Enhancing Scientific Computations with Scientific Workflows

Pegasus Workflow Management System

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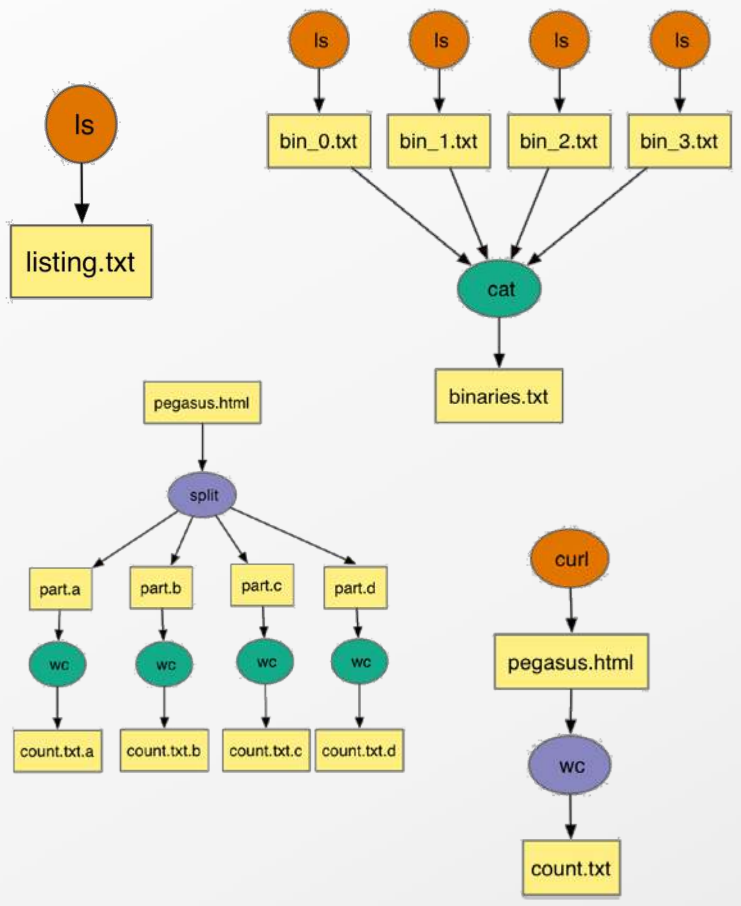
http://pegasus.isi.edu

OUTLINE

Introduction	*Scientific Workflows* *Pegasus Overview* *Successful Stories*
Pegasus Overview	*Basic Concepts* *Features* *System Architecture*
Features	*Data Staging* *Information Catalogs* *Fault-Tolerance*
Break	*10min Break*
Hands On Tutorial	

OUTLINE

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**

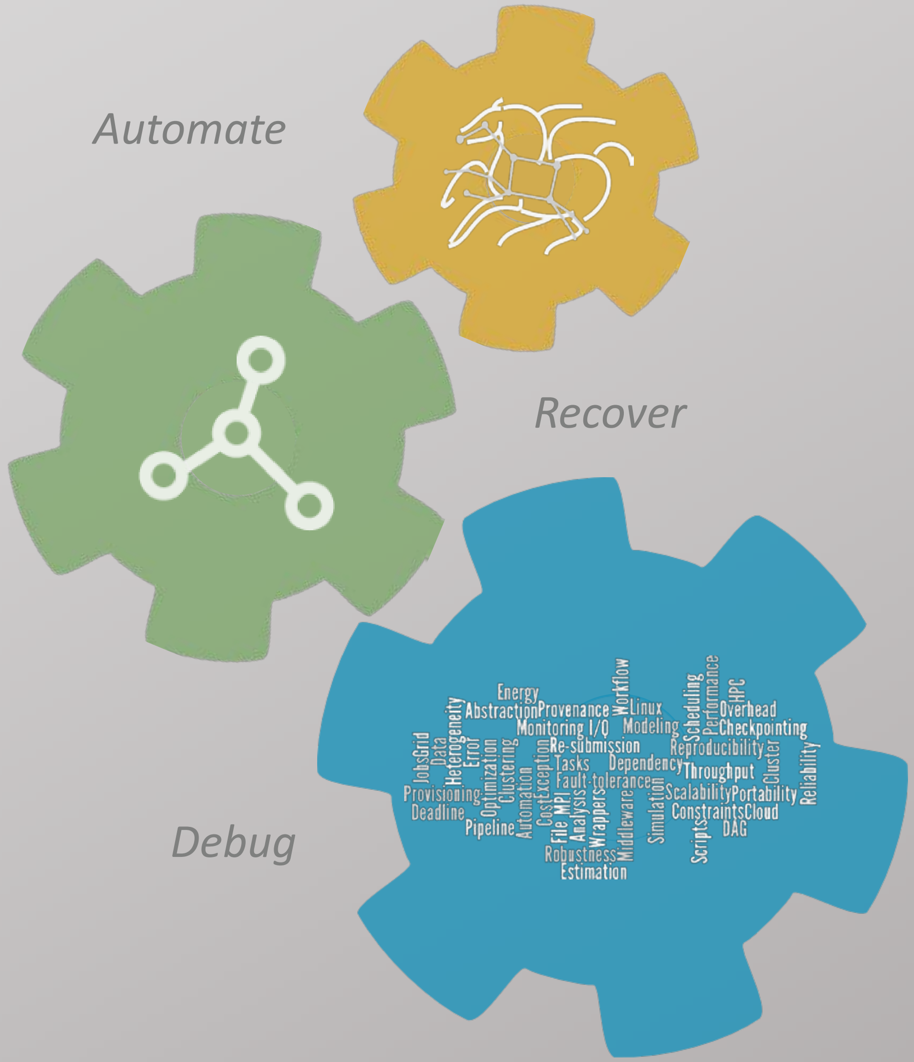
Automatically executes data transfers

Reusable, aids **reproducibility**

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

Handles **failures** with to provide reliability

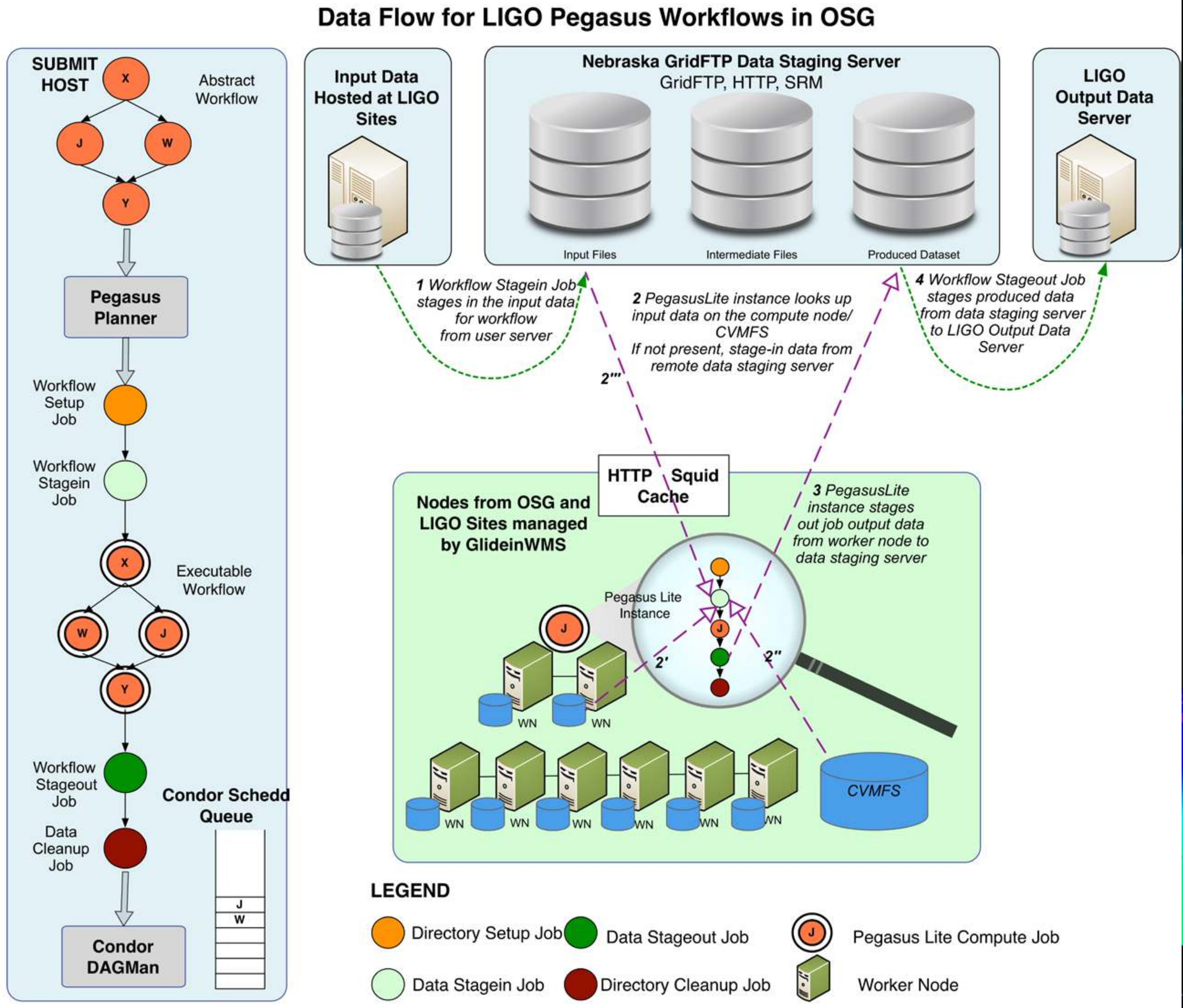
Keeps track of data and **files**



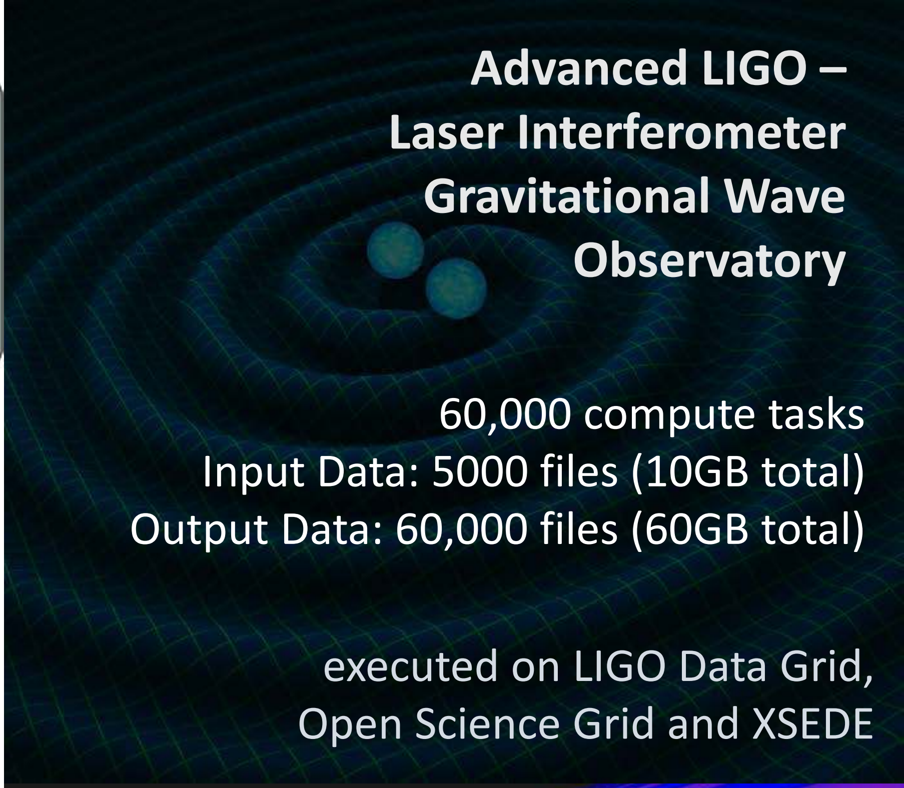
HTCondor High Throughput Computing

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

Some of the successful stories…

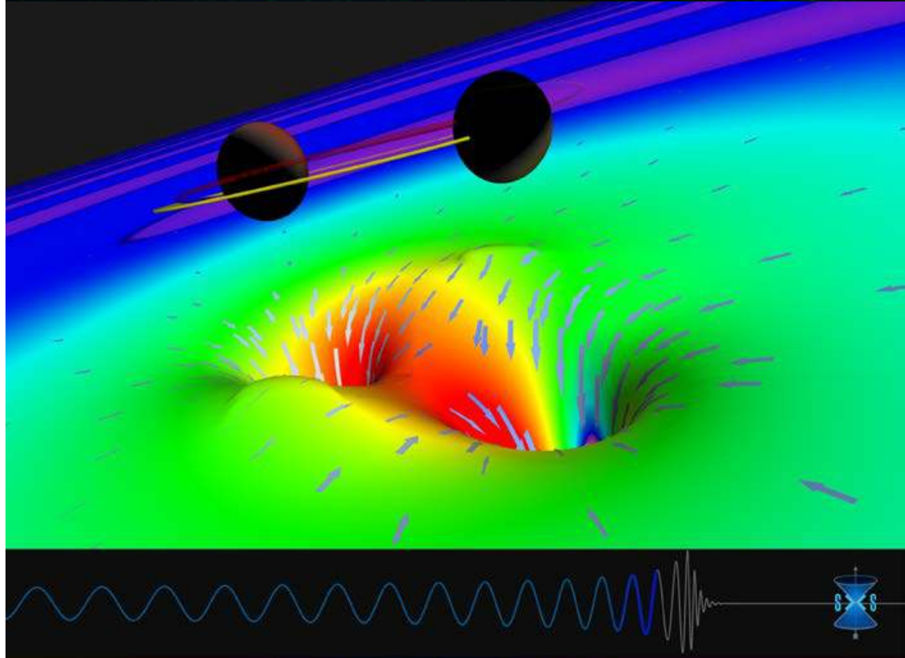

Data Flow for LIGO Pegasus Workflows in OSG
SUBMIT HOST
Abstract Workflow
X
J
W
Y
Pegasus Planner
Workflow Setup Job
Workflow Stagein Job
Executable Workflow
Workflow Stageout Job
Data Cleanup Job
Condor Schedd Queue
Condor DAGMan
Input Data Hosted at LIGO Sites
Nebraska GridFTP Data Staging Server
GridFTP, HTTP, SRM
Input Files
Intermediate Files
Produced Dataset
LIGO Output Data Server
1 Workflow Stagein Job stages in the input data for workflow from user server
2 PegasusLite instance looks up input data on the compute node/ CVMFS
If not present, stage-in data from remote data staging server
4 Workflow Stageout Job stages produced data from data staging server to LIGO Output Data Server
2'''
HTTP Squid Cache
Nodes from OSG and LIGO Sites managed by GlideinWMS
3 PegasusLite instance stages out job output data from worker node to data staging server
Pegasus Lite Instance
2'
2''
WN
CVMFS
LEGEND
Directory Setup Job
Data Stageout Job
Pegasus Lite Compute Job
Data Stagein Job
Directory Cleanup Job
Worker Node

