Pegasus 5.0 Workflows

Workflow Management System

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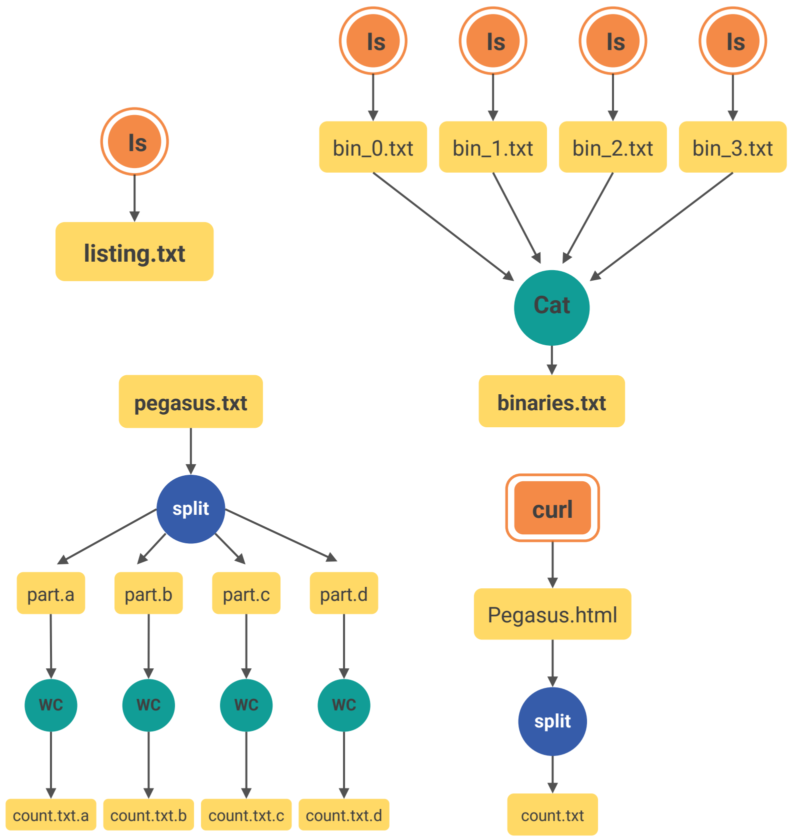
1. Introduction

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.**
  - Resources distributed across Internet.
- **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

Why Pegasus?

Automate
Recover
Debug

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

Workflow Challenges Across Domains

- Describe complex workflows in a simple way
- Access distributed, heterogeneous data and resources (heterogeneous interfaces)
- 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.

