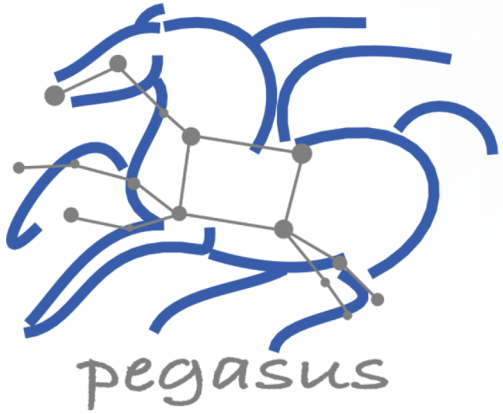

Pegasus
Workflow Management System

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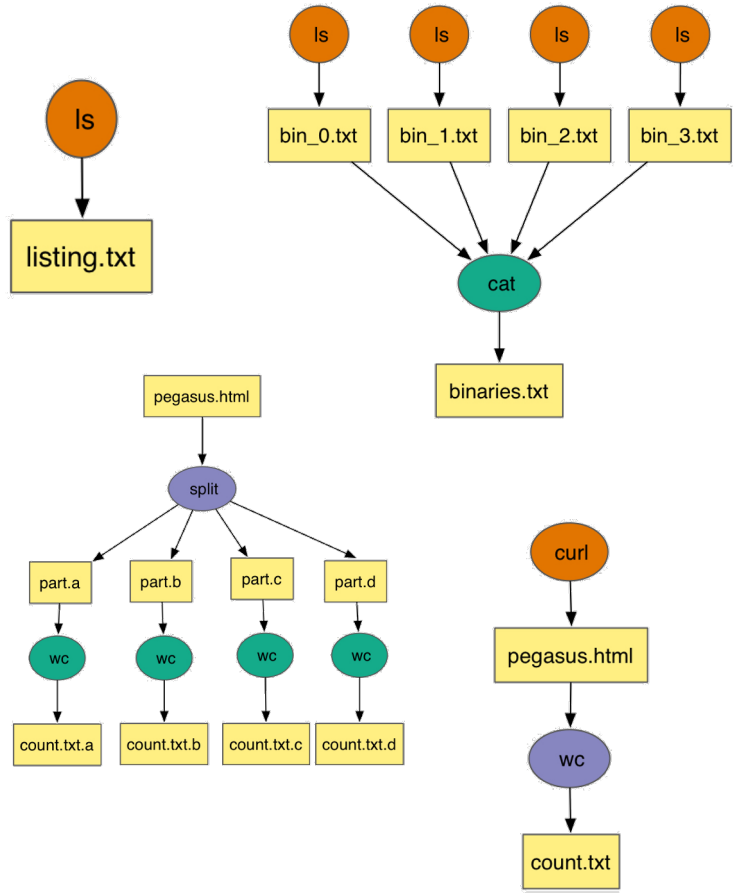
What are Scientific Workflows

- Conducts a series of computational tasks.
  - Resources distributed across Internet.
- Chaining (outputs become inputs) replaces manual hand-offs.
  - Accelerated creation of products.
- Ease of use - gives non-developers access to sophisticated codes.
  - Avoids need to download-install-learn how to use someone else's code.
- Provides framework to host or assemble community set of applications.
  - Honors original codes. Allows for heterogeneous coding styles.
- Framework to define common formats or standards when useful.
  - Promotes exchange of data, products, codes. Community metadata.
- Multi-disciplinary workflows can promote even broader collaborations.
  - E.g., ground motions fed into simulation of building shaking.
- Certain rules or guidelines make it easier to add a code into a workflow.

Workflow Building Blocks



Slide Content Courtesy of David Okaya, SCEC, USC

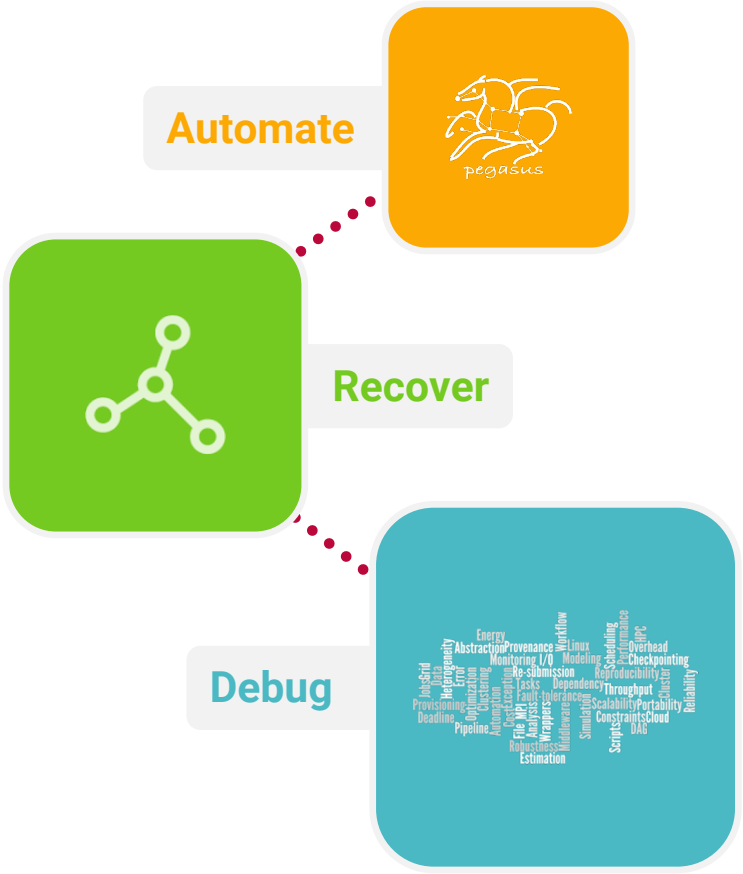
Workflow Challenges Across Domains

- Need to describe complex workflows in a simple way
- Need to access distributed, heterogeneous data and resources (heterogeneous interfaces)
- Need to deal with resources/software that change over time
- Ease of use. Ability to debug and monitor large workflows

Our Focus

- Separation between workflow description and workflow execution
- Workflow planning and scheduling (scalability, performance)
- Task execution (monitoring, fault tolerance, debugging, web dashboard)
- Provide additional assurances that a scientific workflow is not accidentally or maliciously tampered with during its execution.

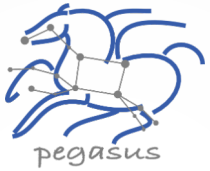
Why Pegasus?



- **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**
- Ensures **Data Integrity** during workflow execution

HTCondor High Throughput Computing

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



Some of The Success Stories...

Southern California Earthquake Center's CyberShake

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

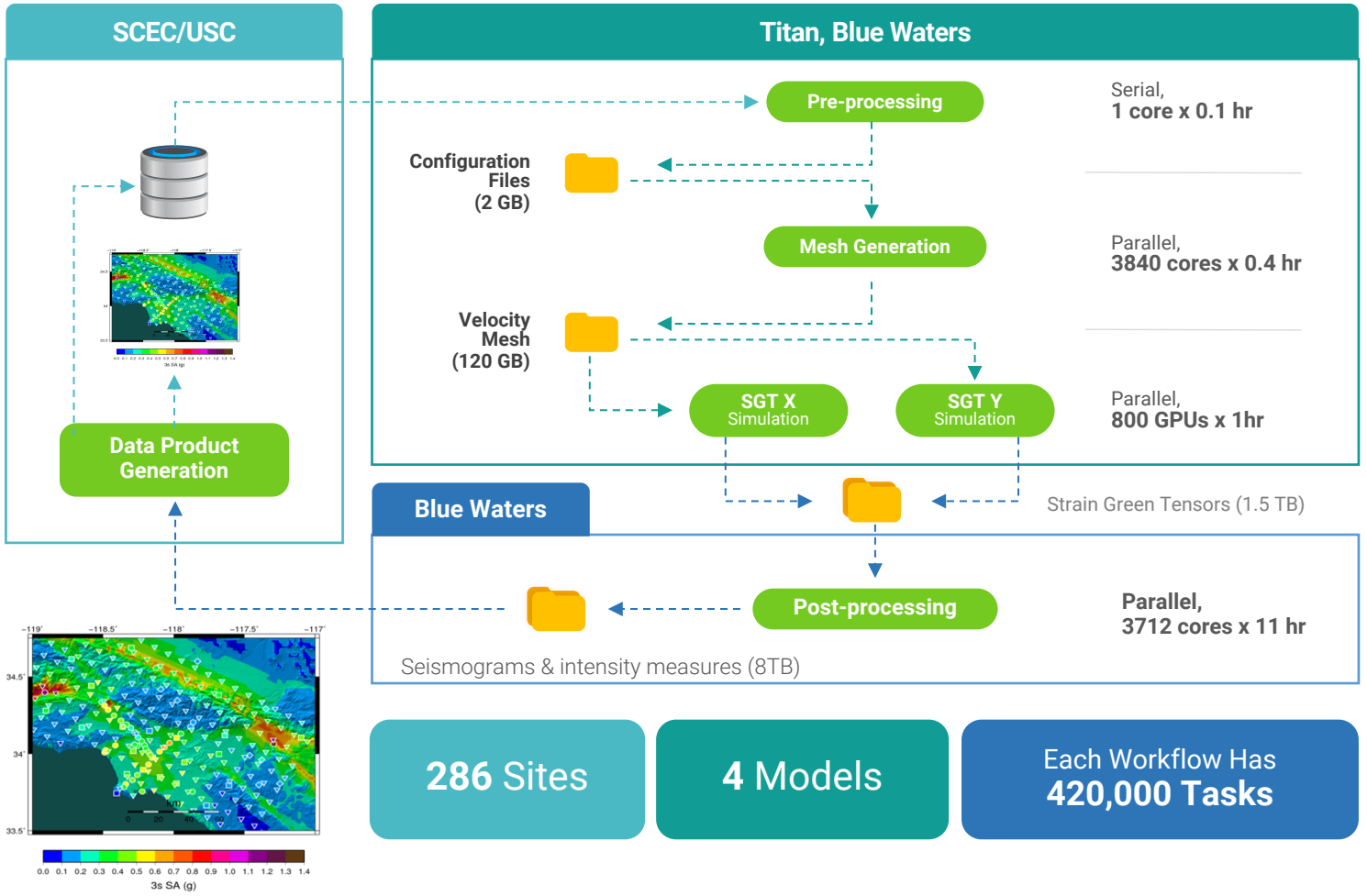
GPU jobs:
439,000 node-hours
AWP-ODC finite-difference code
5 billion points per volume, 23,000 timesteps
200 GPUs for 1 hour