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

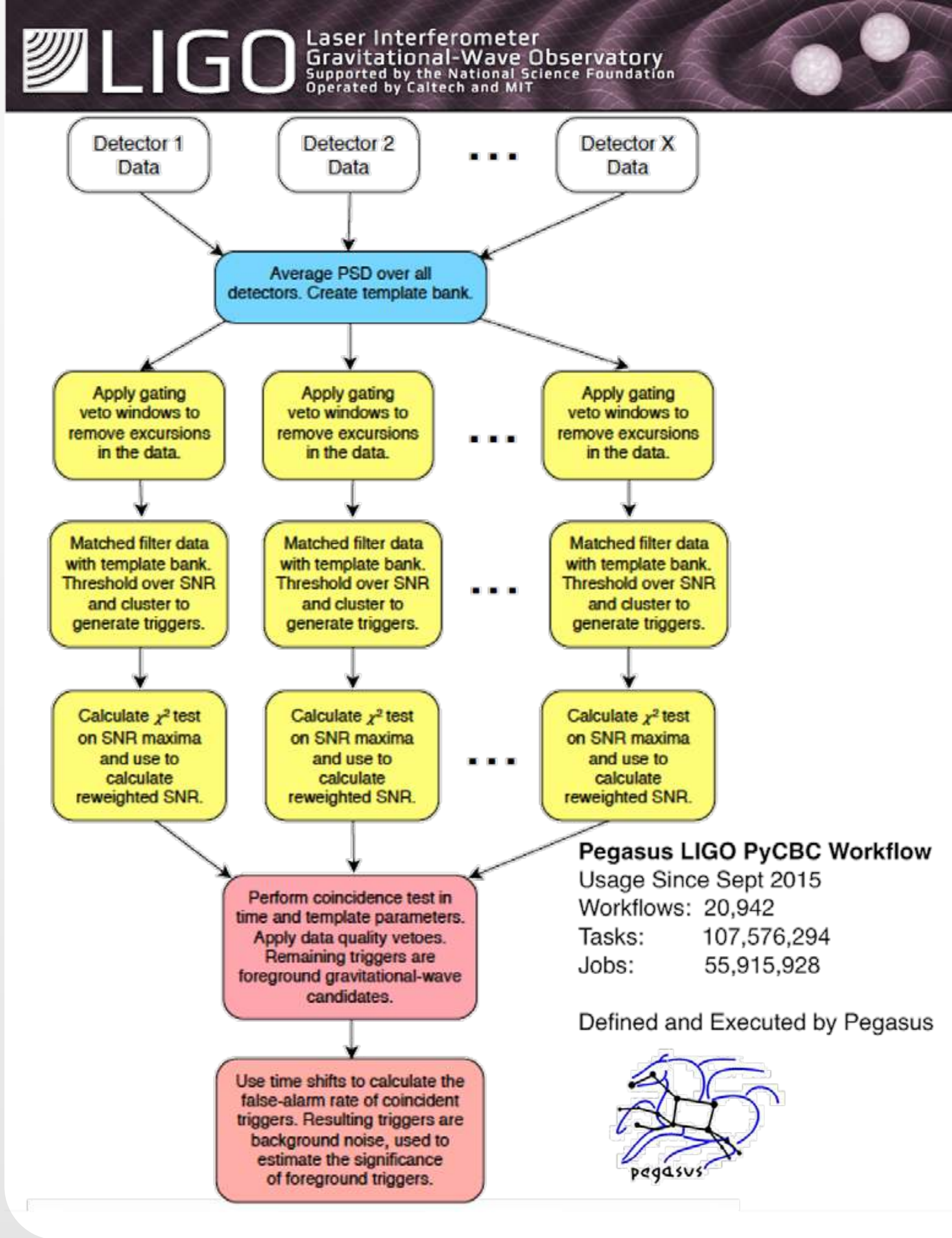
Contains **100's of thousands of jobs** and accesses on order of **terabytes of data**

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**


LIGO
Laser Interferometer Gravitational-Wave Observatory
Supported by the National Science Foundation
Operated by Caltech and MIT
Detector 1 Data
Detector 2 Data
Detector X Data
Average PSD over all detectors. Create template bank.
Apply gating veto windows to remove excursions in the data.
Matched filter data with template bank. Threshold over SNR and cluster to generate triggers.
Calculate χ^2 test on SNR maxima and use to calculate reweighted SNR.
Perform coincidence test in time and template parameters. Apply data quality vetoes. Remaining triggers are foreground gravitational-wave candidates.
Use time shifts to calculate the false-alarm rate of coincident triggers. Resulting triggers are background noise, used to estimate the significance of foreground triggers.
pegasus

Pegasus LIGO PyCBC Workflow

Usage Since Sept 2015

Workflows:	20,942
Tasks:	107,576,294
Jobs:	55,915,928

Defined and Executed by 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.*

Southern California Earthquake Center's CyberShake

Builders ask seismologists: What will the peak ground motion be at my new building in the next 50 years?

Seismologists answer this question using Probabilistic Seismic Hazard Analysis (PSHA)

CPU jobs (Mesh generation, seismogram synthesis): 1,094,000 node-hours

GPU jobs: 439,000 node-hours

AWP-ODC finite-difference code

5 billion points per volume, 23000 timesteps

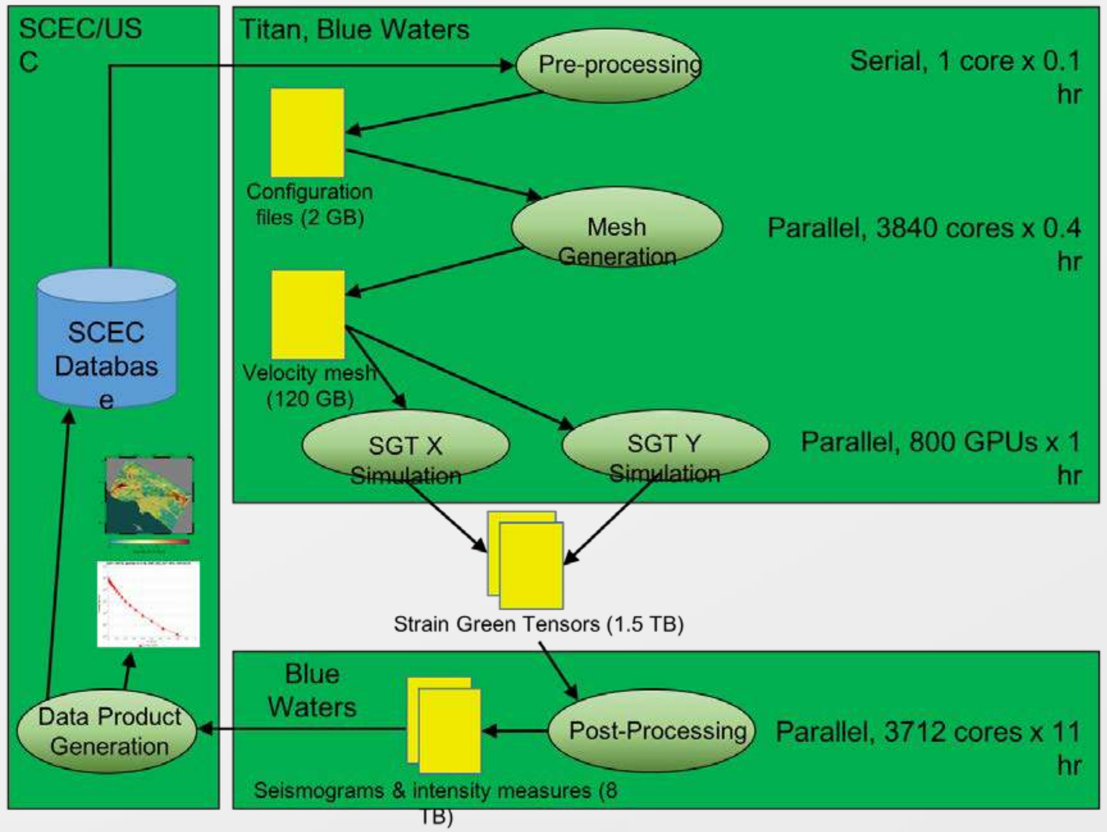
200 GPUs for 1 hour

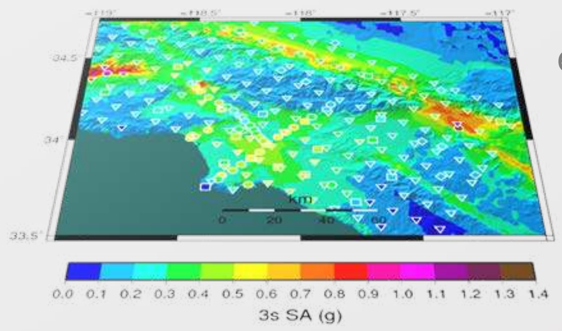
Titan:

421,000 CPU node-hours, 110,000 GPU node-hours

Blue Waters:

673,000 CPU node-hours, 329,000 GPU node-hours





286 sites, 4 models
each workflow has **420,000 tasks**

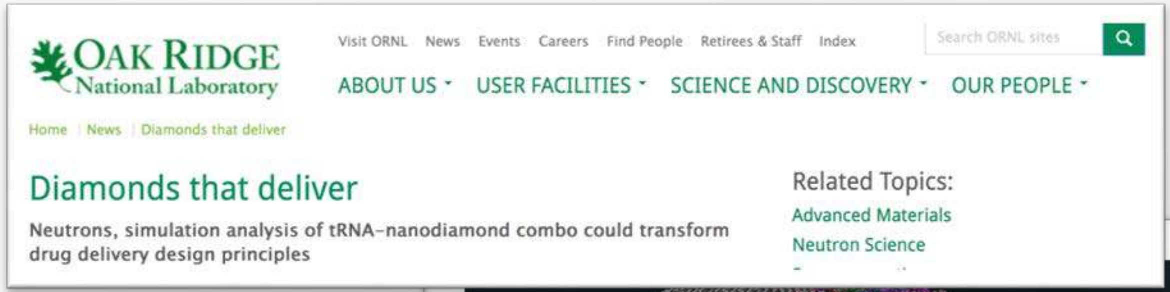
Impact on DOE Science

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

Ran on a Cray XE6 at NERSC using 400,000 CPU hours, and generated 3TB of data.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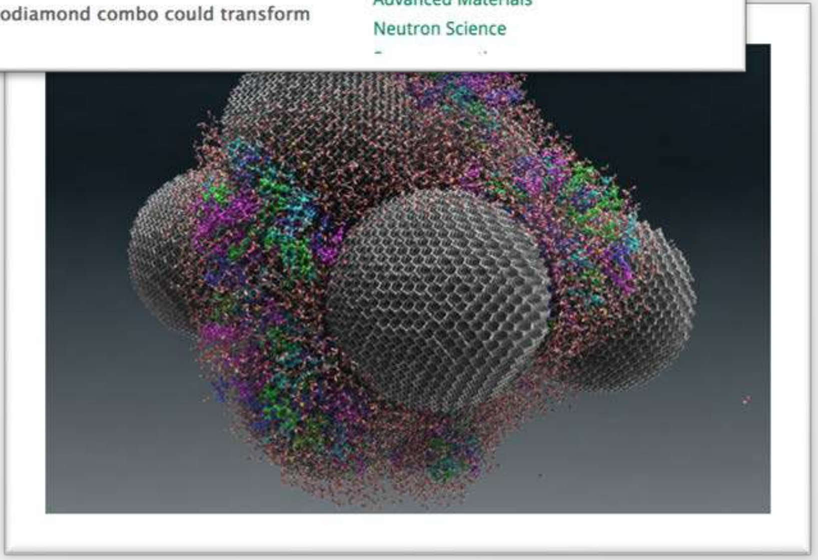
Diamonds that deliver

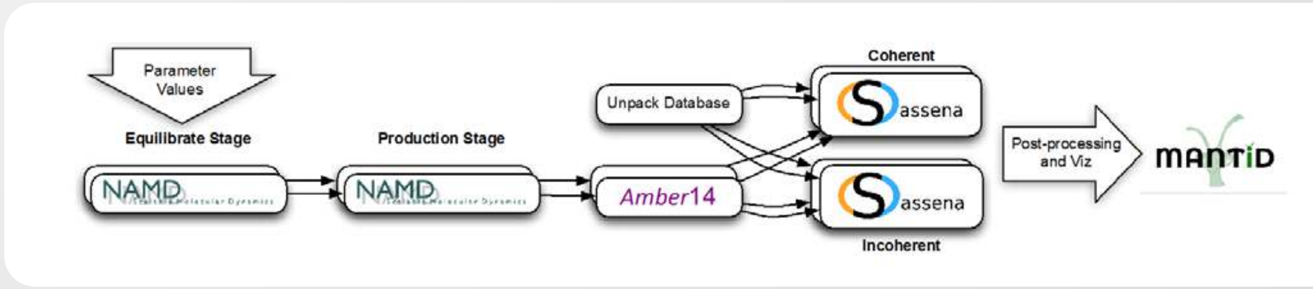
Neutrons, simulation analysis of tRNA–nanodiamond combo could transform drug delivery design principles

