- Worker nodes do not share a file system
- Data is pulled / pushed from a staging site, possibly not co-located with the computation

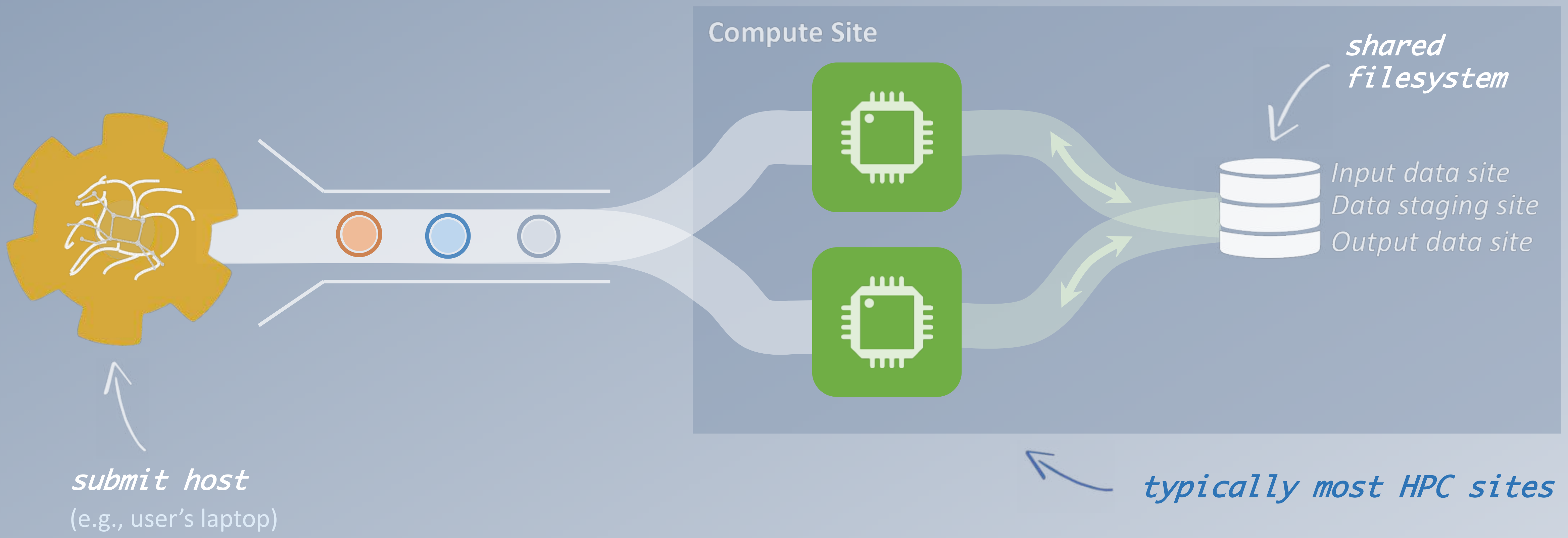
Shared File System (HPC sites, XSEDE, Campus clusters, …)