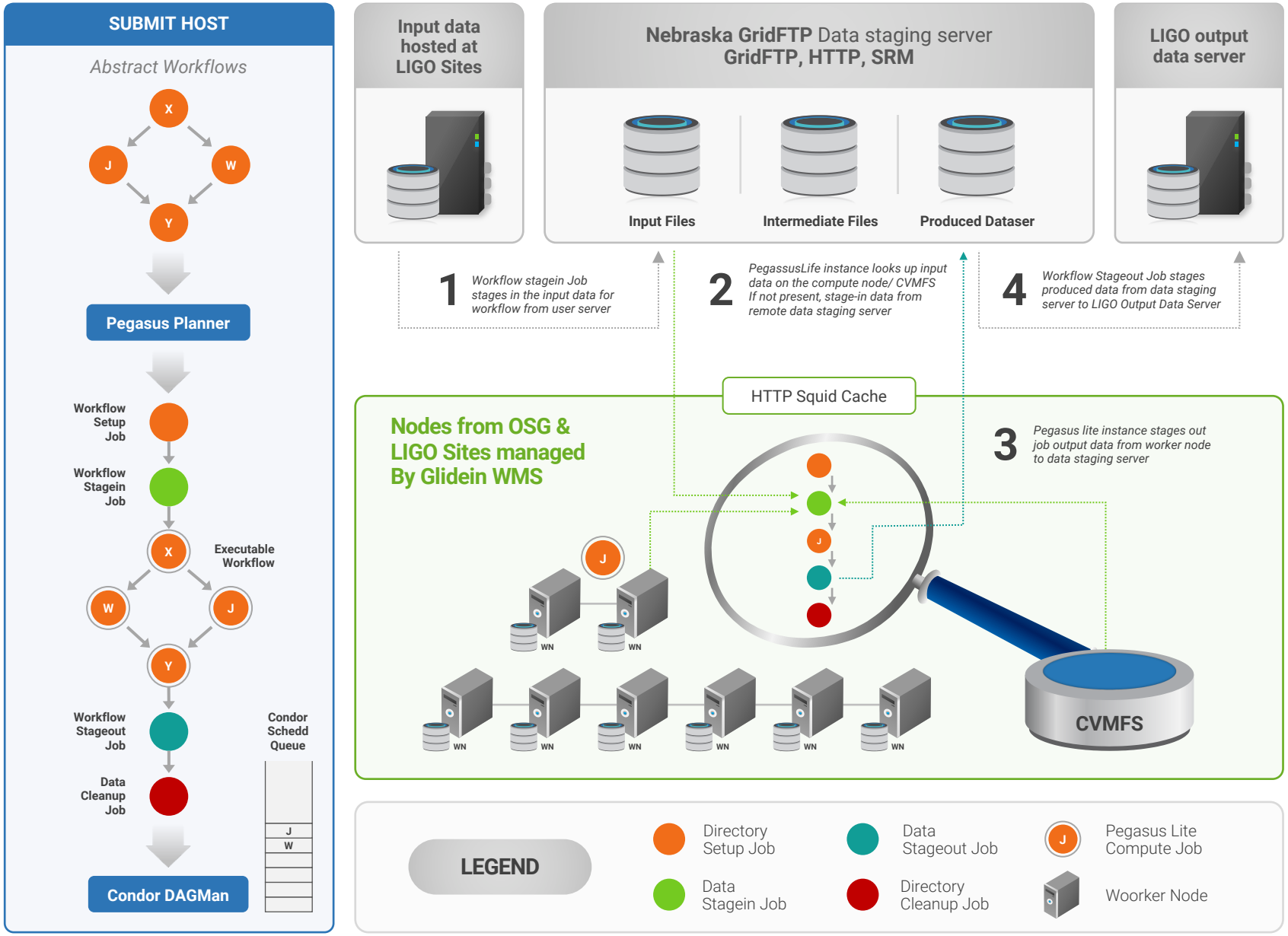
Titan:
421,000 CPU node-hours, 110,000 GPU node-hours

Blue Waters:
673,000 CPU node-hours, 329,000 GPU node-hours

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)





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)

Processed Data: 725 GB

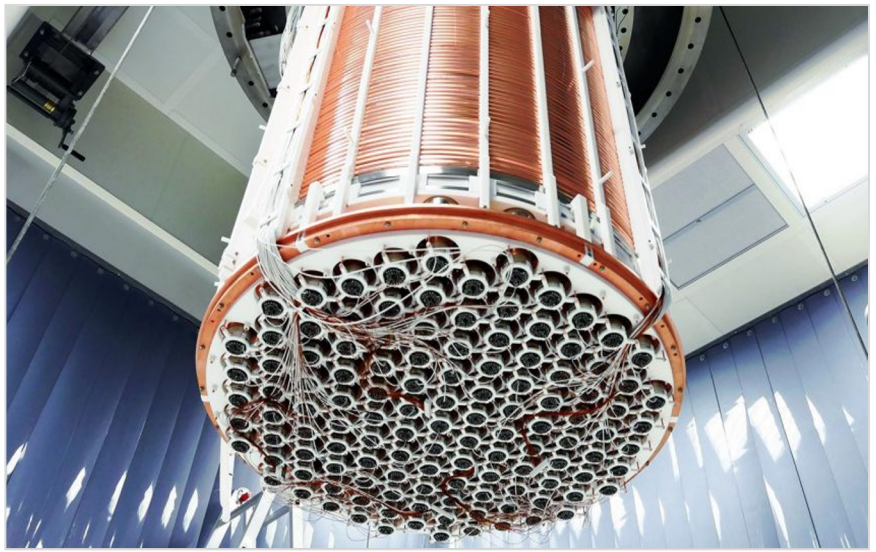
Executed on **LIGO Data Grid, EGI, Open Science Grid and XSEDE**

XENONnT - Dark Matter Search

Two Workflows

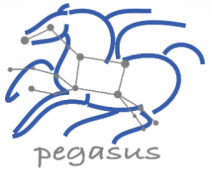
Monte Carlo simulations and the main processing pipeline.

- Workflows execute across Open Science Grid (OSG) & **European Grid Infrastructure (EGI)**
- Rucio for data management
- MongoDB instance to track science runs and data products.



```
------------------------------------------------------------------------------
Type           Succeeded Failed  Incomplete  Total     Retries   Total+Retries
Tasks          4000      0       0           4000      267       4267
Jobs           4484      0       0           4484      267       4751
Sub-Workflows  0         0       0           0         0         0
------------------------------------------------------------------------------

Workflow wall time                                       : 5 hrs, 2 mins
Cumulative job wall time                                 : 136 days, 9 hrs
Cumulative job wall time as seen from submit side        : 141 days, 16 hrs
Cumulative job badput wall time                          : 1 day, 2 hrs
Cumulative job badput wall time as seen from submit side : 4 days, 20 hrs
```

Main processing pipeline is being developed for XENONnT - data taking will start at the end of 2019. Workflow in development:



Basic Concepts...