Related Topics:

Advanced Materials

Neutron Science


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.*

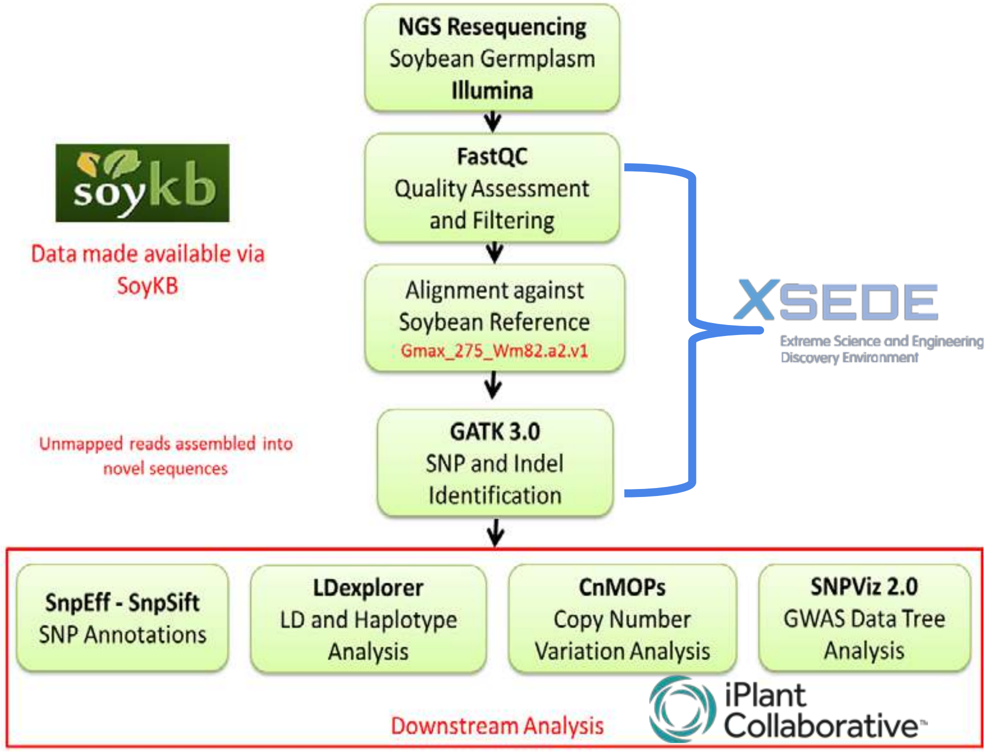
Soybean Workflow

TACC Wrangler as Execution Environment

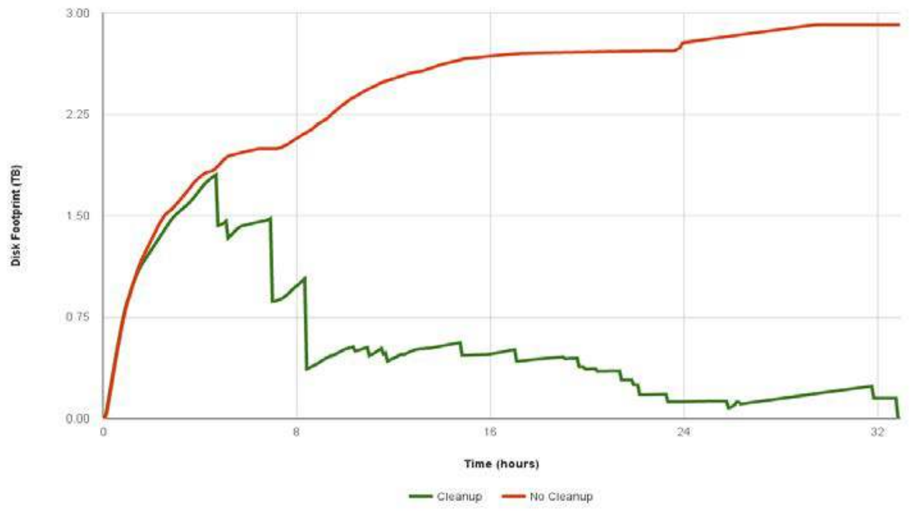
Flash Based Shared Storage

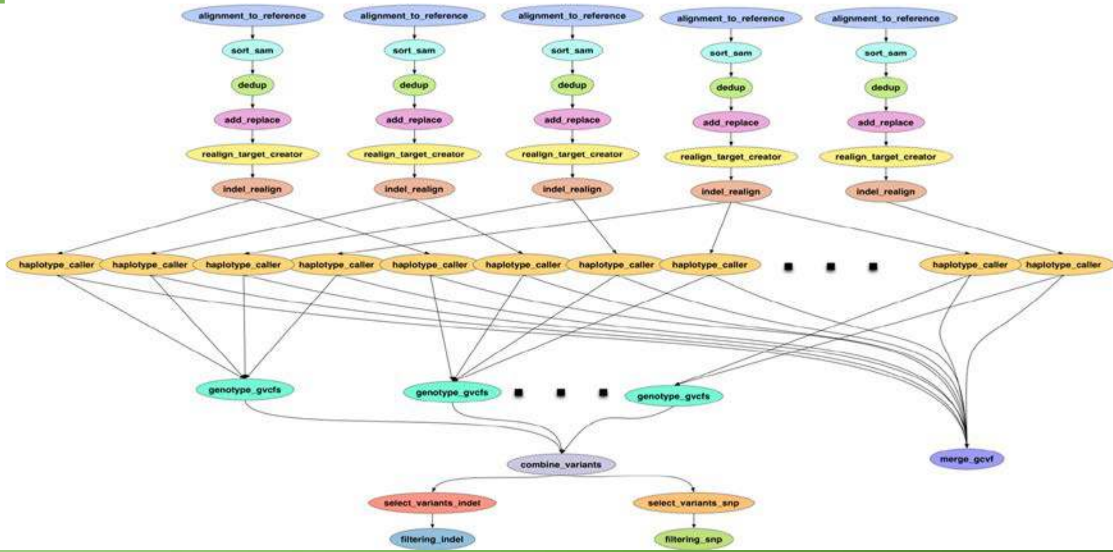
Switched to glideins (pilot jobs) - Brings in remote compute nodes and joins them to the HTCondor pool on the submit host - Workflow runs at a finer granularity

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



NGS Resequencing
Soybean Germplasm
Illumina
FastQC
Quality Assessment and Filtering
Alignment against Soybean Reference
Gmax_275_Wm82.a2.v1
GATK 3.0
SNP and Indel Identification
soykb
Data made available via SoyKB
Unmapped reads assembled into novel sequences
XSEDE
Extreme Science and Engineering Discovery Environment
SnpEff - SnpSift
SNP Annotations
LDexplorer
LD and Haplotype Analysis
CnMOPs
Copy Number Variation Analysis
SNPViz 2.0
GWAS Data Tree Analysis
iPlant Collaborative
Downstream Analysis





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Basic concepts…

Key Pegasus Concepts

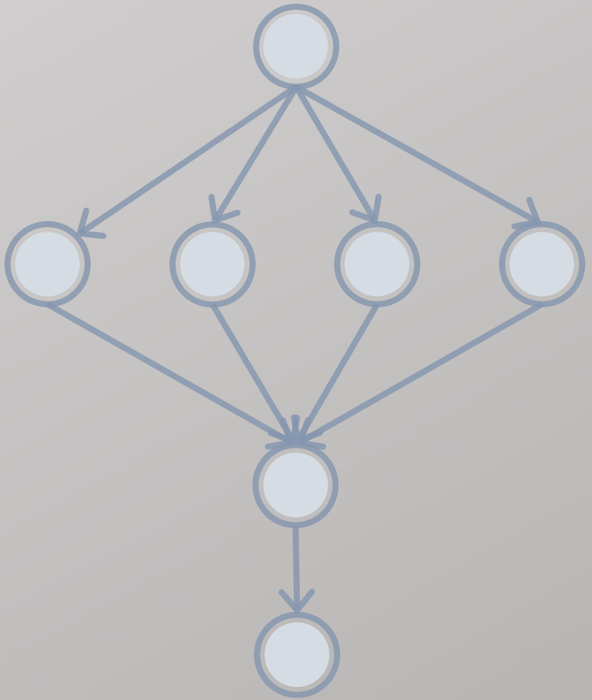
HTCondor
High Throughput Computing

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

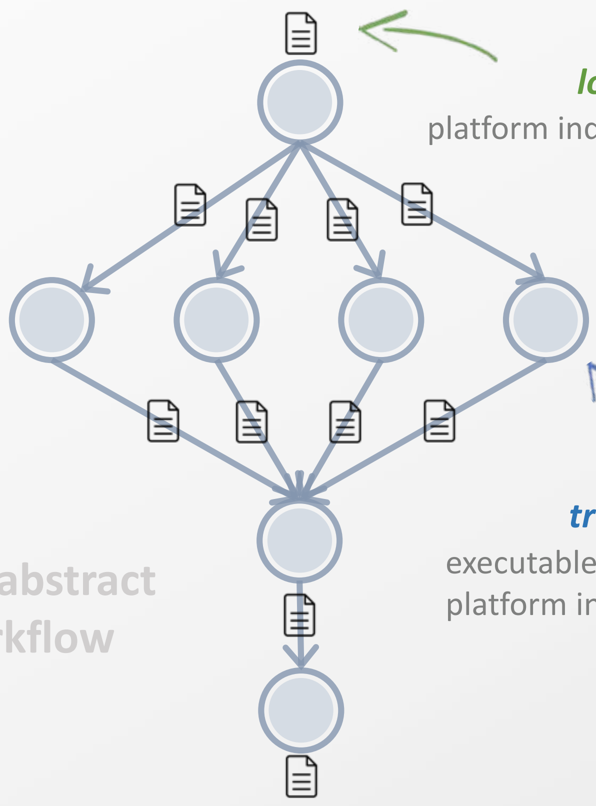
Planning converts an abstract workflow into a concrete, executable workflow

- Planner is like a compiler

DAX
DAG in XML

Portable Description

Users do not worry about low level execution details

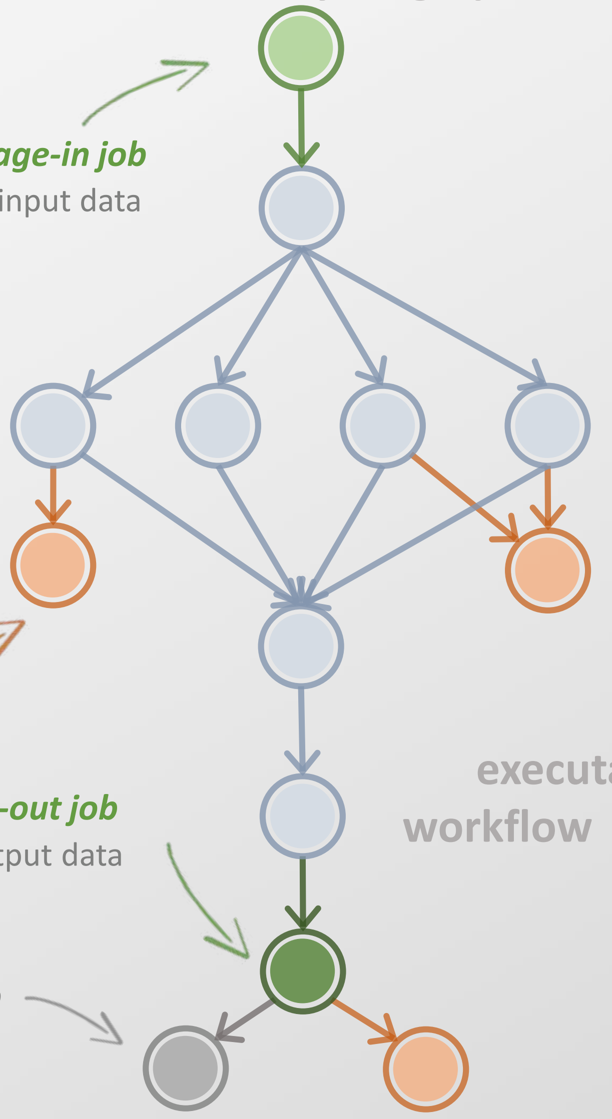


logical filename (LFN)
platform independent (abstraction)

transformation
executables (or programs) platform independent

abstract workflow

DAG
directed-acyclic graphs



stage-in job
Transfers the workflow input data

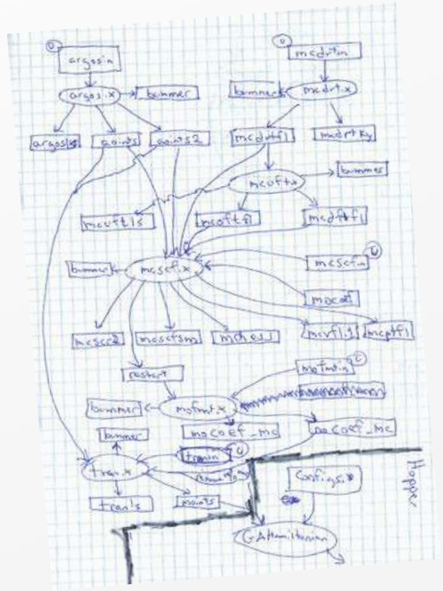
cleanup job
Removes unused data

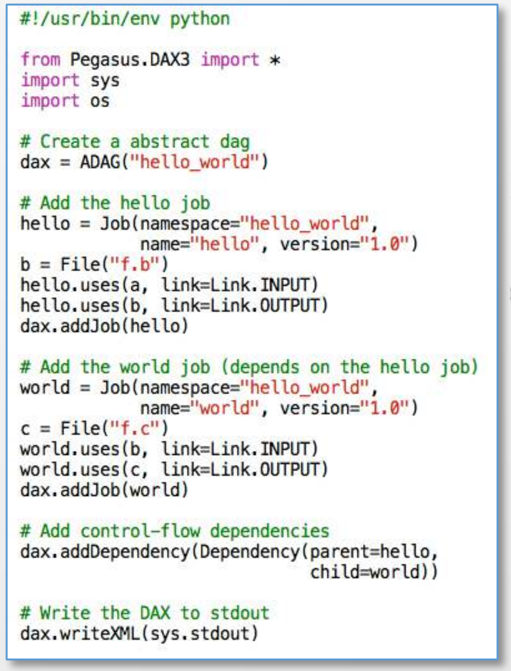
stage-out job
Transfers the workflow output data

registration job
Registers the workflow output data

executable workflow

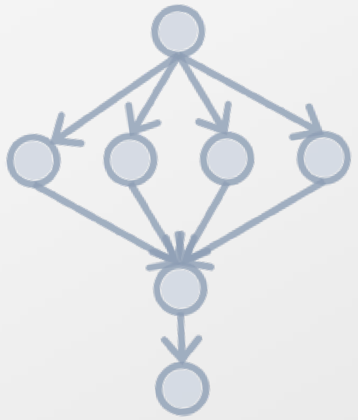
Pegasus also provides tools to generate the abstract workflow