- I/O is directly against the shared file system



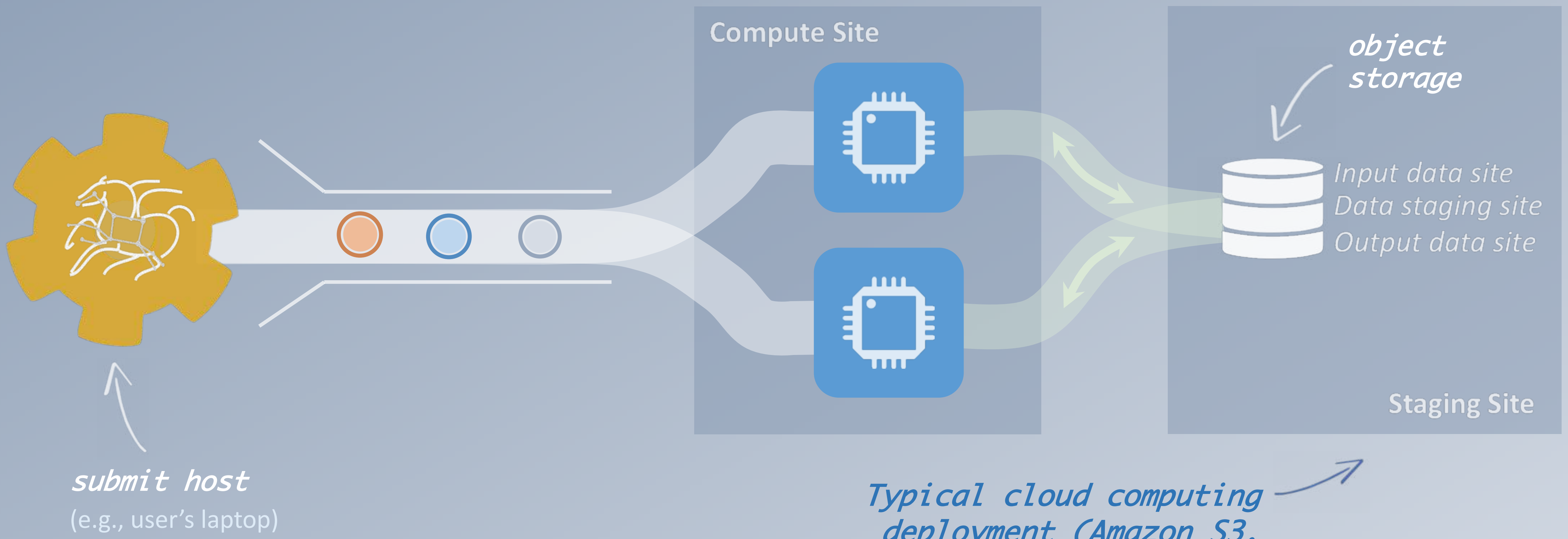
High Performance Computing

There are several possible configurations…