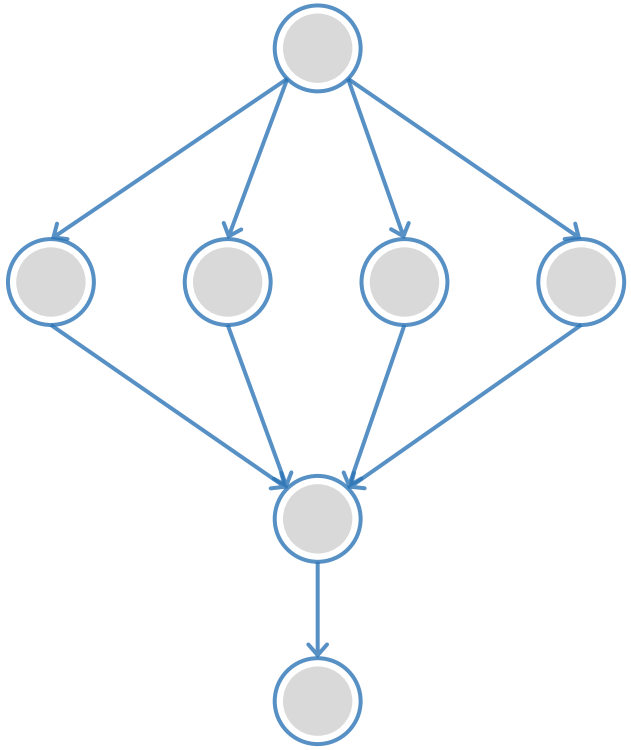
Key Pegasus Concepts

- **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



Input Workflow Specification YAML formatted

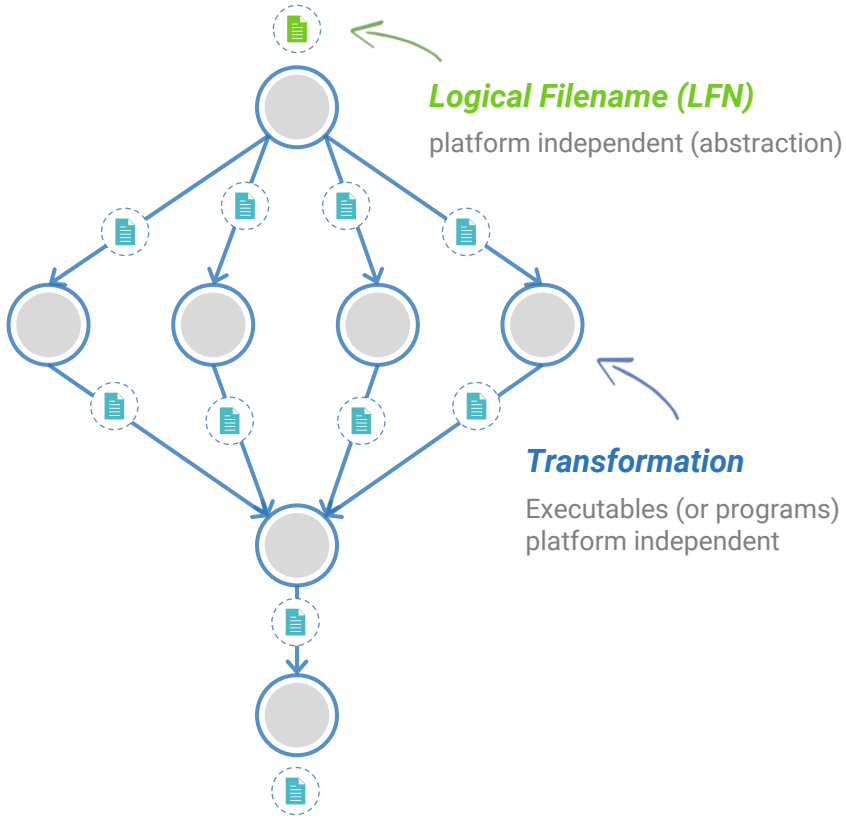
directed-acyclic graphs

Output Workflow

Portable Description

Users do not worry about low level execution details

ABSTRACT WORKFLOW

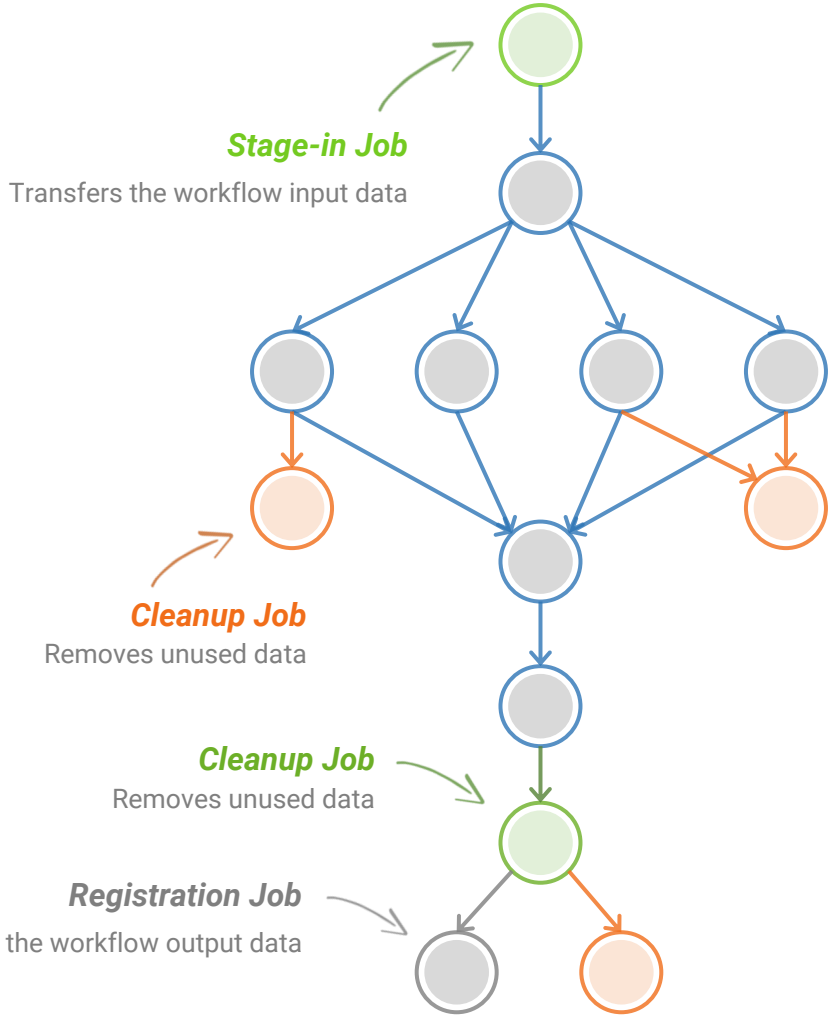


Logical Filename (LFN)

platform independent (abstraction)

Transformation

Executables (or programs)
platform independent



Stage-in Job

Transfers the workflow input data

Cleanup Job

Removes unused data

Cleanup Job

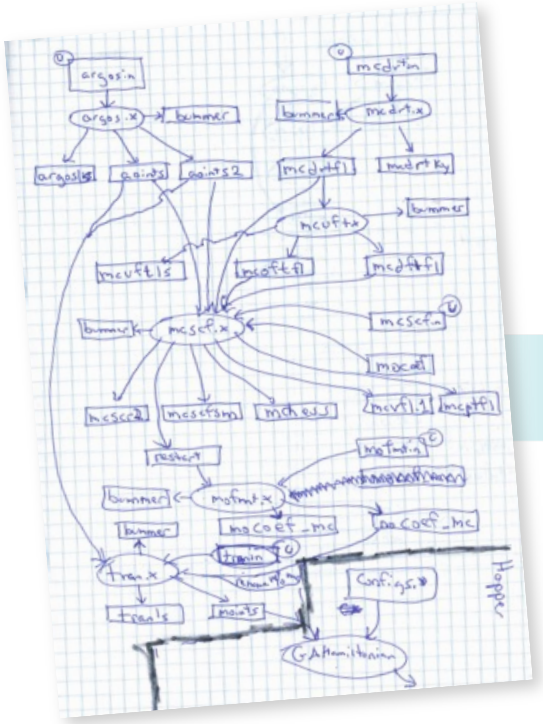
Removes unused data

Registration Job

Registers the workflow output data

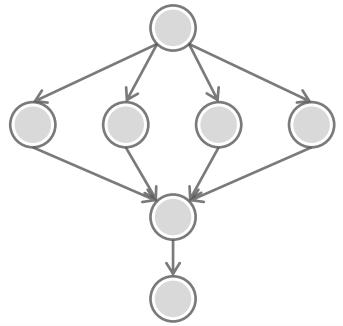
EXECUTABLE WORKFLOW

Pegasus also provides tools to generate the Abstract Workflow



```python
#!/usr/bin/env python3

import os
import logging
from pathlib import Path
from argparse import ArgumentParser

logging.basicConfig(level=logging.DEBUG)

# --- Import Pegasus API ------------------
from Pegasus.api import *

# --- Create Abstract Workflow ------------
wf = Workflow("pipeline")

webpage = File("pegasus.html")

# --- Create Parent Job -------------
curl_job = (
    Job("curl")
    .add_args("-o", webpage, "http://pegasus.isi.edu")
    .add_outputs(webpage, stage_out=False, register_replica=False)
)

count = File("count.txt")

# --- Create Dependent Job ----------
wc_job = (
    Job("wc")
    .add_args("-l", webpage)
    .add_inputs(webpage)
    .set_stdout(count, stage_out=True, register_replica=True)
)
# --- Add jobs to the Abstract Workflow -------
wf.add_jobs(curl_job, wc_job)

# --- Add control flow dependency ----------
wf.add_dependency(wc_job, parents=[curl_job])

# --- Write out the Abstract Workflow ----------
wf.write()
```