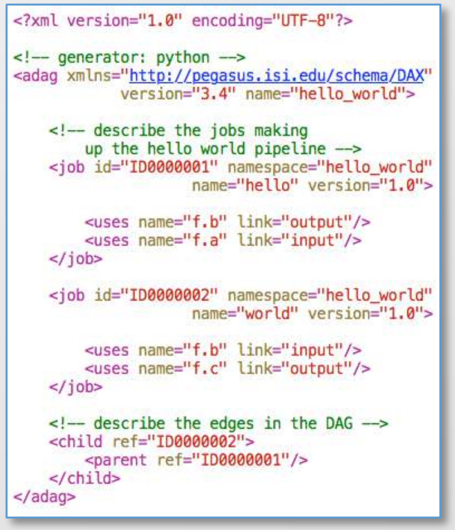




```
#!/usr/bin/env python

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

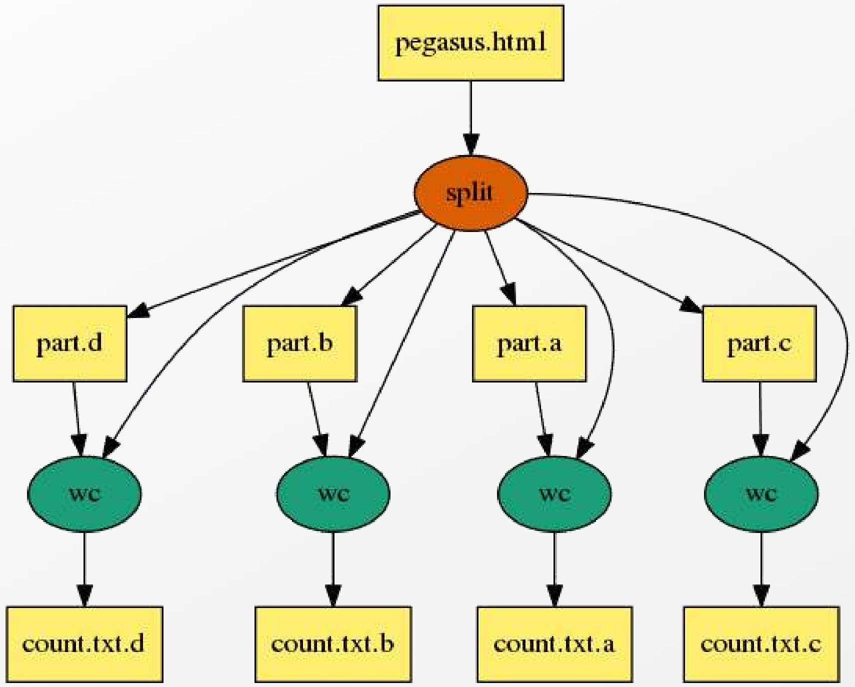




```
<?xml version="1.0" encoding="UTF-8"?>

<!-- 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

An example
Split Workflow



Visualization Tools:

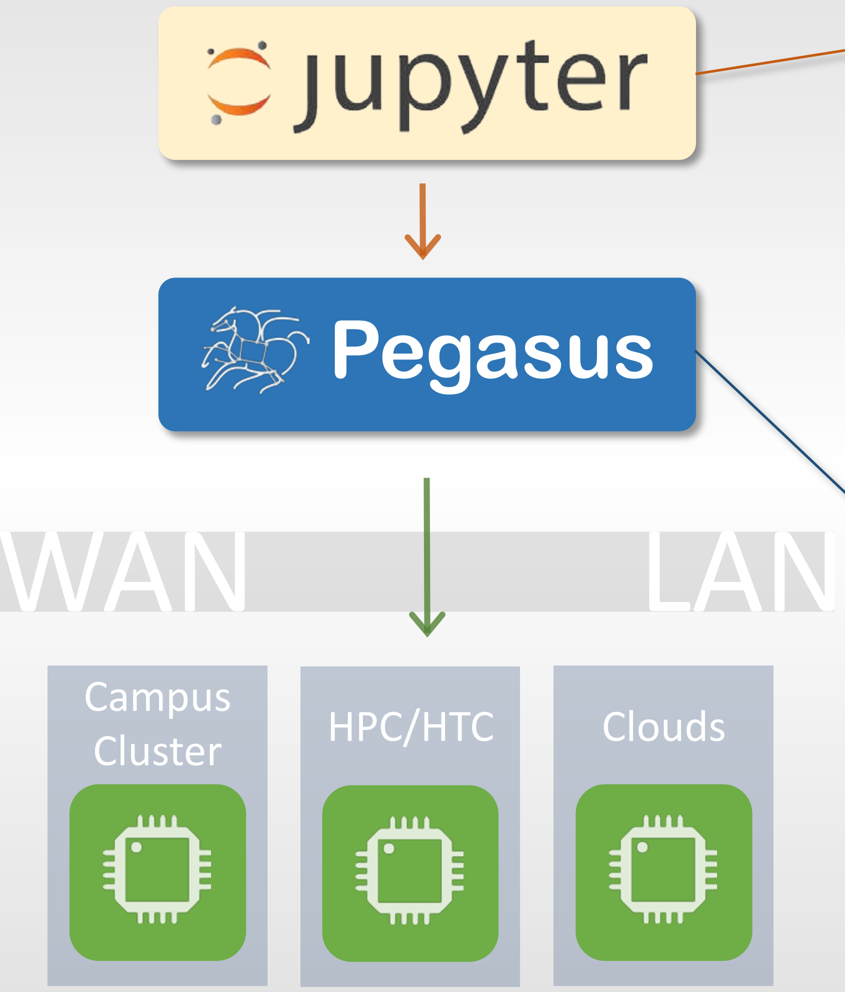
pegasus-graphviz

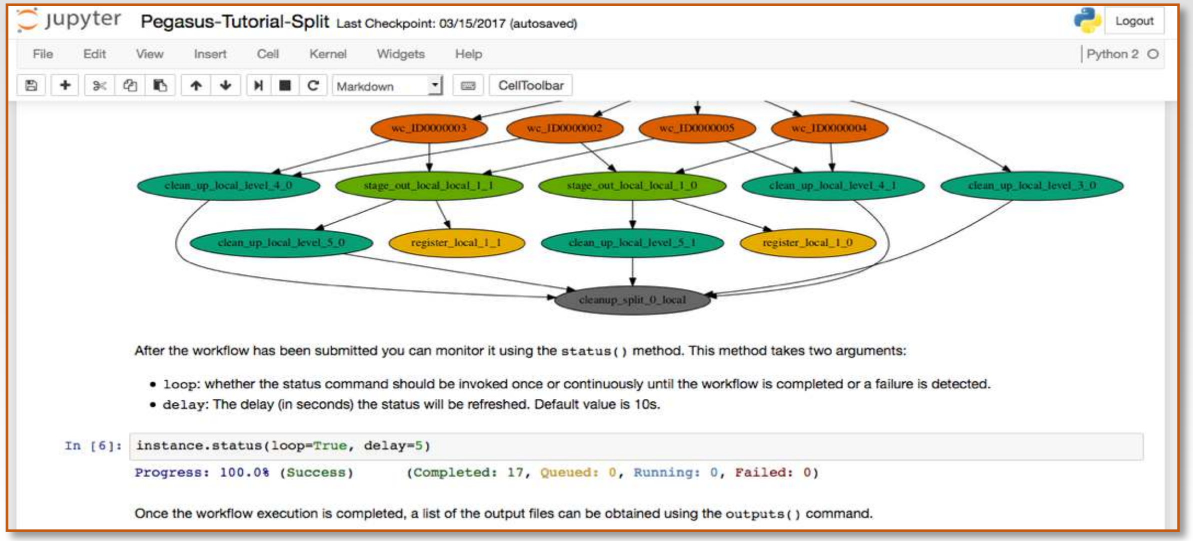
pegasus-plots

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()
```

Running Pegasus workflows with Jupyter



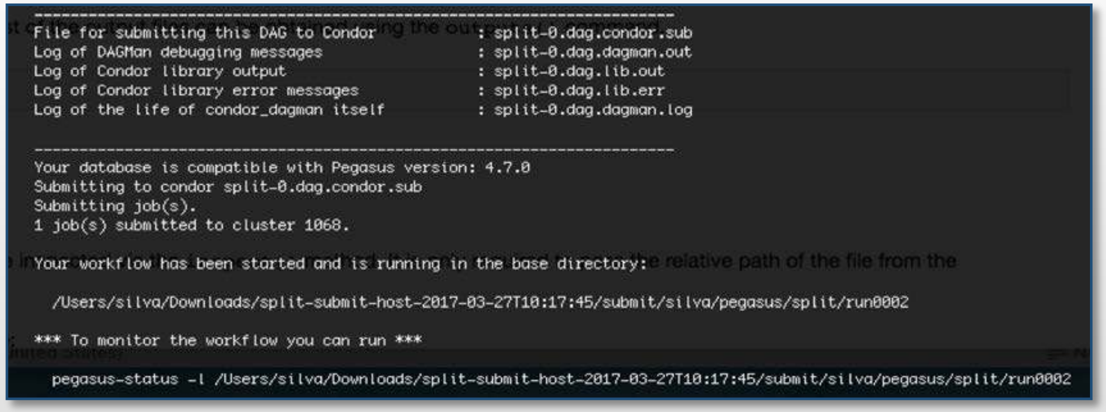


After the workflow has been submitted you can monitor it using the `status()` method. This method takes two arguments:

- `loop`: whether the status command should be invoked once or continuously until the workflow is completed or a failure is detected.
- `delay`: The delay (in seconds) the status will be refreshed. Default value is 10s.

```
In [6]: instance.status(loop=True, delay=5)
        Progress: 100.0% (Success)      (Completed: 17, Queued: 0, Running: 0, Failed: 0)
```

Once the workflow execution is completed, a list of the output files can be obtained using the `outputs()` command.



```
-----------------------------------------------------------------------
File for submitting this DAG to Condor           : split-0.dag.condor.sub
Log of DAGMan debugging messages                 : split-0.dag.dagman.out
Log of Condor library output                     : split-0.dag.lib.out
Log of Condor library error messages             : split-0.dag.lib.err
Log of the life of condor_dagman itself          : split-0.dag.dagman.log

-----------------------------------------------------------------------
Your database is compatible with Pegasus version: 4.7.0
Submitting to condor split-0.dag.condor.sub
Submitting job(s).
1 job(s) submitted to cluster 1068.

Your workflow has been started and is running in the base directory:

  /Users/silva/Downloads/split-submit-host-2017-03-27T10:17:45/submit/silva/pegasus/split/run0002