Cloud Computing

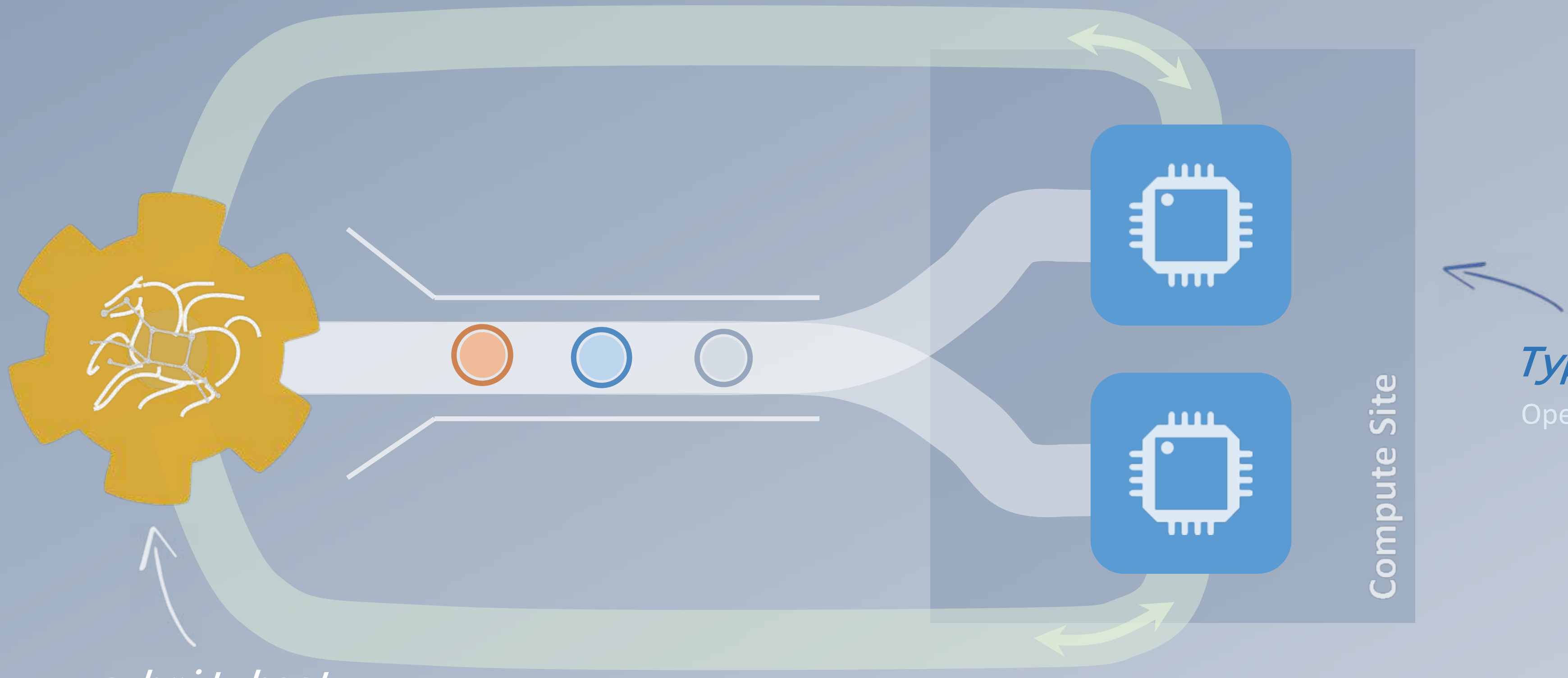
high-scalable object storages



Typical cloud computing deployment (Amazon S3, Google Storage)