python™ Java R jupyter

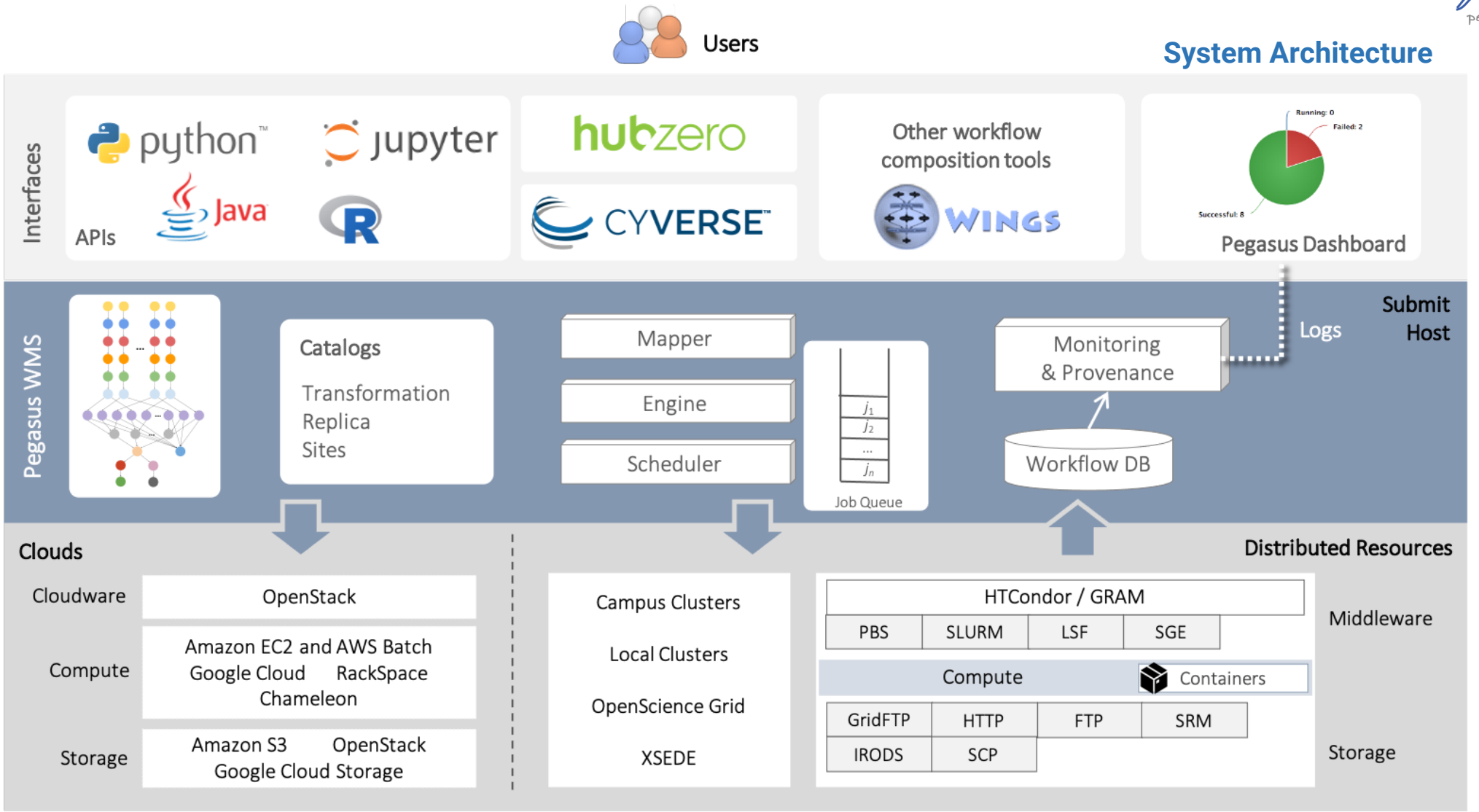


```yaml
x-pegasus:
  apiLang: python
  createdBy: vahi
  createdOn: 11-19-20T14:57:58Z
pegasus: '5.0'
name: pipeline
jobs:
- type: job
  name: curl
  id: ID0000001
  arguments:
  - -o
  - pegasus.html
  - http://pegasus.isi.edu
  uses:
  - lfn: pegasus.html
    type: output
    stageOut: false
    registerReplica: false
- type: job
  name: wc
  id: ID0000002
  stdout: count.txt
  arguments:
  - -l
  - pegasus.html
  uses:
  - lfn: count.txt
    type: output
    stageOut: true
    registerReplica: true
  - lfn: pegasus.html
    type: input
jobDependencies:
- id: ID0000001
  children:
  - ID0000002
```

YAML Formatted

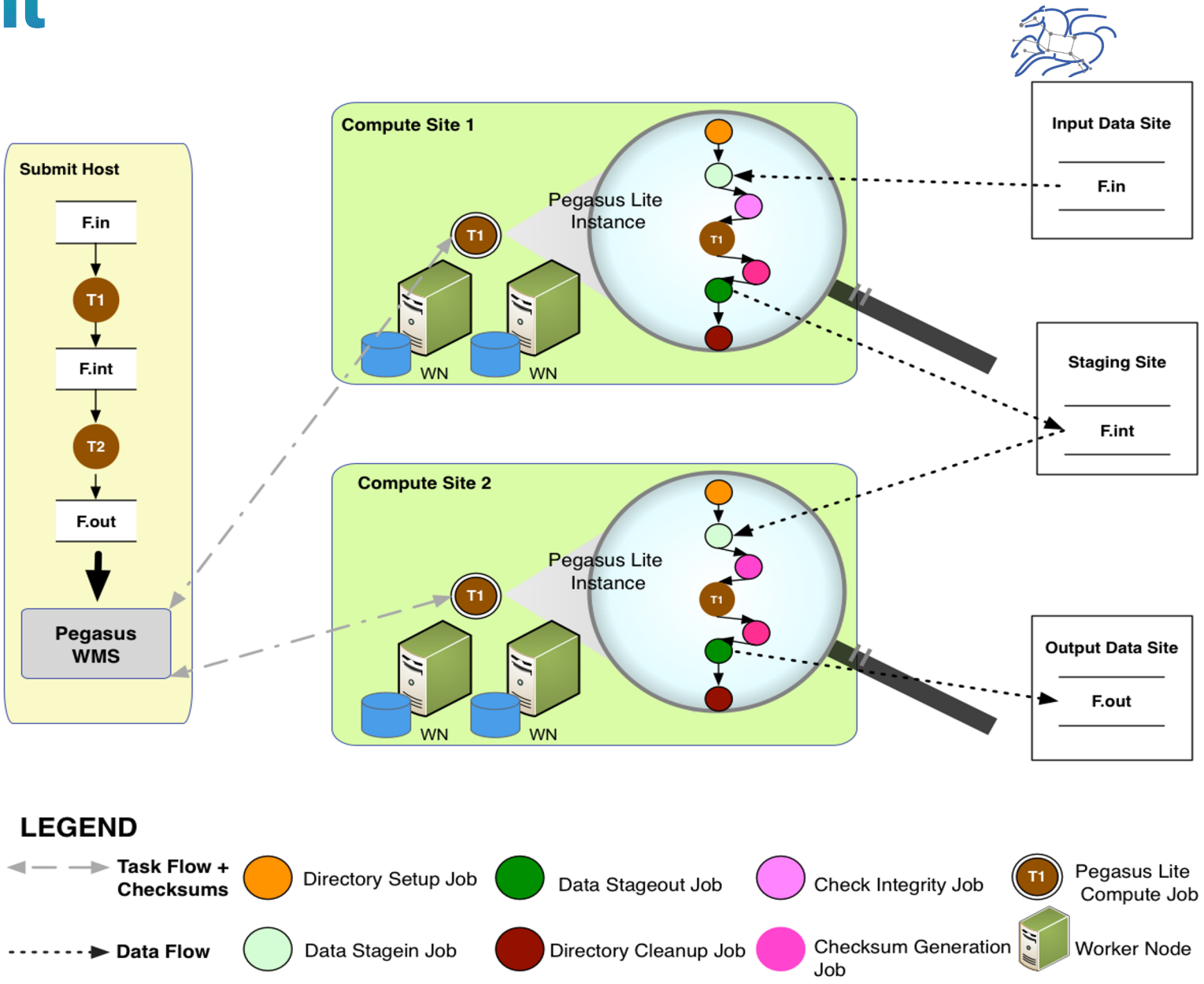
Abstract Workflow

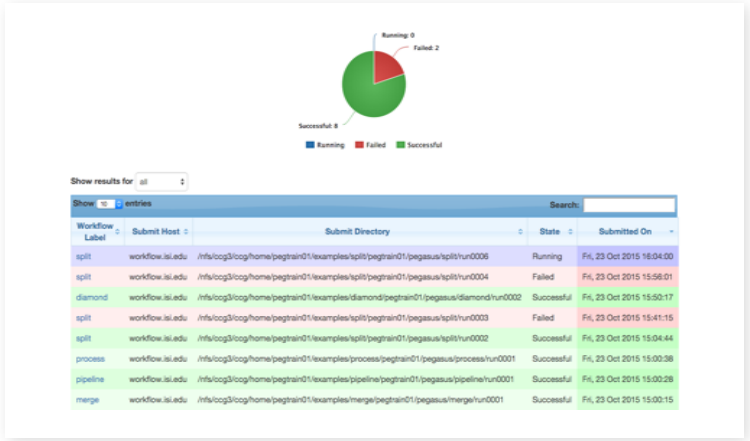
System Architecture



Pegasus Deployment

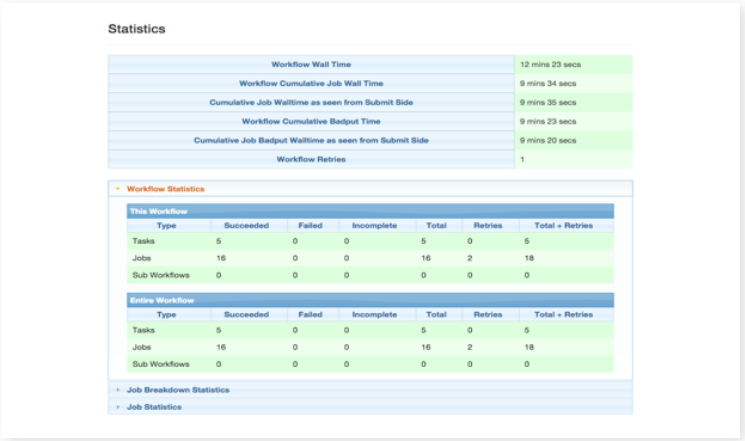
- Workflow Submit Node
  - Pegasus WMS
  - HTCondor
- One or more Compute Sites
  - Compute Clusters
  - Cloud
  - OSG
- Input Sites
  - Host Input Data
- Data Staging Site
  - Coordinate data movement for workflow
- Output Site
  - Where output data is placed