*** To monitor the workflow you can run ***

  pegasus-status -l /Users/silva/Downloads/split-submit-host-2017-03-27T10:17:45/submit/silva/pegasus/split/run0002
```

Pegasus-Jupyter Python API

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

importing the API

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

creating an instance of the DAX

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

running a workflow

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

monitoring a workflow execution

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

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)

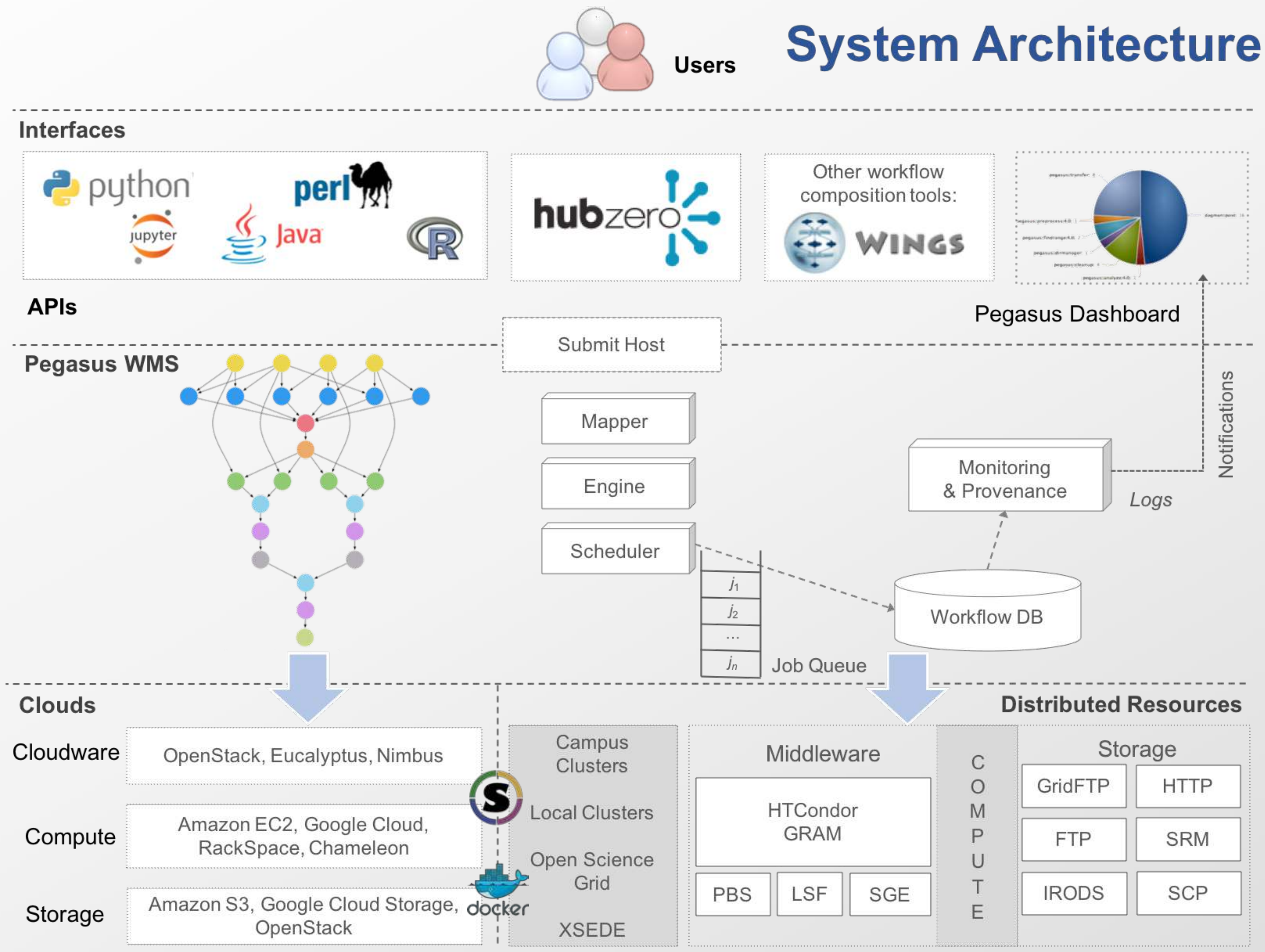
Data Management for Containers

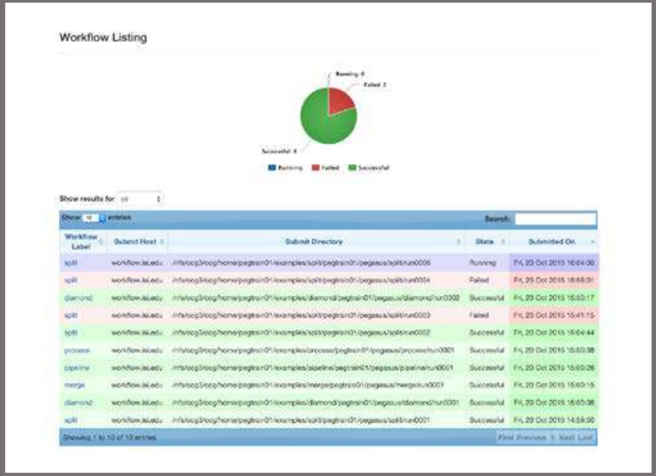
- Users can refer to container images as
  - Docker or Singularity Hub URL’s
  - Docker Image exported as a TAR file and available at a server , just like any other input dataset.

- 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.

System Architecture





Workflow Listing

Show results for: all

Show 10 entries Search:

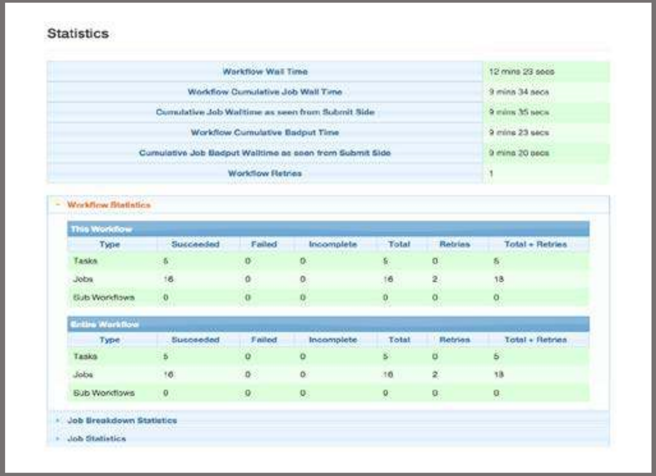
Workflow Label	Submit Host	Submit Directory	State	Submitted On
split	workflow.isi.edu	/nfs/ccg3/ccg/home/pegtrain01/examples/split/pegtrain01/pegasus/split/run0005	Running	Fri, 23 Oct 2015 16:04:30
split	workflow.isi.edu	/nfs/ccg3/ccg/home/pegtrain01/examples/split/pegtrain01/pegasus/split/run0004	Failed	Fri, 23 Oct 2015 16:48:01
diamond	workflow.isi.edu	/nfs/ccg3/ccg/home/pegtrain01/examples/diamond/pegtrain01/pegasus/diamond/run0002	Successful	Fri, 23 Oct 2015 15:53:17
split	workflow.isi.edu	/nfs/ccg3/ccg/home/pegtrain01/examples/split/pegtrain01/pegasus/split/run0003	Failed	Fri, 23 Oct 2015 15:41:15
split	workflow.isi.edu	/nfs/ccg3/ccg/home/pegtrain01/examples/split/pegtrain01/pegasus/split/run0002	Successful	Fri, 23 Oct 2015 15:04:44
process	workflow.isi.edu	/nfs/ccg3/ccg/home/pegtrain01/examples/process/pegtrain01/pegasus/process/run0001	Successful	Fri, 23 Oct 2015 15:03:38
pipeline	workflow.isi.edu	/nfs/ccg3/ccg/home/pegtrain01/examples/pipeline/pegtrain01/pegasus/pipeline/run0001	Successful	Fri, 23 Oct 2015 15:03:26
merge	workflow.isi.edu	/nfs/ccg3/ccg/home/pegtrain01/examples/merge/pegtrain01/pegasus/merge/run0001	Successful	Fri, 23 Oct 2015 15:03:15
diamond	workflow.isi.edu	/nfs/ccg3/ccg/home/pegtrain01/examples/diamond/pegtrain01/pegasus/diamond/run0001	Successful	Fri, 23 Oct 2015 15:03:06
split	workflow.isi.edu	/nfs/ccg3/ccg/home/pegtrain01/examples/split/pegtrain01/pegasus/split/run0001	Successful	Fri, 23 Oct 2015 14:59:50

Showing 1 to 10 of 10 entries First Previous 1 Next Last

Pegasus

dashboard

web interface for monitoring
and debugging workflows



Statistics

Workflow Wall Time	12 mins 23 secs
Workflow Cumulative Job Wall Time	9 mins 34 secs
Cumulative Job Walltime as seen from Submit Side	9 mins 35 secs
Workflow Cumulative Badput Time	9 mins 23 secs
Cumulative Job Badput Walltime as seen from Submit Side	9 mins 20 secs
Workflow Retries	1

– Workflow Statistics

This Workflow

Type	Succeeded	Failed	Incomplete	Total	Retries	Total + Retries
Tasks	5	0	0	5	0	5
Jobs	16	0	0	16	2	18
Sub Workflows	0	0	0	0	0	0

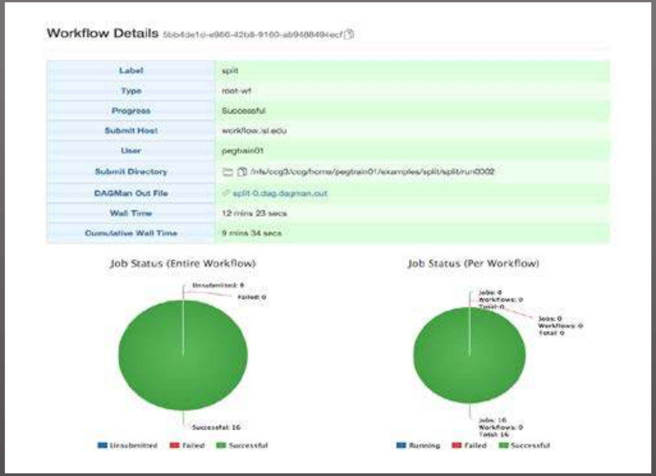
Entire Workflow

Type	Succeeded	Failed	Incomplete	Total	Retries	Total + Retries
Tasks	5	0	0	5	0	5
Jobs	16	0	0	16	2	18
Sub Workflows	0	0	0	0	0	0

+ Job Breakdown Statistics

+ Job Statistics

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.



Workflow Details 5bb4de1c-e966-42b8-9160-ab948849ecf

Label	split
Type	root-wf
Progress	Successful
Submit Host	workflow.isi.edu
User	pegtrain01
Submit Directory	/nfs/ccg3/ccg/home/pegtrain01/examples/split/split/run0002
DAGMan Out File	split-0.dag.dagman.out
Wall Time	12 mins 23 secs
Cumulative Wall Time	9 mins 34 secs

Real-time Monitoring

Reporting

Debugging

Troubleshooting

RESTful API

Pegasus dashboard

web interface for monitoring and debugging workflows

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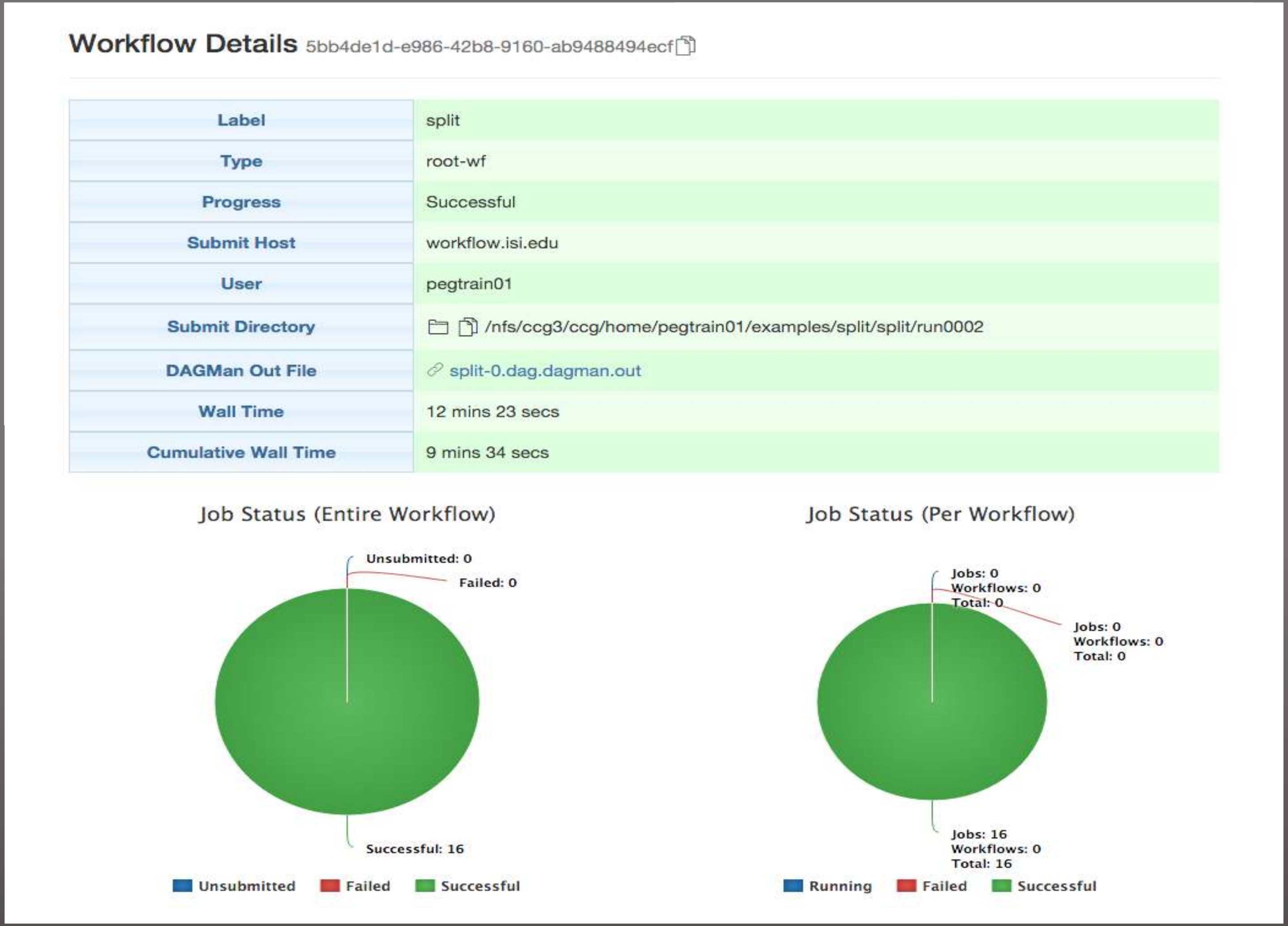

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DAGMan Out File	split-0.dag.dagman.out
Wall Time	12 mins 23 secs
Cumulative Wall Time	9 mins 34 secs

Job Status (Entire Workflow)
Unsubmitted: 0
Failed: 0
Successful: 16
🟦 Unsubmitted 🟥 Failed 🟩 Successful
Job Status (Per Workflow)
Jobs: 0 Workflows: 0 Total: 0
Jobs: 0 Workflows: 0 Total: 0
Jobs: 16 Workflows: 0 Total: 16
🟦 Running 🟥 Failed 🟩 Successful

>_ 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

Pegasus

http://pegasus.isi.edu

Pegasus est. 2001

Automate, recover, and debug scientific computations.

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pegasus-users@isi.edu

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

HipChat

Confluence — Product announcement email copy - edited by William Smith

William Smith — Here's the final email TIS_Email_Promo.png

Image

Cassie Owens — great! let's send it

William Smith — sent!

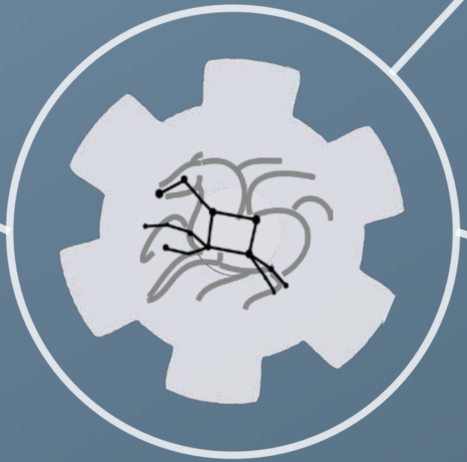
Ryan Lee — tweets are already rolling in! https://twitter.com/andgenth/status/402881643452452864

OUTLINE

Introduction	*Scientific Workflows* *Pegasus Overview* *Successful Stories*
Pegasus Overview	*Basic Concepts* *Features* *System Architecture*
Features	*Data Staging* *Information Catalogs* *Fault-Tolerance*
Break	*10min Break*
Hands On Tutorial	

Understanding Pegasus features…

So, what information does Pegasus need?



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

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

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>
```