Grid Computing

local data management



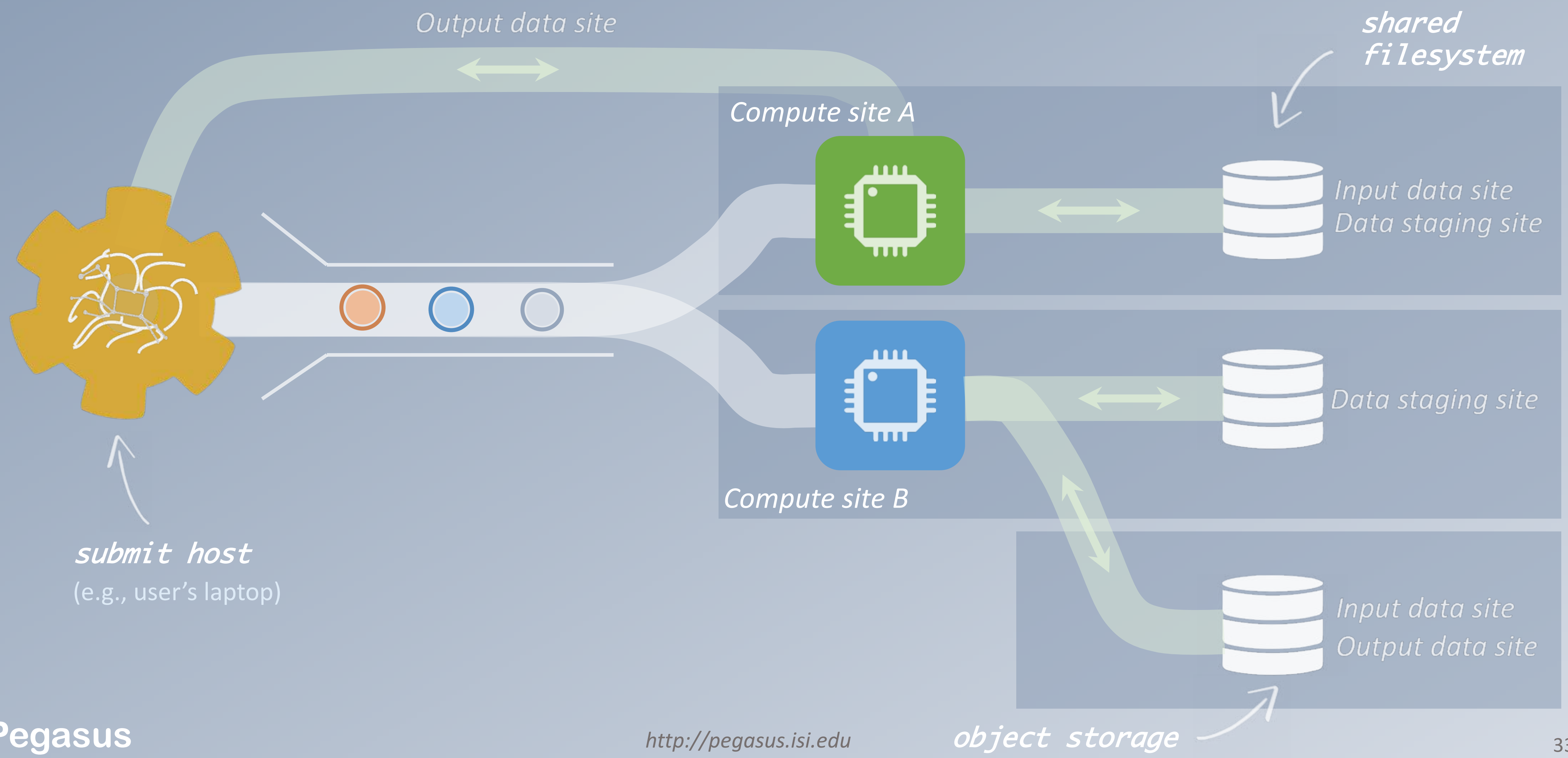
Typical OSG sites