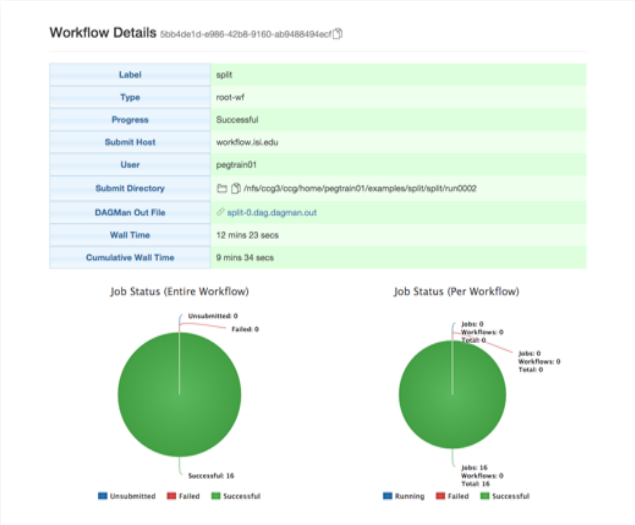
PEGASUS DASHBOARD

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

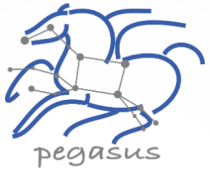
command-line…

```
$ 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



Understanding Pegasus Features...

Data Staging Configurations

HTCondor I/O (HTCondor pools, OSG, …)

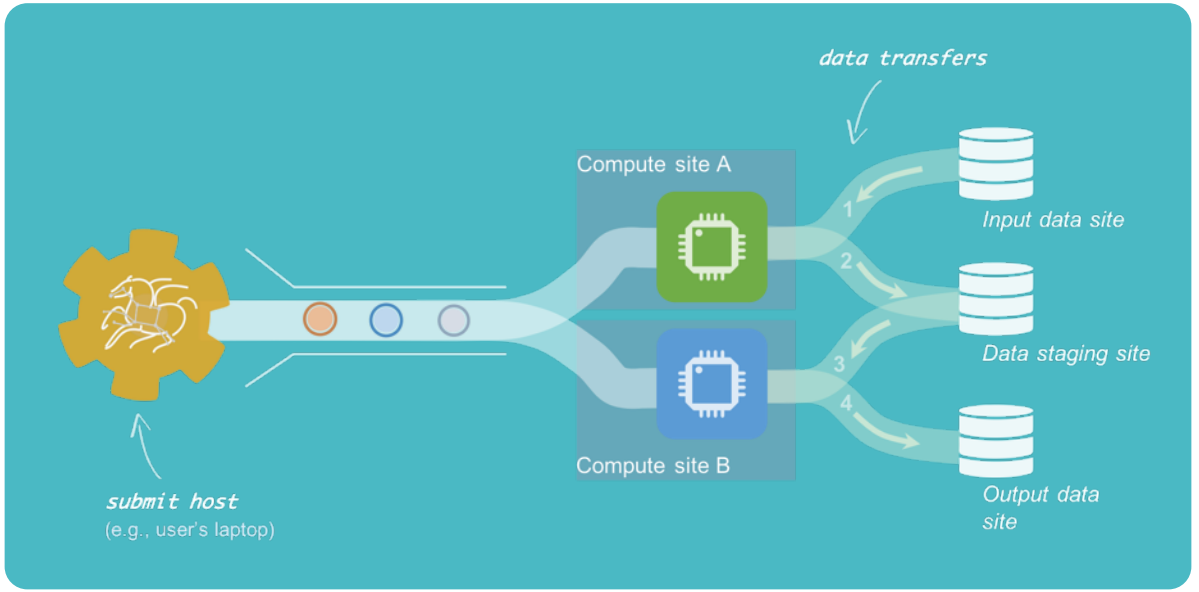
- Worker nodes do not share a file system
- Data is pulled from / pushed to the submit host via HTCondor file transfers
- Staging site is the submit host

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



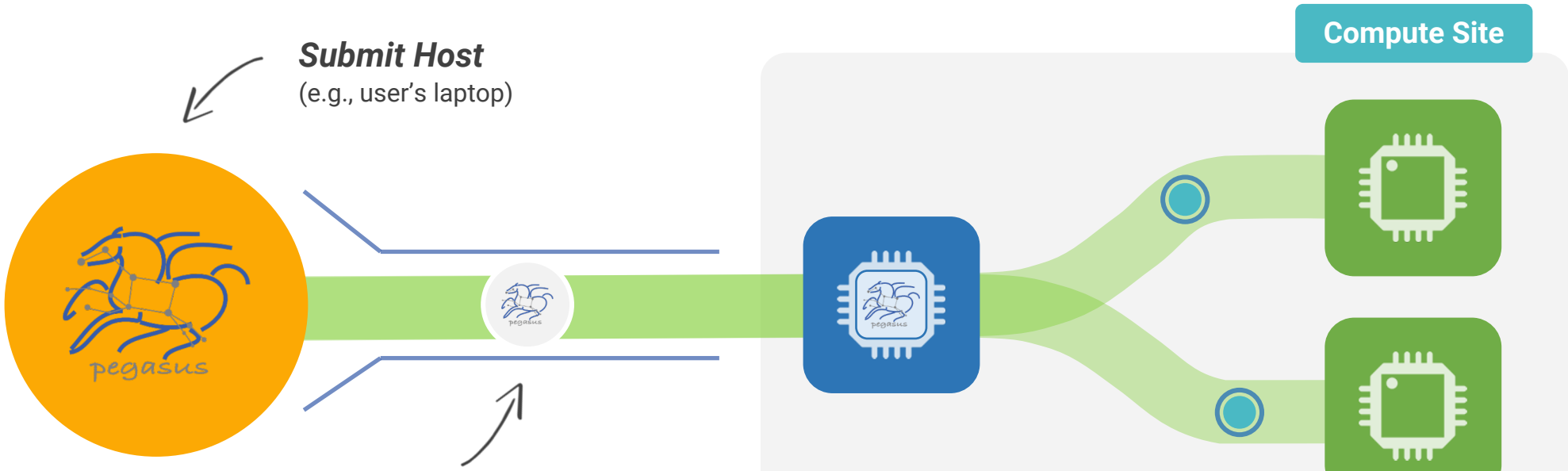
Pegasus-transfer

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

- **Directory creation, file removal**
  - If protocol can support it, also 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
Rucio
cp
ln -s
```

Running fine-grained workflows on HPC systems…



Workflow wrapped as an MPI job

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

Challenges to Scientific Data Integrity

Modern IT systems are not perfect - errors creep in.

At modern “Big Data” sizes we are starting to see checksums breaking down.

Plus there is the threat of intentional changes: malicious attackers, insider threats, etc.