How does it know where the executables are or which ones to use?

executables description

list of executables locations per site

physical executables

mapped from logical transformations

transformation type

whether it is installed or
available to stage

```
...
# This is the transformation catalog. It lists information about
# each of the executables that are used by the workflow.

tr ls {
  site PegasusVM {
    pfn "/bin/ls"
    arch "x86_64"
    os "linux"
    type "INSTALLED”
  }
}
...
```

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"
```

Data Staging Configurations

HTCondor I/O (HTCondor pools, OSG, …)

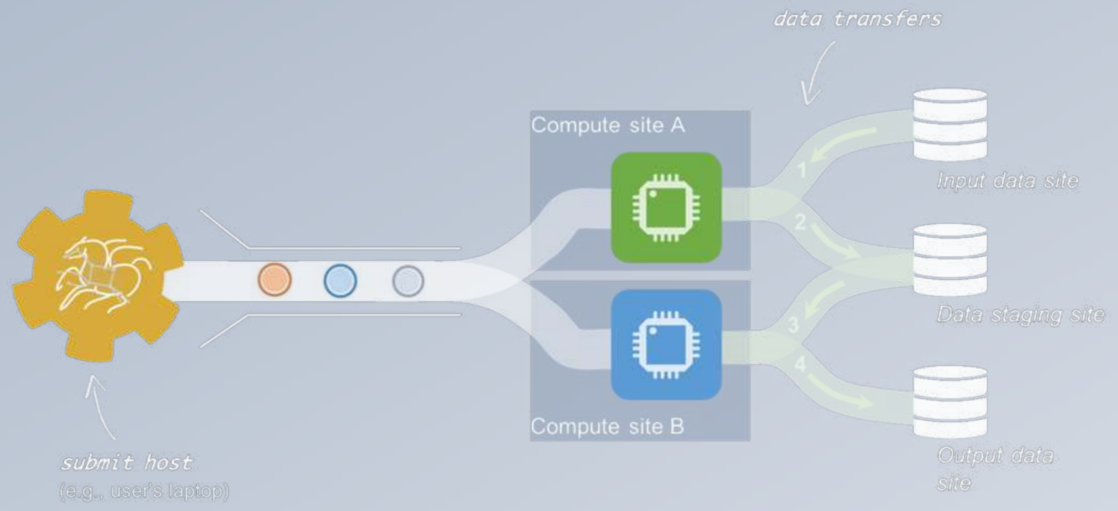
- Worker nodes do not share a file system
- Data is pulled from / pushed to the submit host via HTCondor file transfers
- Staging site is the submit host

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

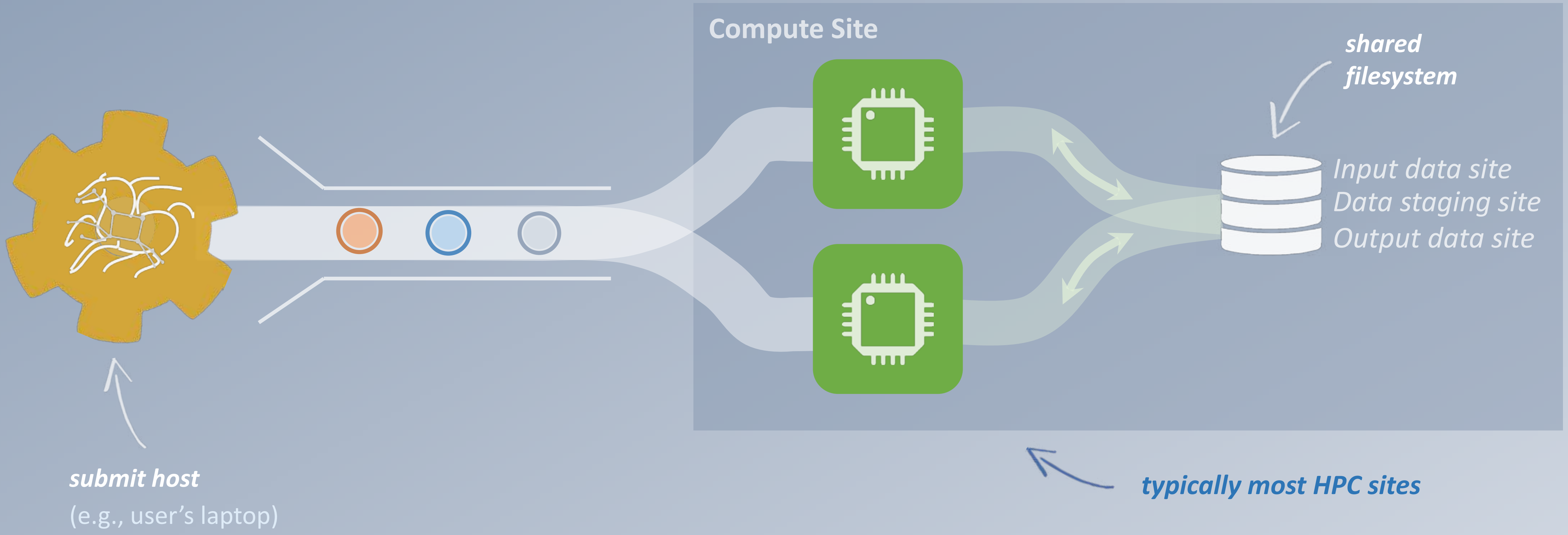
Shared File System (HPC sites, XSEDE, Campus clusters, …)

- I/O is directly against the shared file system



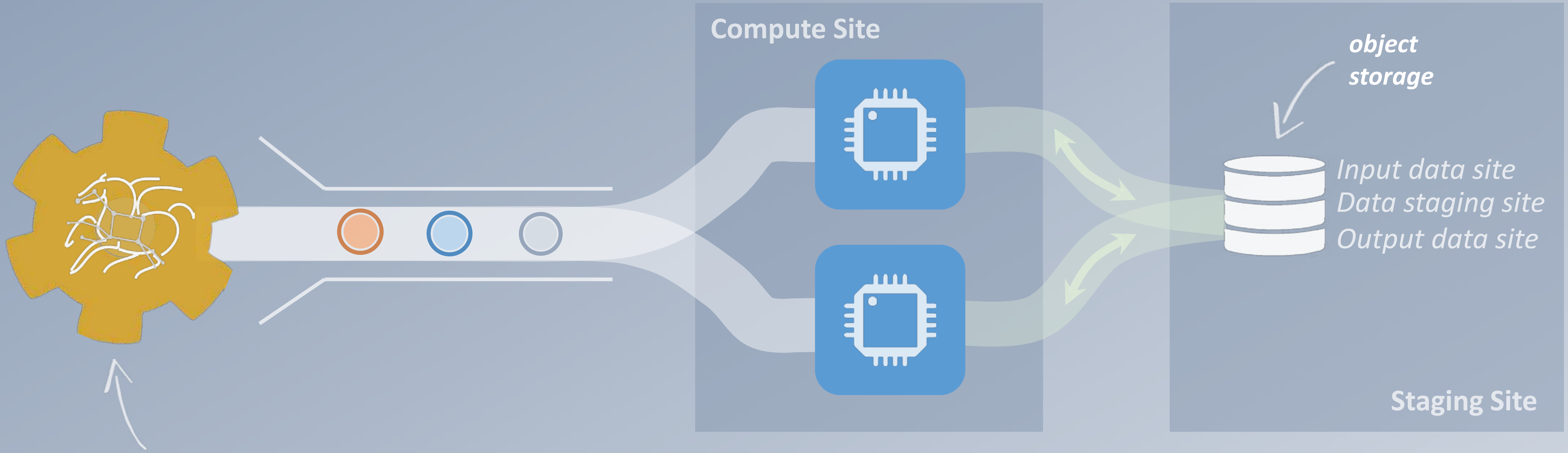
High Performance Computing

There are several possible configurations…



Cloud Computing

high-scalable object storages

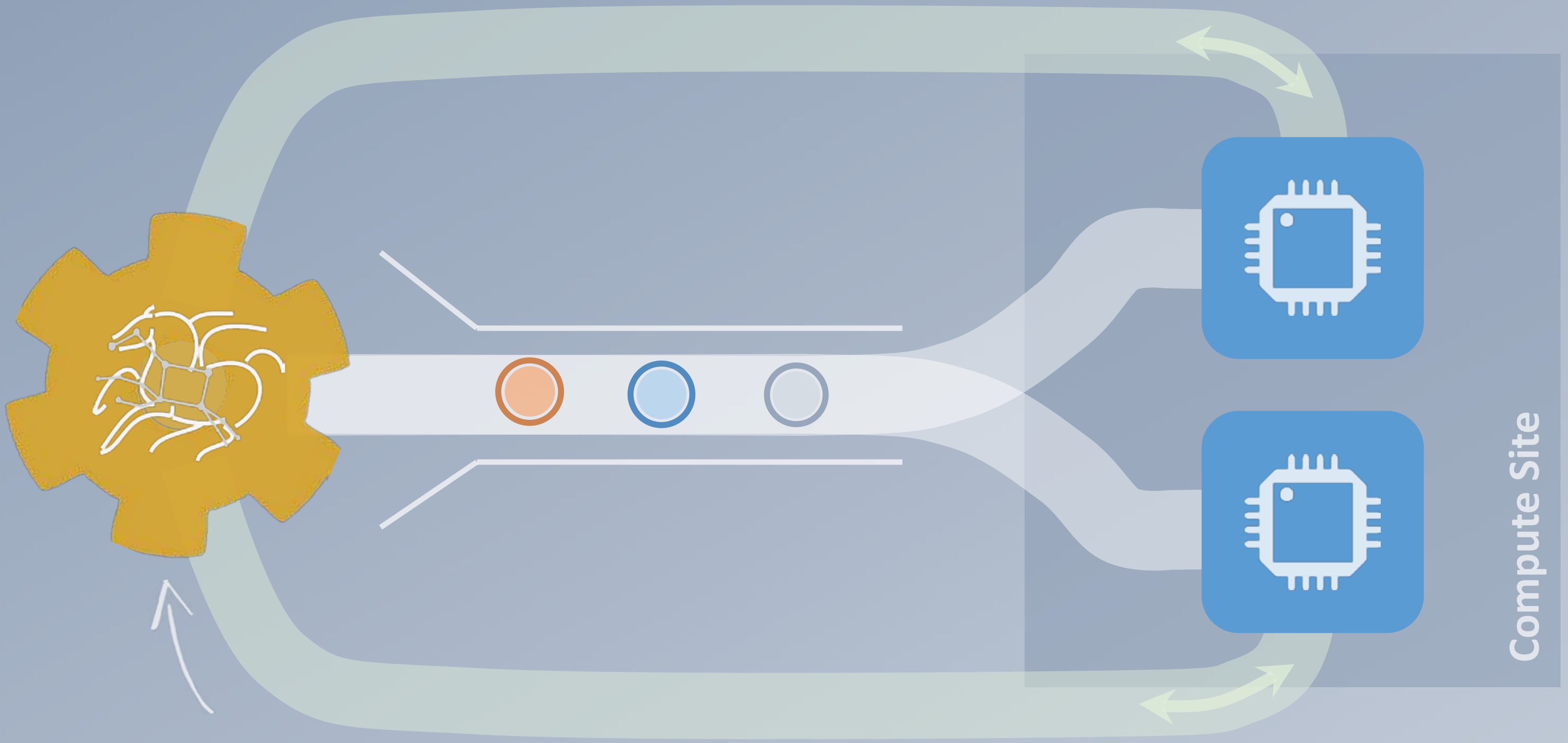


submit host
(e.g., user's laptop)

Typical cloud computing deployment (Amazon S3, Google Storage)

Grid Computing

local data management



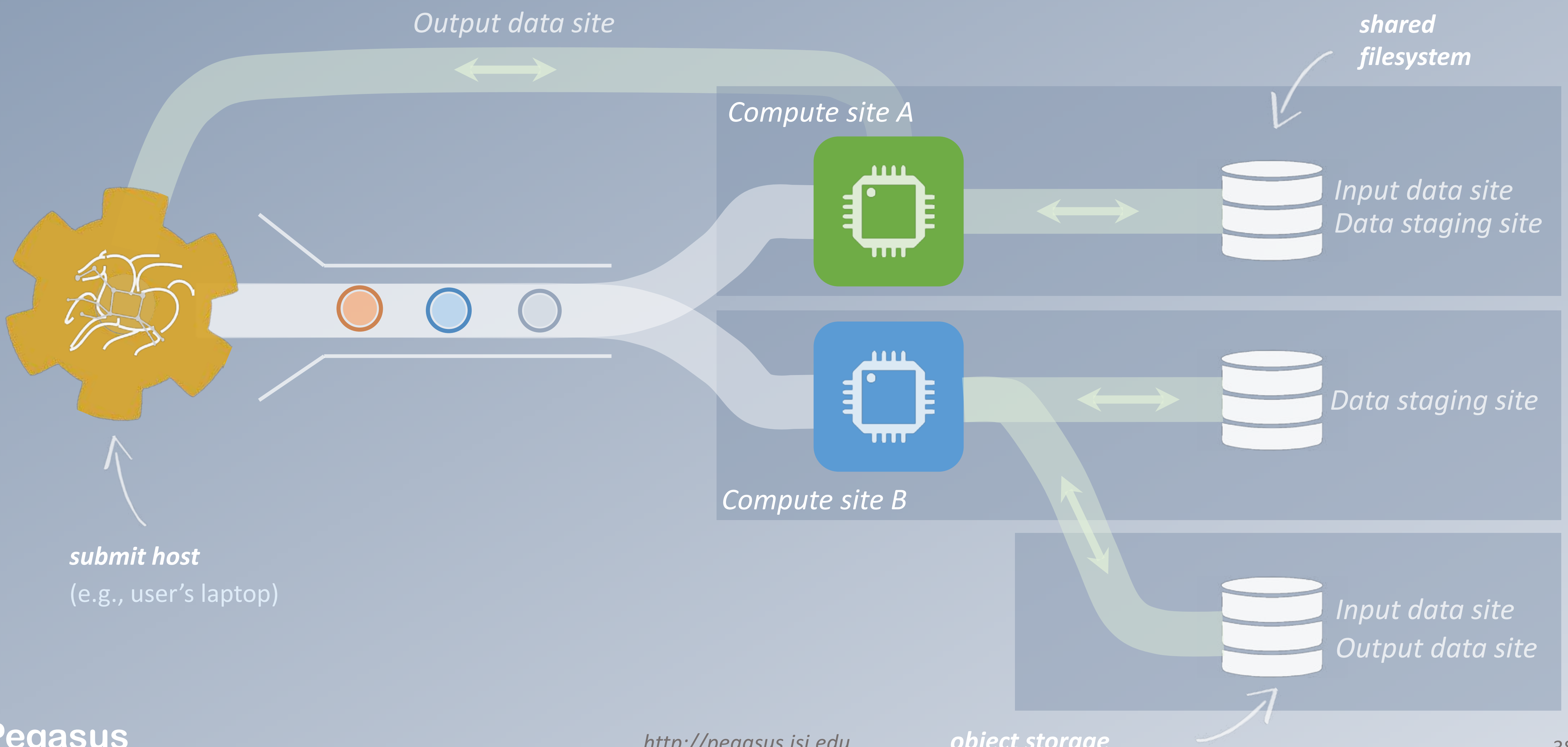
Typical OSG sites

Open Science Grid

submit host

(e.g., user's laptop)

And yes… you can mix everything!



Running workflows on AWS

There are many different ways to set up an execution environment in Amazon EC2

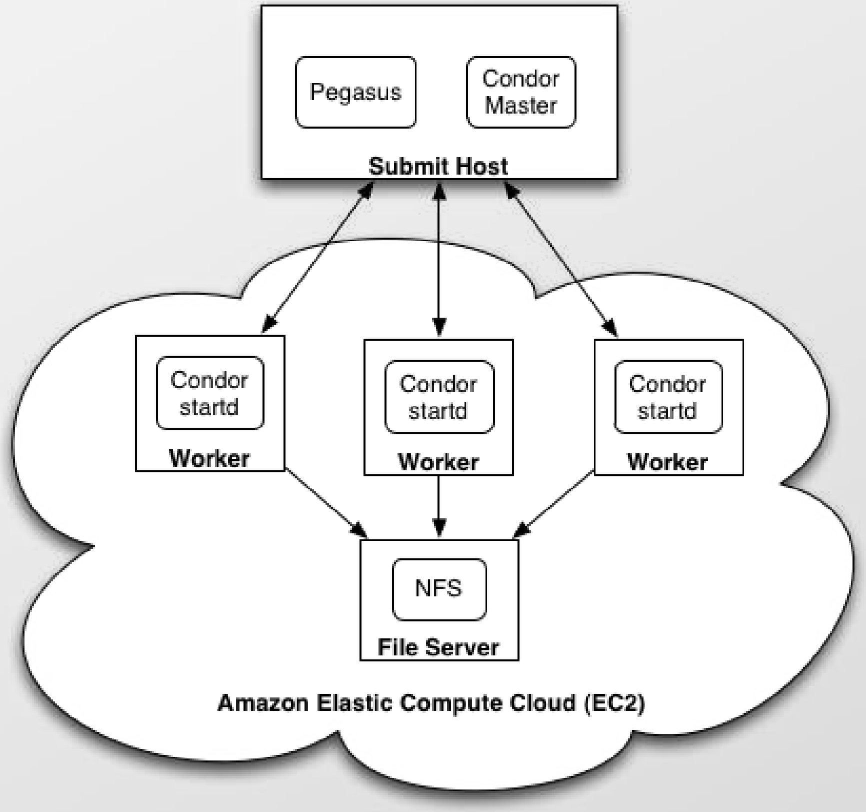
The simplest way is to use a submit machine outside the cloud, and to provision several worker nodes and a file server node in the cloud

1. Launch the VM (Condor Worker) – requires configuration
2. The VM will appear as a new compute resource
3. Spawn job to the cloud VM
4. VMs shutdown itself in the absence of work

Guidelines for Tutorial VM:

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

Amazon EC2



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
```