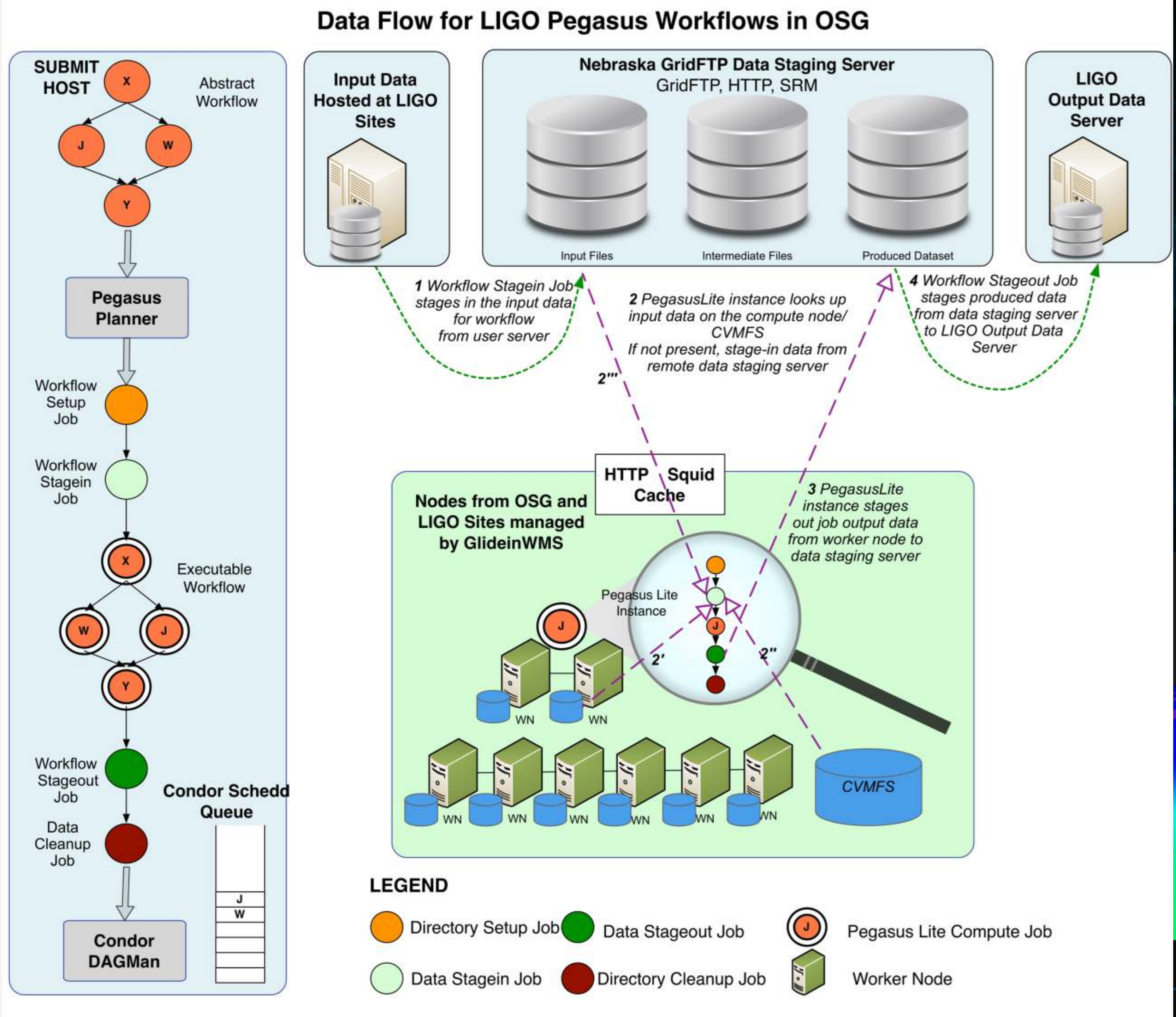
Open Science Grid

submit host

(e.g., user's laptop)

And yes… you can mix everything!