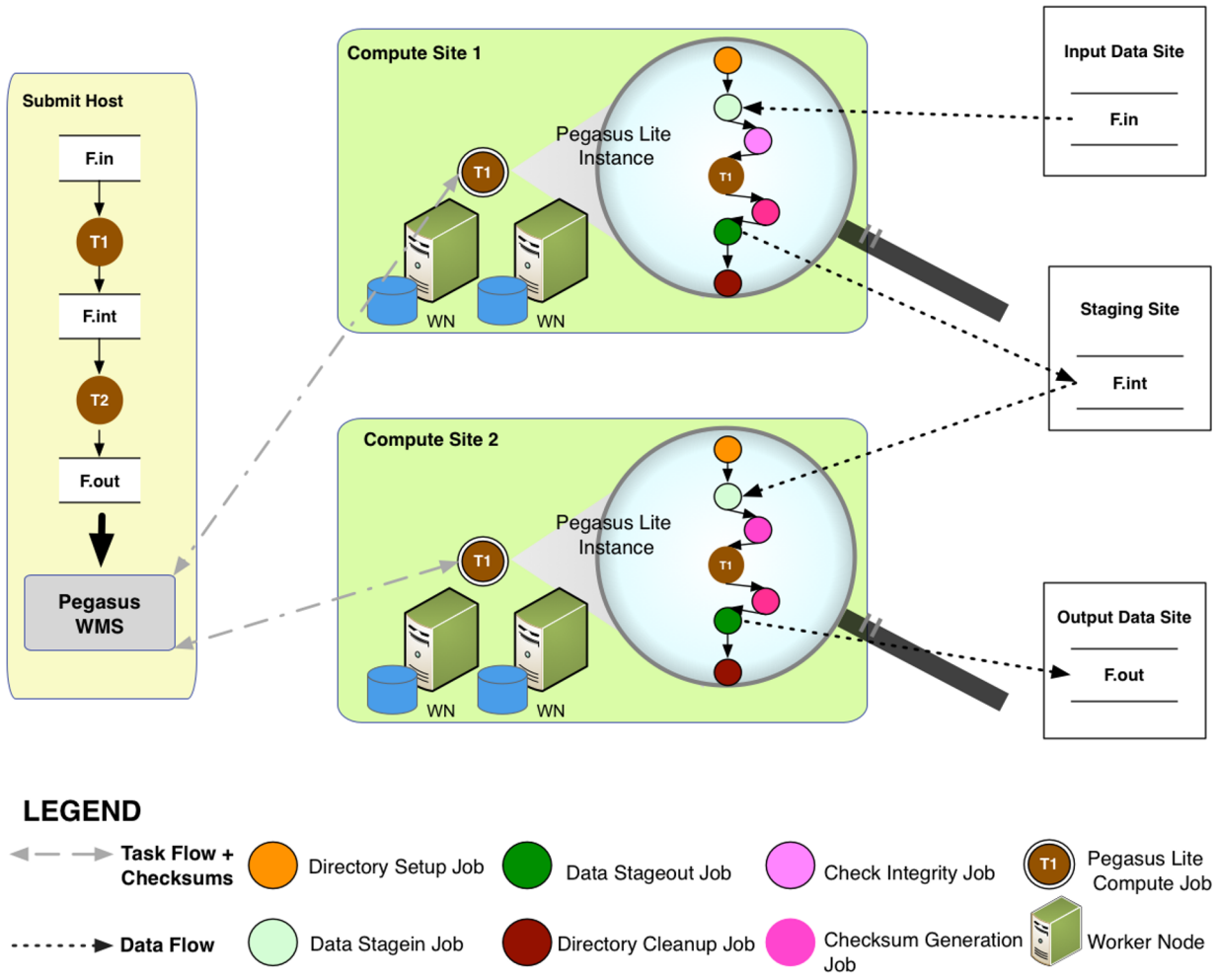
User Perception: “Am I not already protected? I have heard about TCP checksums, encrypted transfers, checksum validation, RAID and erasure coding – is that not enough?”

Automatic Integrity Checking in Pegasus

Pegasus performs integrity checksums on input files right before a job starts on the remote node.

- For raw inputs, checksums specified in the input replica catalog along with file locations
- All intermediate and output files checksums are generated and tracked within the system.
- Support for sha256 checksums

Job failure is triggered if checksums fail



Pegasus Container Support

Users can refer to **containers** in the **Transformation Catalog** with their executable preinstalled

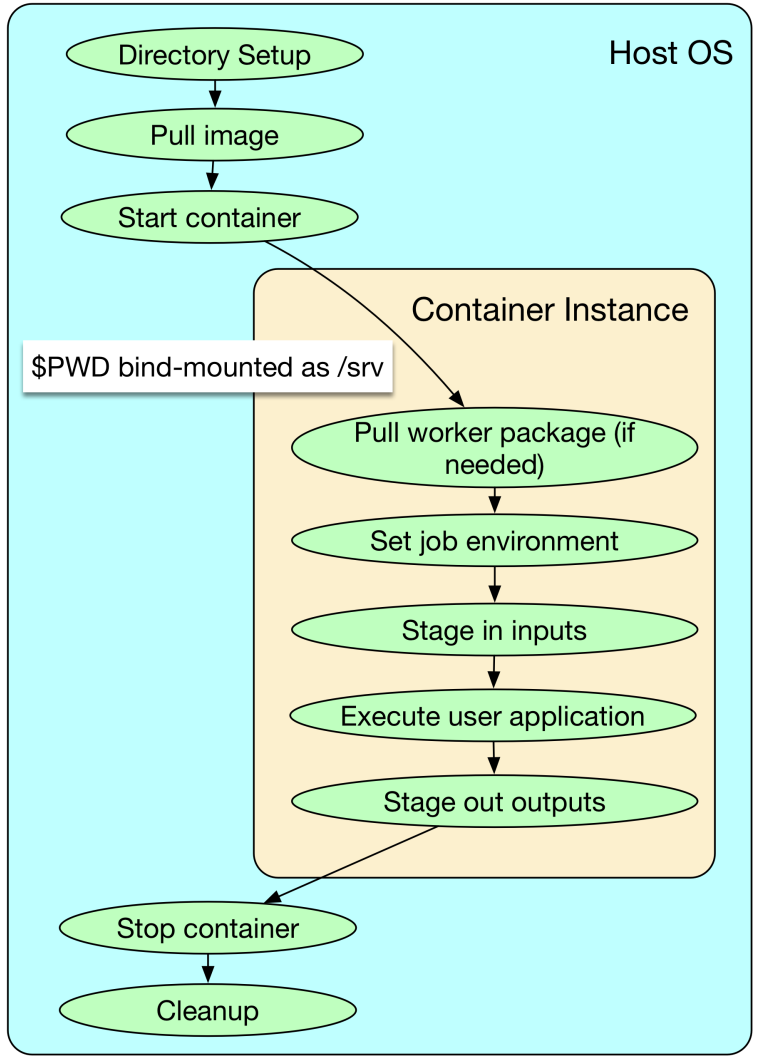
Users can **refer** to a **container** they want to **use – Pegasus stages** their executables and containers to the node

- Useful if you want to use a site recommended/standard container image.
- Users are using generic image with executable staging.

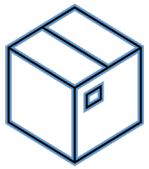
Future Plans

- Users can specify an image buildfile for their jobs.
- *Pegasus will build the Docker image as separate jobs in the executable workflow, export them as a tar file and ship them around*

Containers Execution Model



Data Management for Containers



Containers are data too!

Pegasus treats containers as input data dependency

- Staged to compute node if not present
- Docker or Singularity Hub URL's
- Docker Image exported as a TAR file and available at a server, just like any other input dataset

Scaling up for larger workflows

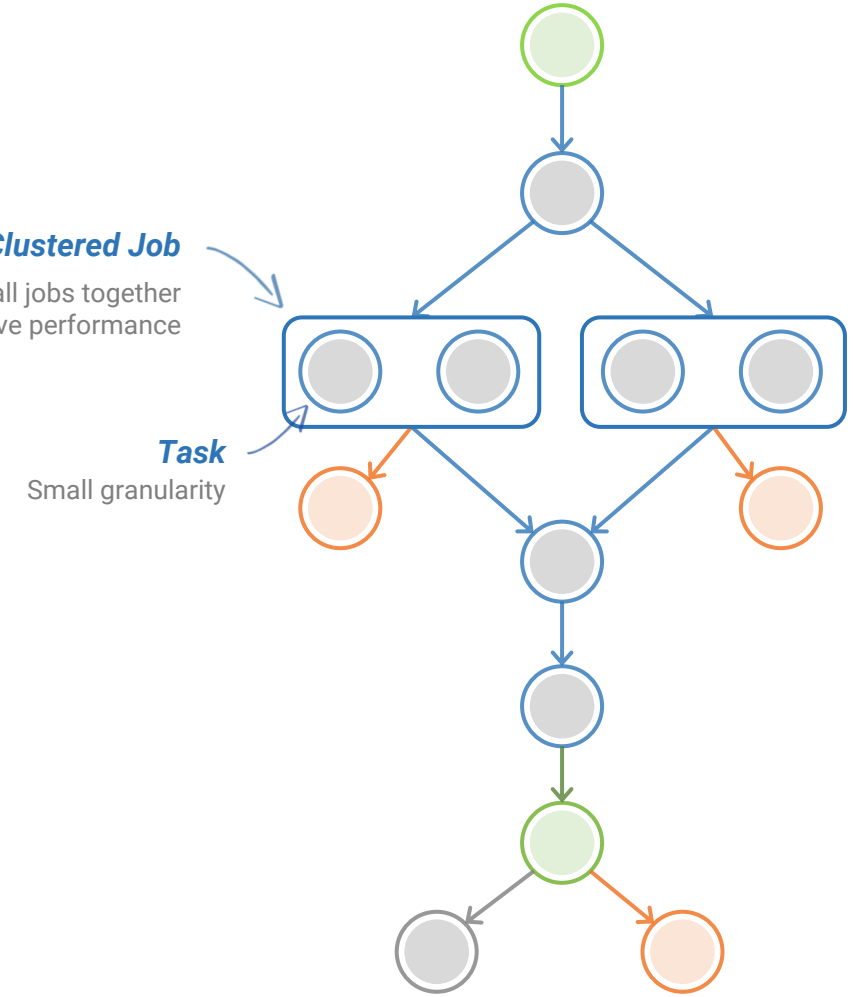
- The image is pulled down as a tar file as part of data stage-in jobs in the workflow
- The exported tar file is then shipped with the workflow and made available to the jobs
- Pricing considerations. You are now charged if you exceed a certain rate of pulls from Hubs