And if a job fails?

Job Failure Detection

detects non-zero exit code
output parsing for success or failure message
exceeded timeout
do not produced expected output files

Job Retry

helps with transient failures
set number of retries per job and run

Checkpoint Files

job generates checkpoint files
staging of checkpoint files is automatic on restarts

Rescue DAGs

workflow can be restarted from checkpoint file
recover from failures with minimal loss

A few more features…

Metadata

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

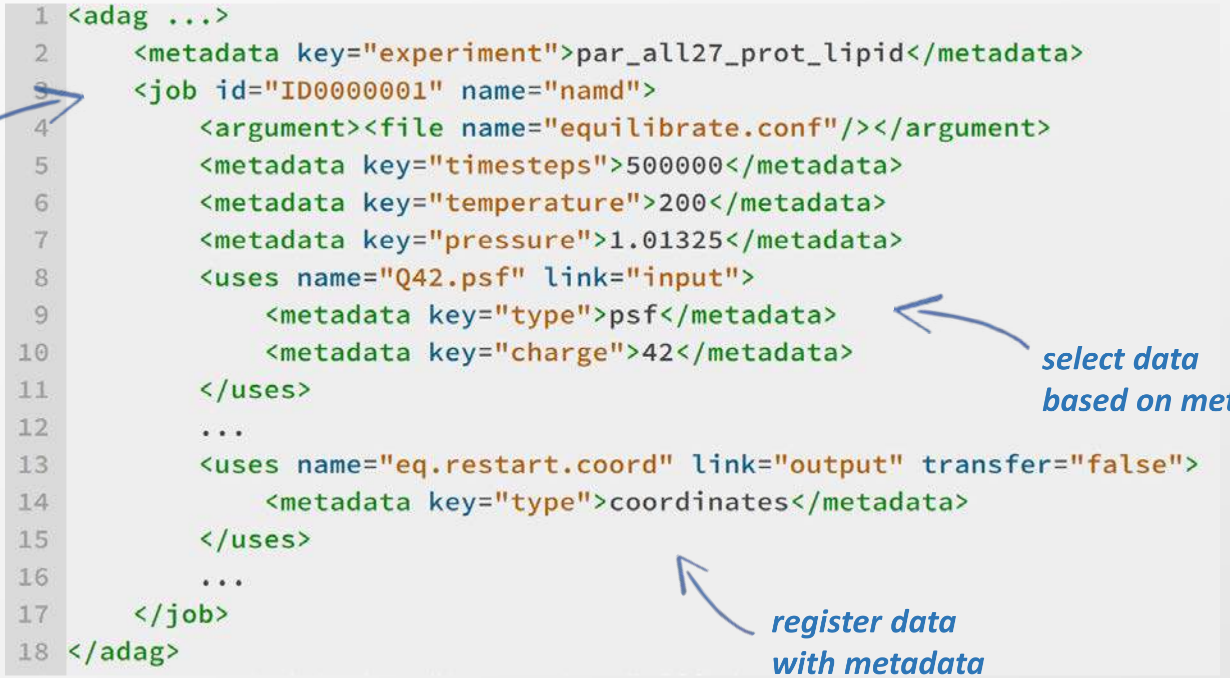
Data registration

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

Static and runtime metadata

Static: application parameters

Runtime: performance metrics

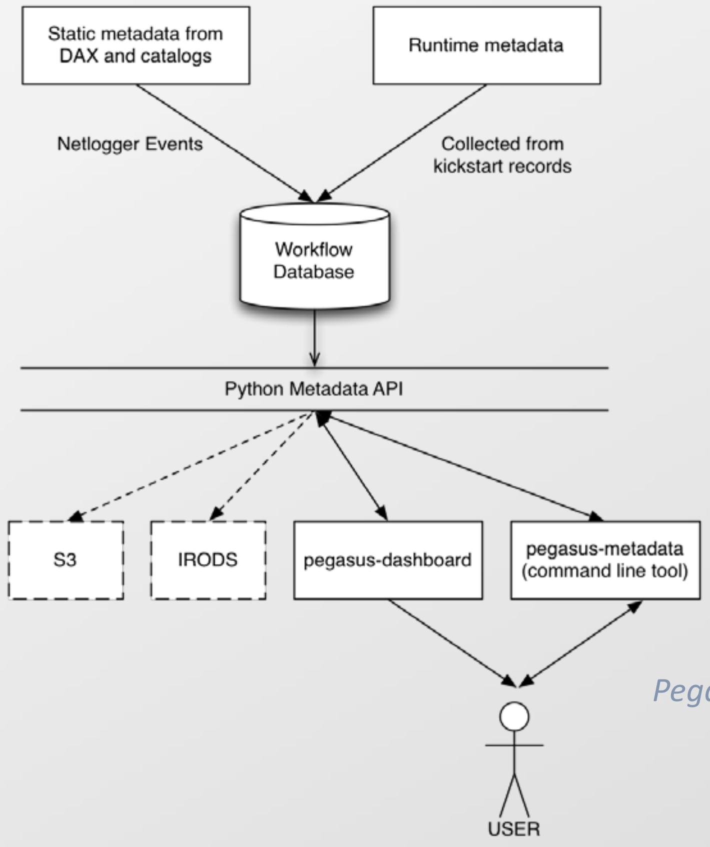


```
<adag ...>
    <metadata key="experiment">par_all27_prot_lipid</metadata>
    <job id="ID0000001" name="namd">
        <argument><file name="equilibrate.conf"/></argument>
        <metadata key="timesteps">500000</metadata>
        <metadata key="temperature">200</metadata>
        <metadata key="pressure">1.01325</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>
```