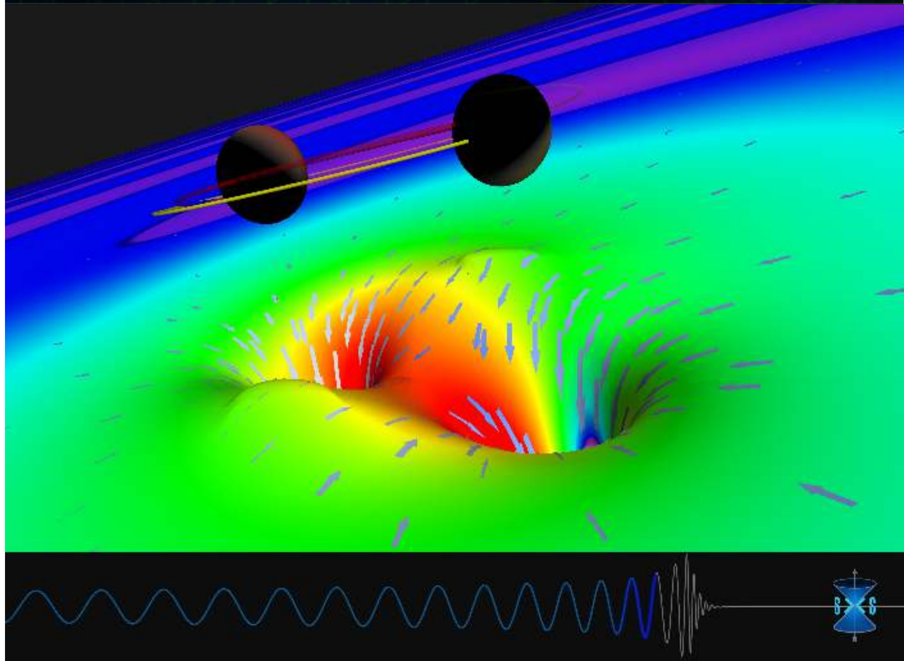




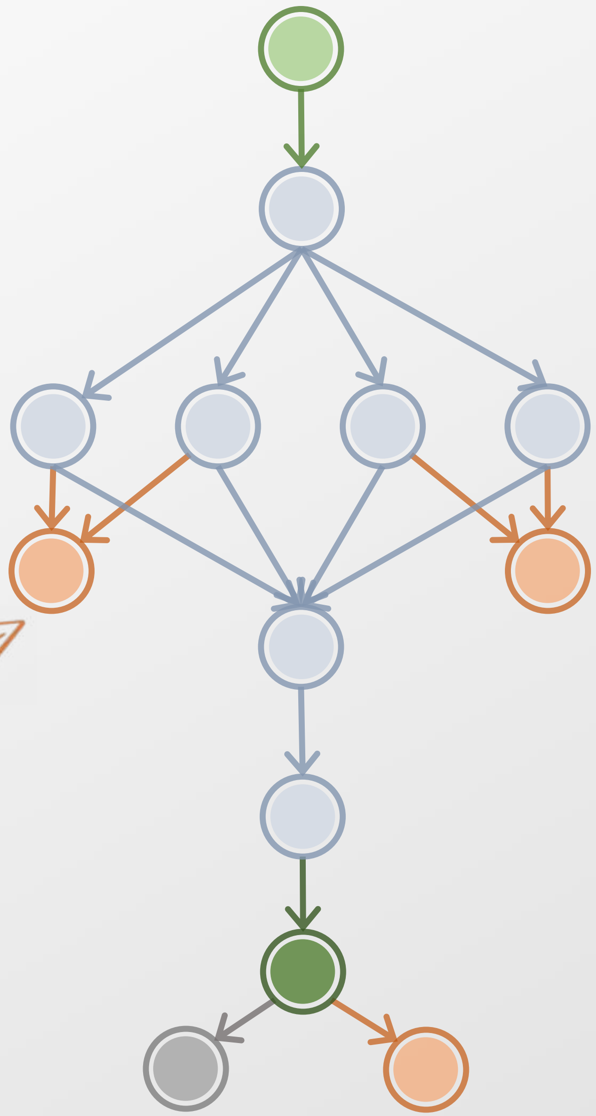
Advanced LIGO – Laser Interferometer Gravitational Wave Observatory