Other Optimizations

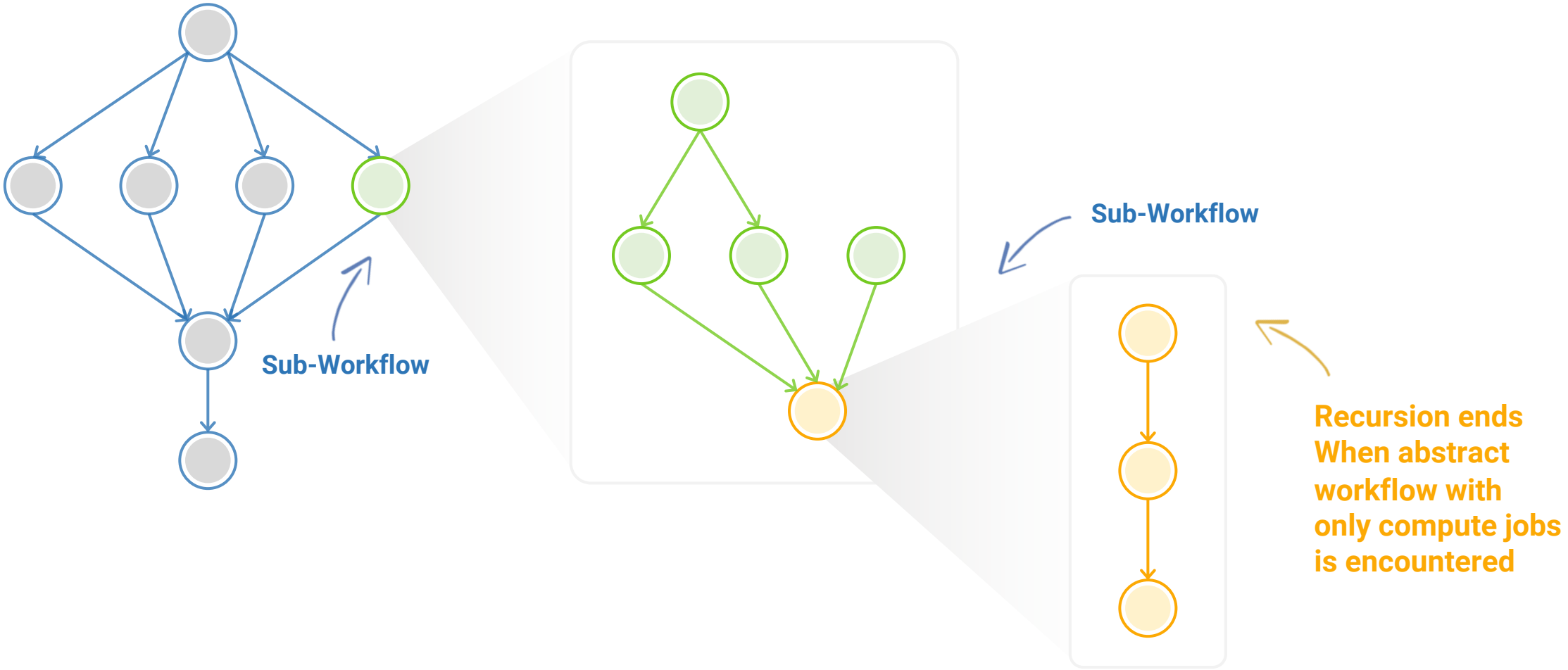
- Symlink against existing images on shared filesystem such as **CVMFS**
- The exported tar file is then shipped with the workflow and made available to the jobs

Performance.

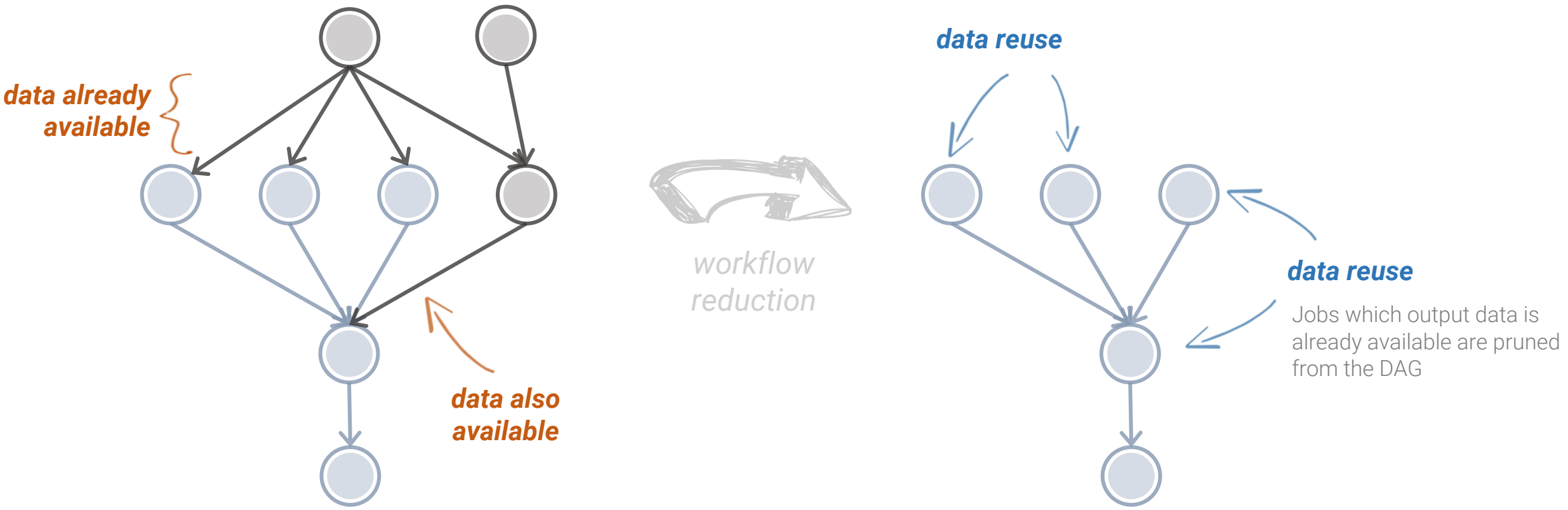
Why not improve it?



Pegasus also handles large-scale workflows



Data Reuse prune jobs if output data already exists



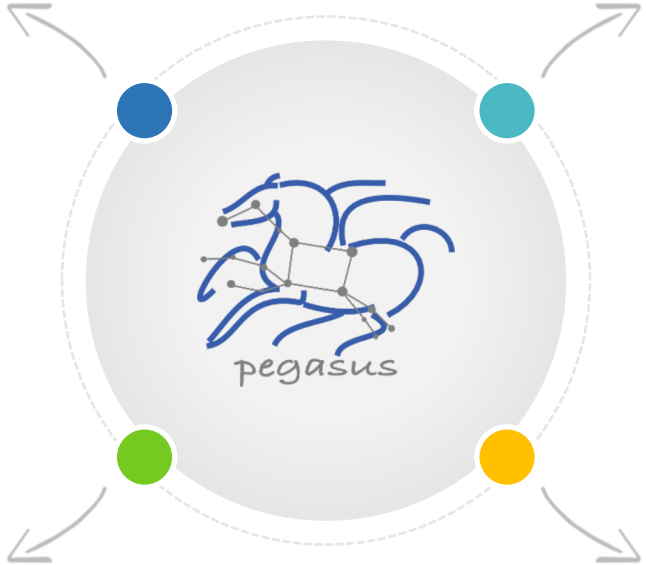
And if a job fails?

Postscript

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

Job Submissions

LOCAL

Submit Machine

Personal HTCondor

Local Campus Cluster accessible via Submit Machine **

HTCondor via BLAHP

*** Both Glite and BOSCO build on HTCondor BLAHP*

Currenty supported schedulers:
SLURM SGE PBS MOAB

REMOTE

BOSCO + SSH**

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

BOSCO based Glideins**

SSH based submission of glideins

PyGlidein

IceCube glidein service

OSG using glideinWMS

Infrastructure provisioned glideins

CREAMCE

Uses CondorG

Globus GRAM

Uses CondorG

Credentials Management

Credentials required for two purposes

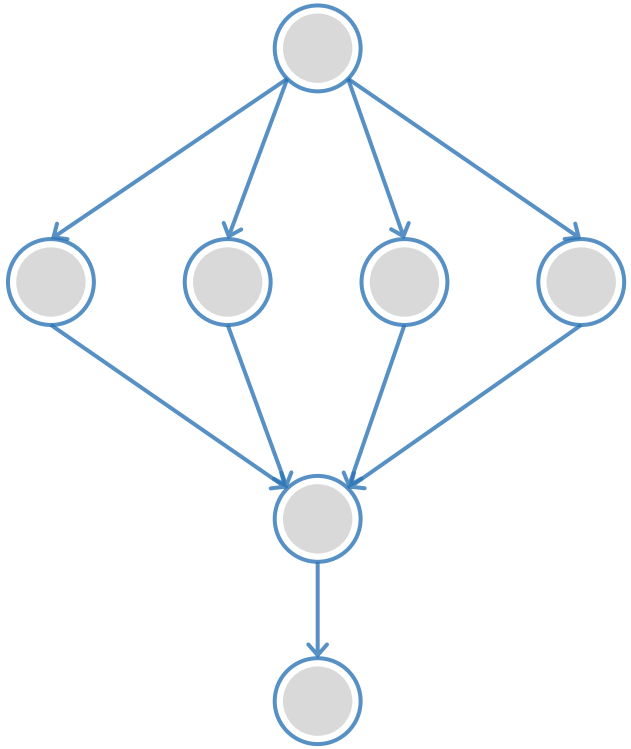
- Job Submission
- Data transfers to **stage-in** input and **stage-out** generated outputs when a job executes