workflow, job, file

select data based on metadata

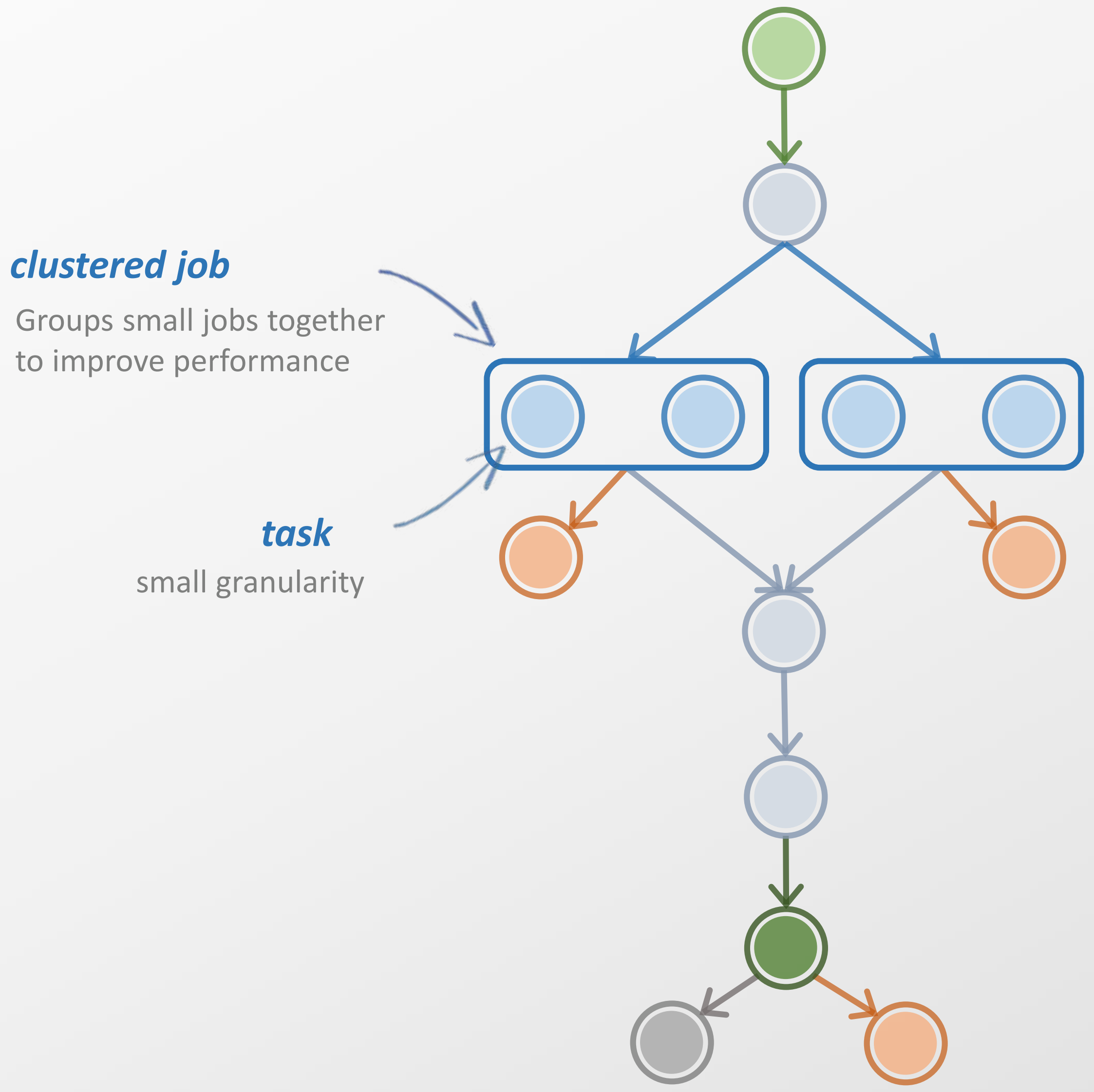
register data with metadata



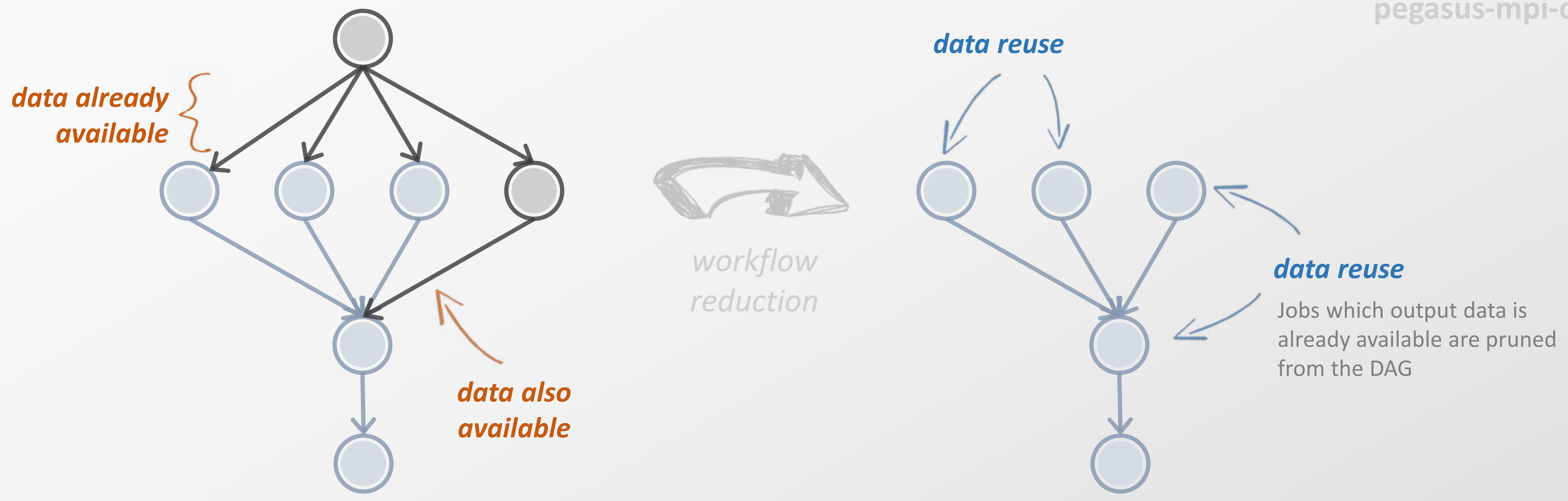
Static metadata from DAX and catalogs
Runtime metadata
Netlogger Events
Collected from kickstart records
Workflow Database
Python Metadata API
S3
IRODS
pegasus-dashboard
pegasus-metadata (command line tool)
USER

since Pegasus 4.6

Performance, why not improve it?

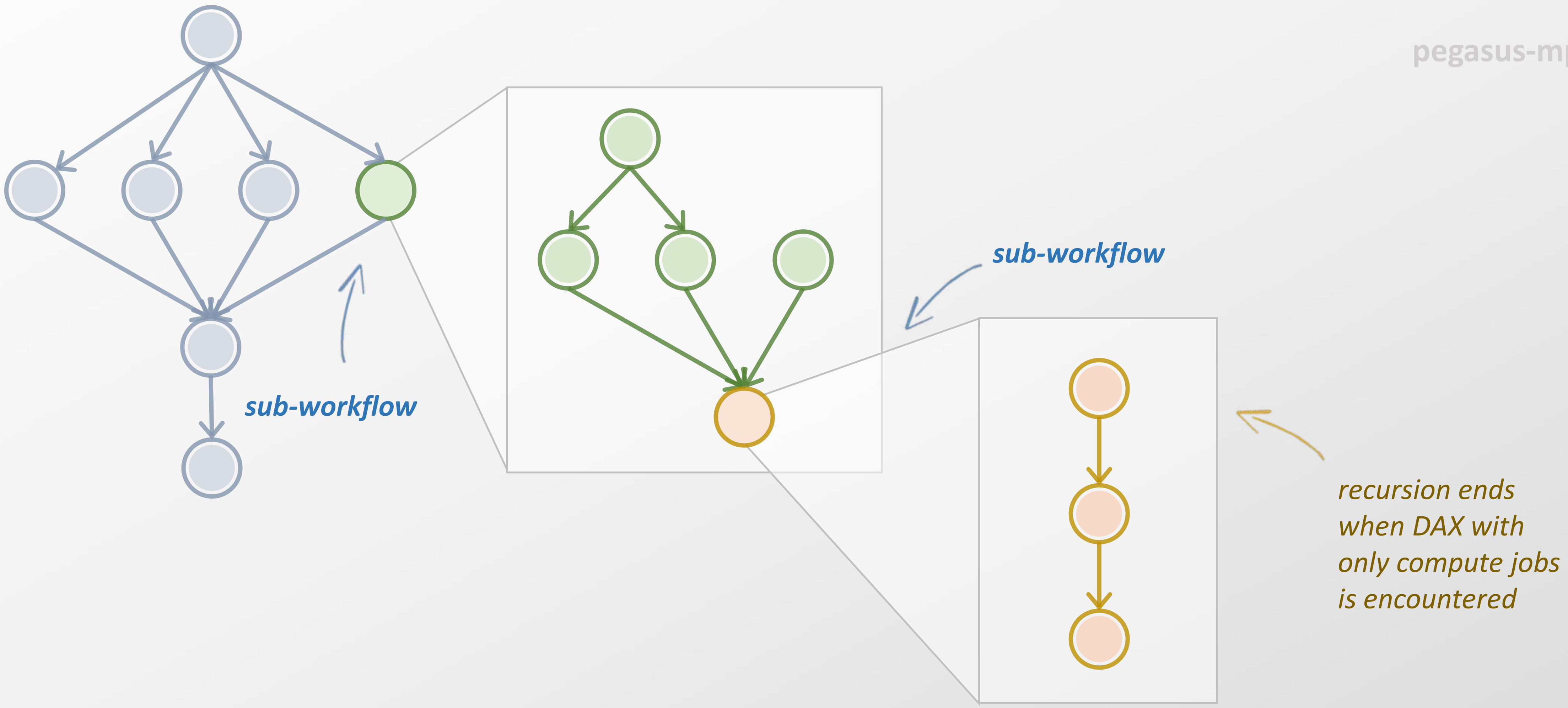


What about **data reuse**?

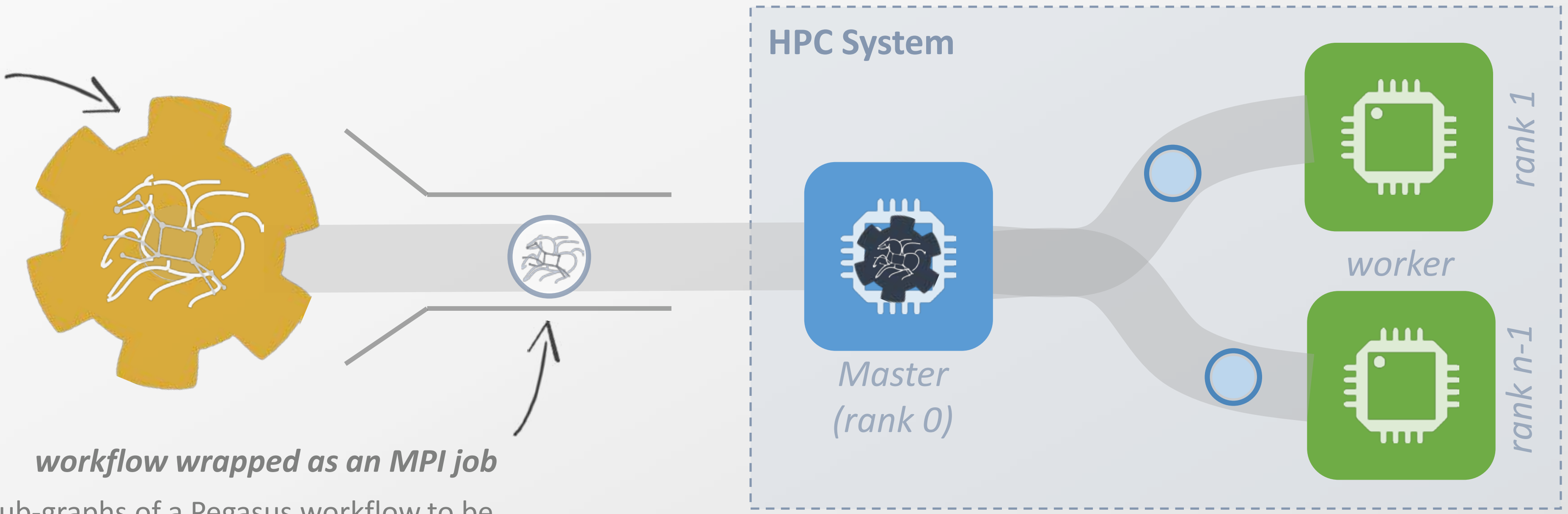


Jobs which output data is already available are pruned from the DAG

Pegasus also handles **large-scale workflows**


sub-workflow
sub-workflow
recursion ends when DAX with only compute jobs is encountered

Running **fine-grained** workflows on HPC systems…



submit host
(e.g., user's laptop)

workflow wrapped as an MPI job

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

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Hands On Tutorial	

Hands-On Pegasus Tutorial…

Pegasus Tutorial

- SSH to our training machine
    - You need to be connected to the '**utk-open**' network
    - Login with your user's tutorial login and password

```
ssh pegtrain42@workflow.isi.edu
```

Split Workflow Execution Steps

- Step 1: Change directory to split workflow dir
  ```
  cd  ~/tutorial/split_example
  ```
- Step 2: Generate the Pegasus DAX file
  ```
  ./daxgen.py split.dax
  ```
- Step 3: Plan and submit the split workflow
  ```
  ./plan_dax.sh split.dax
  ```
- Step 4: Observe the progress of the workflow
  ```
  watch pegasus-status -l submit/USERNAME/pegasus/split_wf/run0001
  ```

Pegasus Dashboard

- Step 1: Change workflow db permissions

```
chmod –R 755 ~/.pegasus
```

- Step 2: Go to your browser and open
  `https://workflow.isi.edu:8443`

- Step 3: Login with your user’s tutorial login and password

NAMD Workflow Execution Steps

- Step 1: Change directory to namd workflow dir
```
cd  ~/tutorial/namd_example
```

- Step 2: Generate the Pegasus DAX file
```
./daxgen.py namd.dax
```

- Step 3: Plan and submit the namd workflow
```
./plan_dax.sh namd.dax
```

- Step 4: Observe the progress of the workflow
```
watch pegasus-status -l submit/USERNAME/pegasus/namd_wf/run0001
```

NAMD Workflow With Docker

- Step 1: Create a docker image with NAMD pre-installed
  There is already on here: https://hub.docker.com/r/papajim/namd_image
- Step 2: Edit the transformation catalog to use docker

```
cont namd_image {
  type “docker”
  image “docker:///papajim/namd_image:latest”
}
tr namd {
  site condorpool {
    container “namd_image”
    pfn “file:///opt/NAMD_2.12_Linux-x86_64-multicore/namd2”
    arch “x86_64”
    os “LINUX”
    type “INSTALLED”
}}
```

NAMD Workflow With Docker

- Step 3: Change directory to namd workflow dir
  cd ~/tutorial/namd_docker

- Step 4: Generate the Pegasus DAX file
  ./daxgen.py namd.dax

- Step 5: Plan and submit the namd workflow
  ./plan_dax.sh namd.dax

- Step 6: Observe the progress of the workflow
  watch pegasus-status –l submit/USERNAME/pegasus/namd_wf/run0001

Jupyter Notebook

- Go to https://workflow.isi.edu:8000
  - Login with your user’s tutorial login and password
  - Click the button to **Launch the Jupyter server**
  - Open the folder ‘**jupyter**’
  - Launch the ‘**Pegasus-DAX3-Tutorial.ipynb**’ notebook
- Instructions on how to execute the notebook
  - Update the ‘**workflow_dir**’ variable with your training account name

```
    workflow_dir = '/scitech/home/pegtrain42/jupyter/wf-split-tutorial’
```

  - Update the ‘**replica catalog**’ entry with your training account name

```
rc = ReplicaCatalog(workflow_dir)
rc.add('pegasus.html', ‘file:///scitech/home/pegtrain42/jupyter/pegasus.html', site='local')
```

NAMD Workflow Execution Steps (NERSC)

- Step 1: Retrieve myproxy credential from NERSC

```
myproxy-logon -s nerscca.nersc.gov:7512 -t 24 -T -l NERSC_USER
```

- Step 2: Change directory to namd workflow dir

```
cd  ~/tutorial/namd_example
```

- Step 3: Edit "plan_dax.sh" and update the execution site

```
pegasus-plan \
    --conf pegasus.properties \
    --dax $DAXFILE \
    --dir $DIR/submit \
    --input-dir $DIR/input \
    --output-dir $DIR/output \
    --sites nersc \
    --cleanup leaf \
    --force \
    --submit
```

NAMD Workflow Execution Steps (NERSC)

- Step 4: Update sites catalog with your NERSC scratch folder

```
<directory type="shared-scratch" path="YOUR_SHARED_SCRATCH_DIR">
  <file-server operation="all" url="gsiftp://corigrid.nersc.gov/YOUR_SHARED_SCRATCH_DIR"/>
</directory>
```

- Step 5: Generate the Pegasus DAX file
  ```
  ./daxgen_nersc.py namd_nersc.dax
  ```

- Step 6: Plan and submit the namd workflow
  ```
  ./plan_dax.sh namd_nersc.dax
  ```

- Step 7: Observe the progress of the workflow
  ```
  watch pegasus-status -l submit/USERNAME/pegasus/namd_wf/run0002
  ```