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



Optimizing storage usage…



cleanup job

Removes unused data

Problem?

- Users run out of disk space while running workflows

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

- Pegasus Solutions
  - Add leaf cleanup nodes to cleanup after workflow finishes.
  - Interleave cleanup nodes
  - Cluster cleanup nodes per level to improve performance

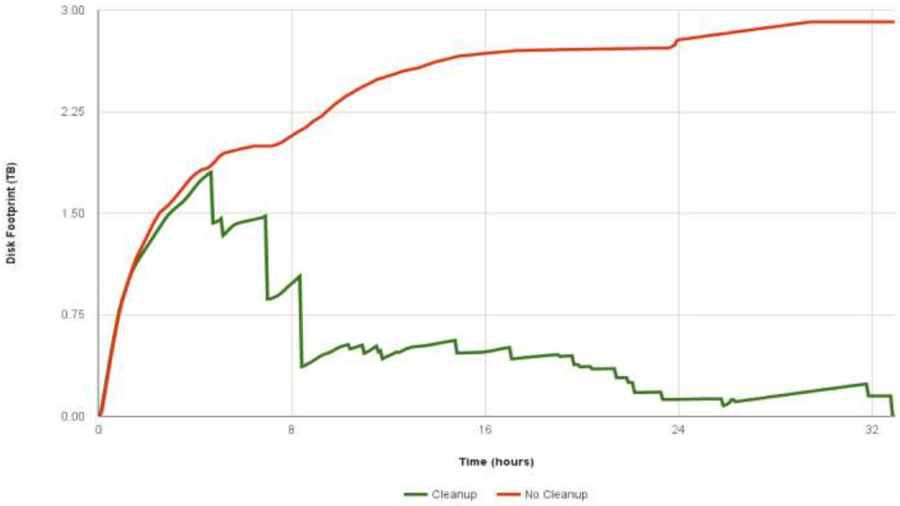
Soybean Workflow

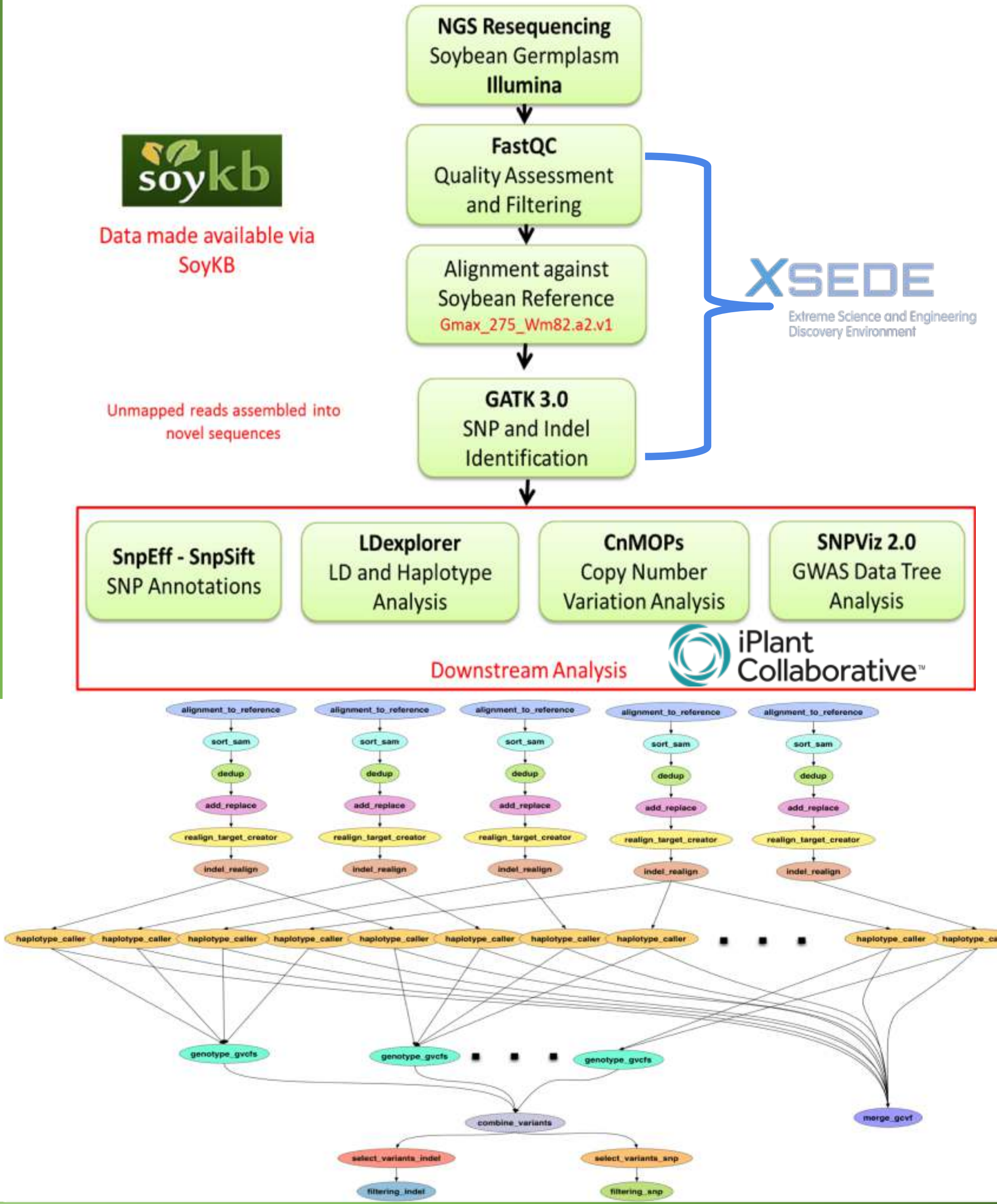
TACC Wrangler as Execution Environment

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)