Specifying Credentials

- Users can specify credentials in a **generic credentials file** on submit host
- Associate credentials with sites in site catalog

Approach

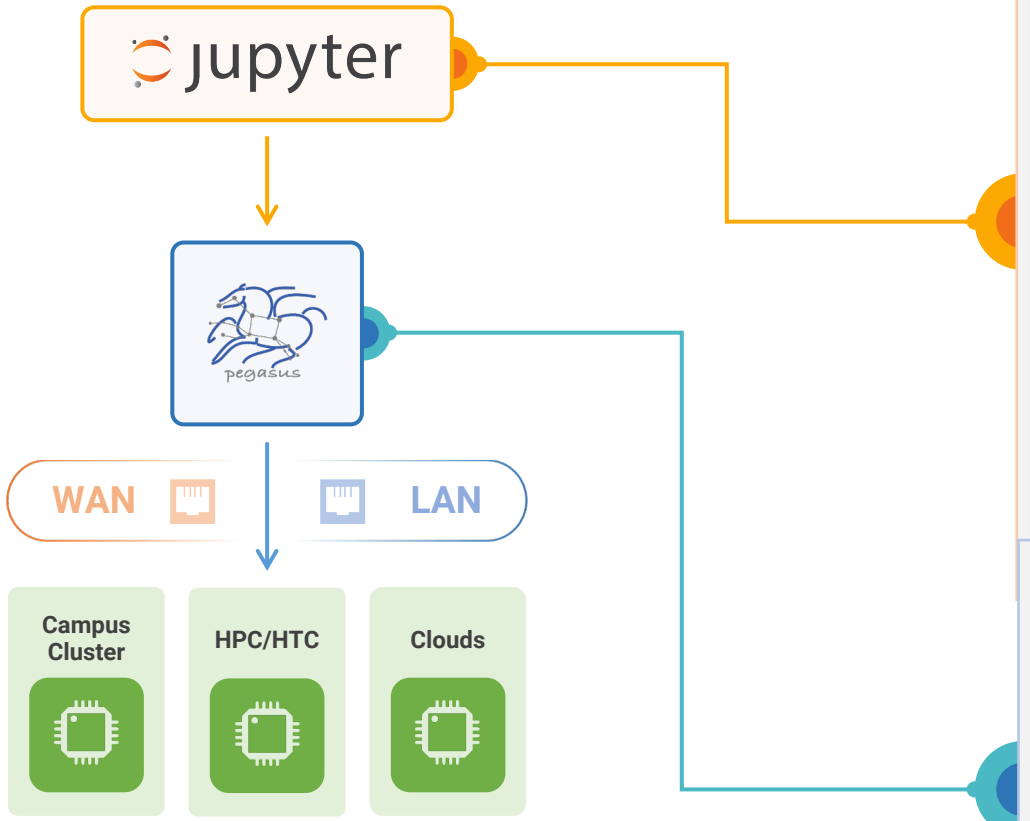
- Planner will **automatically** associate the **required credentials** with each job
- The credentials are **transferred** along with the job
- Usually available **only for the duration** of the job **execution**

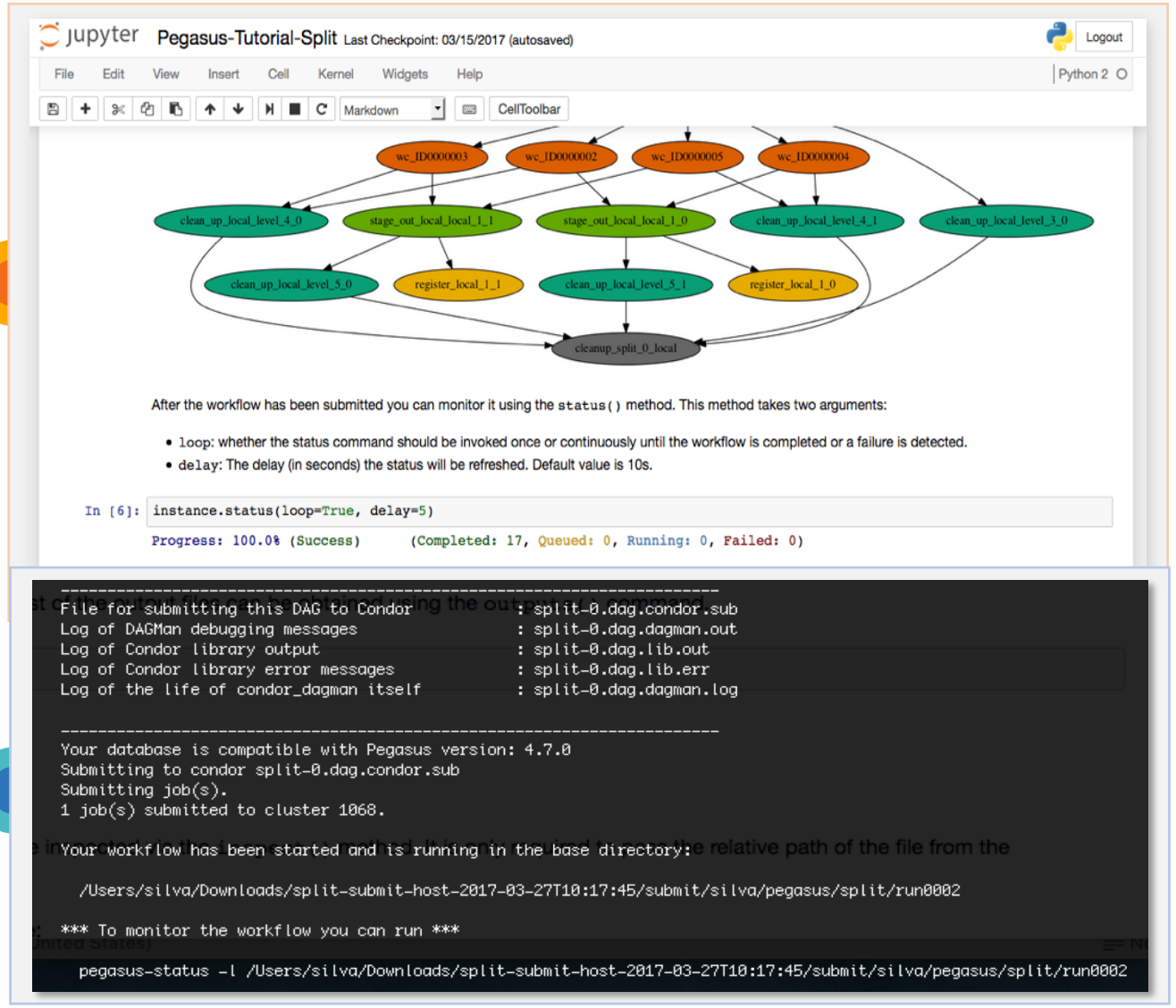


Supported Credentials

- X.509 grid proxies
- Amazon AWS S3 keys,
- Google Cloud Platform OAuth token (.boto file),
- iRods password
- SSH keys
- Web Dav

Running Pegasus workflows with Jupyter





Released Nov, 2020

- New and fresh Python3 API to compose, submit and monitor workflows, and configure catalogs
- New Catalog Formats
- Python 3 Support
  - All Pegasus tools are Python 3 compliant
  - Python PIP packages for workflow composition and monitoring
- Zero configuration required to submit to local HTCondor pool.
- Data Management Improvements
  - New output replica catalog that registers outputs including file metadata such as size and checksums
  - Improved support for hierarchical workflows
- Reworked Documentation and Tutorial

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

```python
#!/usr/bin/env python3
import logging
import sys

from Pegasus.api import *

# logs to be sent to stdout
logging.basicConfig(level=logging.DEBUG, stream=sys.stdout)

# --- Transformations ----------------------------------------
echo = Transformation(
        "echo",
        pfn="/bin/echo",
        site="condorpool"
    )

tc = TransformationCatalog()\
        .add_transformations(echo)

# --- Workflow -----------------------------------------------
Workflow("hello-world", infer_dependencies=True)\
    .add_jobs(
        Job(echo)
            .add_args("Hello World")
            .set_stdout("hello.out")
    ).add_transformation_catalog(tc)\
    .plan(submit=True)\
    .wait()
```

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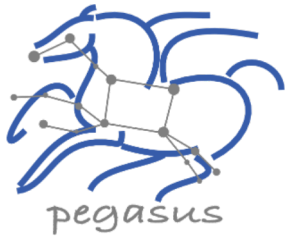

Pegasus

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Automate, recover, and debug scientific computations.

Get Started

- **Pegasus Website**
  https://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