Metadata

Can associate arbitrary key-value pairs with workflows, jobs, and files

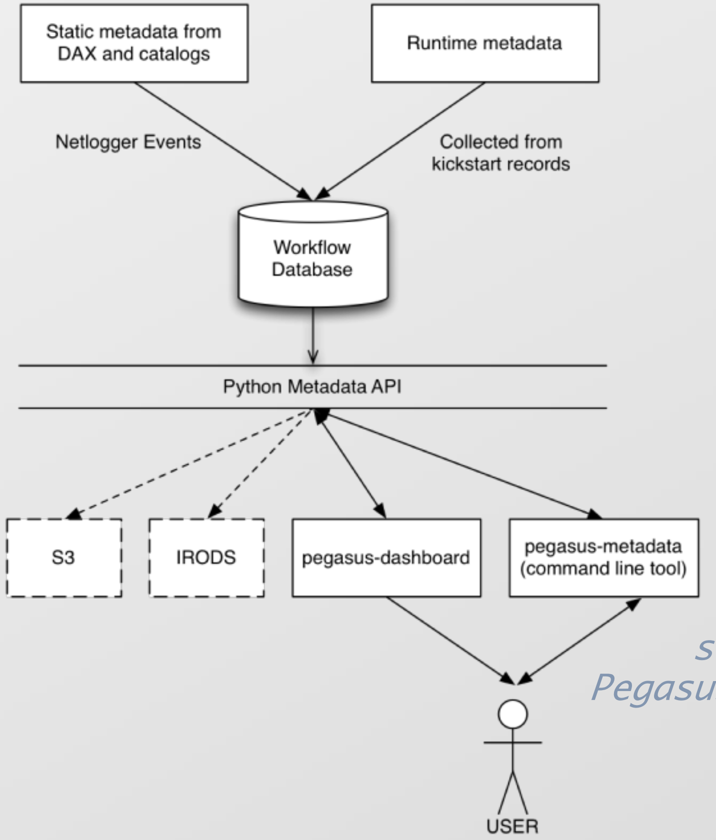
Data registration

Output files get tagged with metadata on registration in the workflow database

Static and runtime metadata

Static: application parameters

Runtime: performance metrics



since Pegasus 4.6

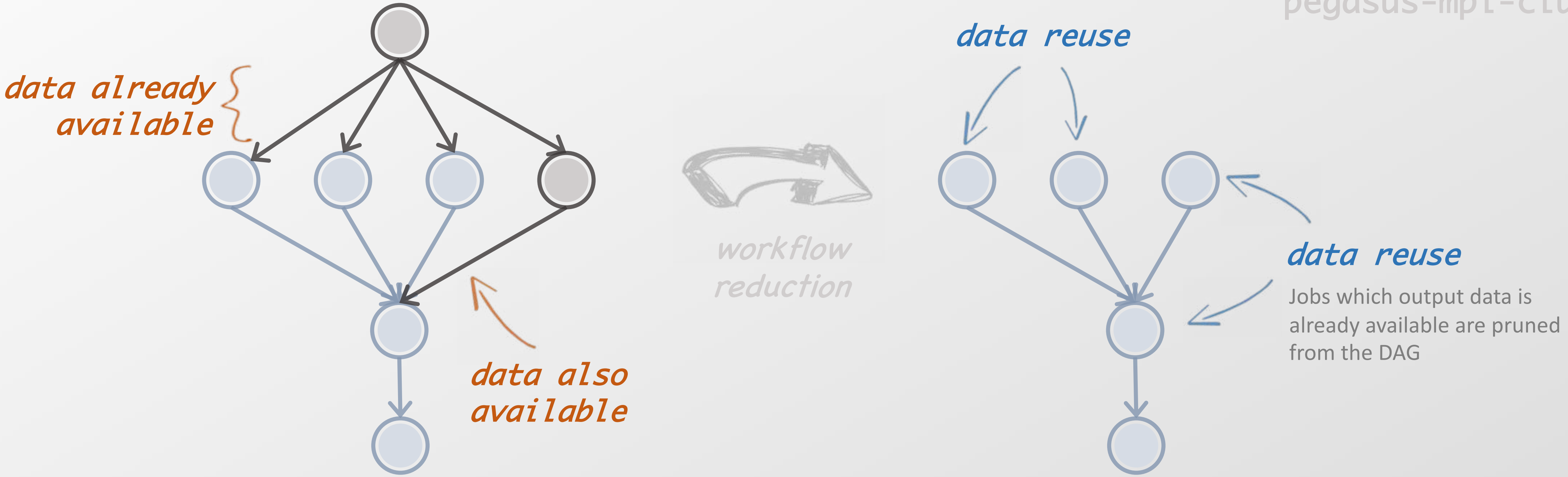
workflow, job, file

```
<adag ...>
    <metadata key="experiment">par_all27_prot_lipid</metadata>
    <job id="ID0000001" name="namd">
        <argument><file name="equilibrate.conf"/></argument>
        <metadata key="timesteps">500000</metadata>
        <metadata key="temperature">200</metadata>
        <metadata key="pressure">1.01325</metadata>
        <uses name="Q42.psf" link="input">
            <metadata key="type">psf</metadata>
            <metadata key="charge">42</metadata>
        </uses>
        ...
        <uses name="eq.restart.coord" link="output" transfer="false">
            <metadata key="type">coordinates</metadata>
        </uses>
        ...
    </job>
</adag>
```

select data based on metadata

register data with metadata

What about data reuse?



Jobs which output data is already available are pruned from the DAG

Data Management for Containers

- Users can refer to container images as
  - Docker or Singularity Hub URL’s
  - Docker Image exported as a TAR file and available at a server , just like any other input dataset.

- We want to avoid hitting Docker/Singularity Hub repeatedly for large workflows
  - Extend pegasus-transfer to pull image from Docker Hub and then export it as tar file, that can be shipped around in the workflow.

- Ensure pegasus worker package gets installed at runtime inside the user container.

Pegasus est. 2001

Automate, recover, and debug scientific computations.

Get Started

Pegasus Website

http://pegasus.isi.edu

Users Mailing List

pegasus-users@isi.edu

Support

pegasus-support@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

HipChat