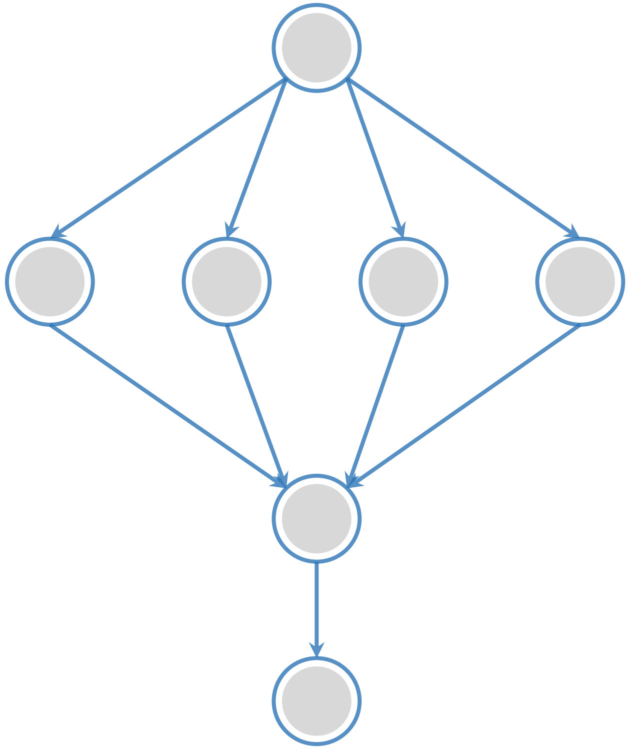
Key Pegasus Concepts

- **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

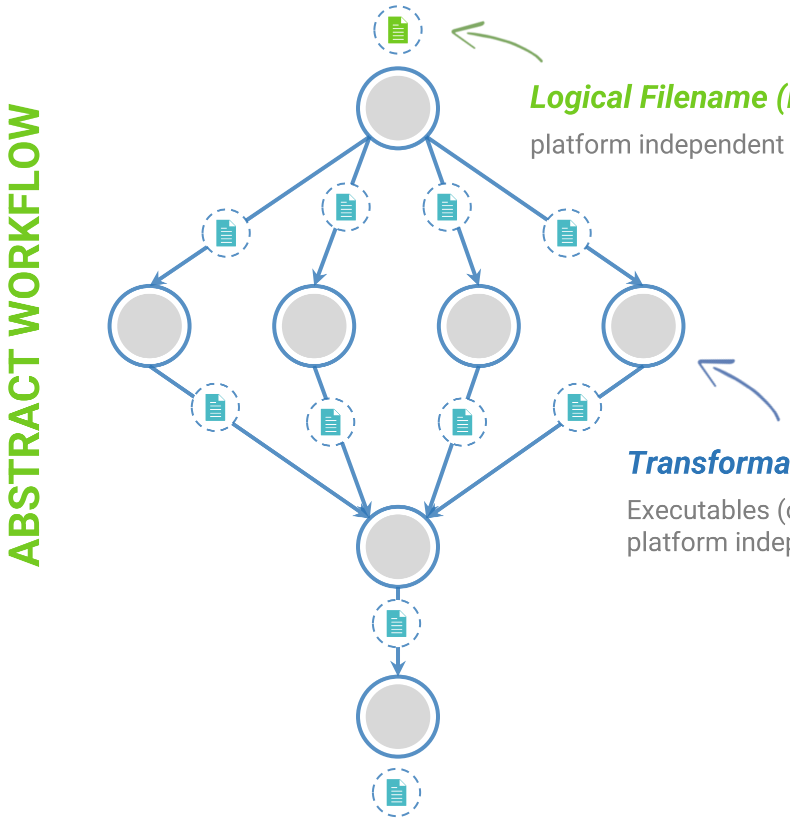


Input Workflow Specification YAML formatted

directed-acyclic graphs Output Workflow

Portable Description

Users do not worry about low level execution details

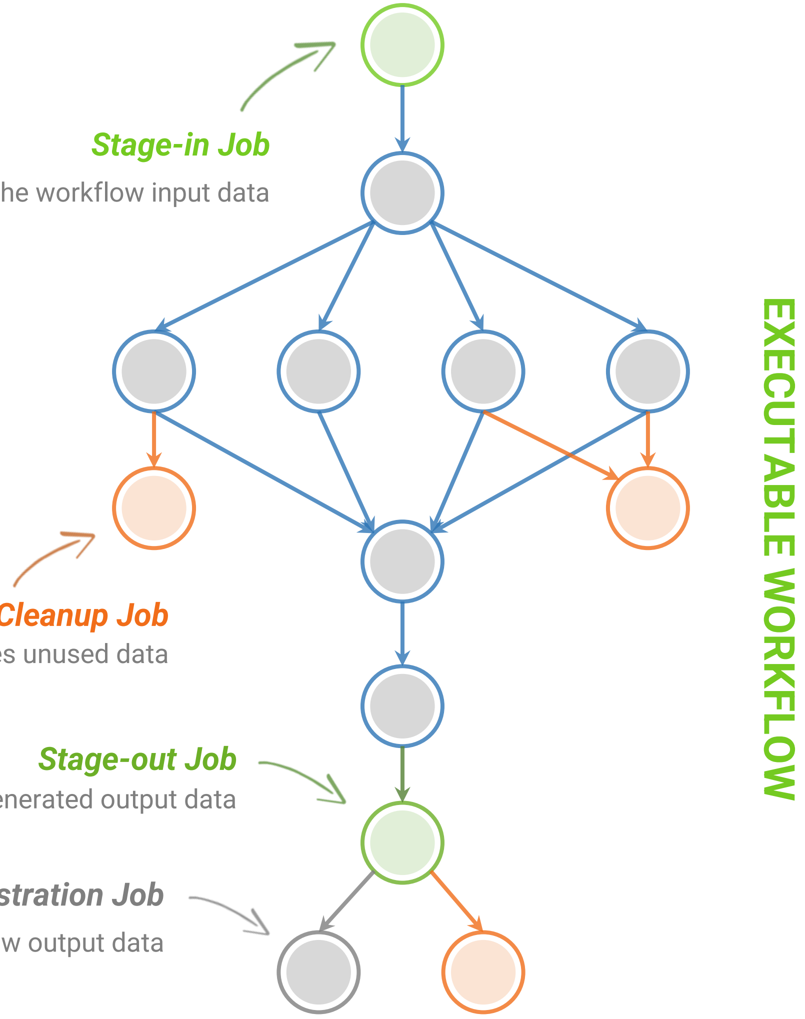


Logical Filename (LFN)

platform independent (abstraction)

Transformation

Executables (or programs)
platform independent



Stage-in Job

Transfers the workflow input data

Cleanup Job

Removes unused data

Stage-out Job

Stage-out generated output data

Registration Job

Registers the workflow output data

Pegasus Deployment

Workflow Submit Node

- Pegasus WMS
- HTCondor

One or more Compute Sites

- Compute Clusters
- Cloud
- OSG

Input Sites

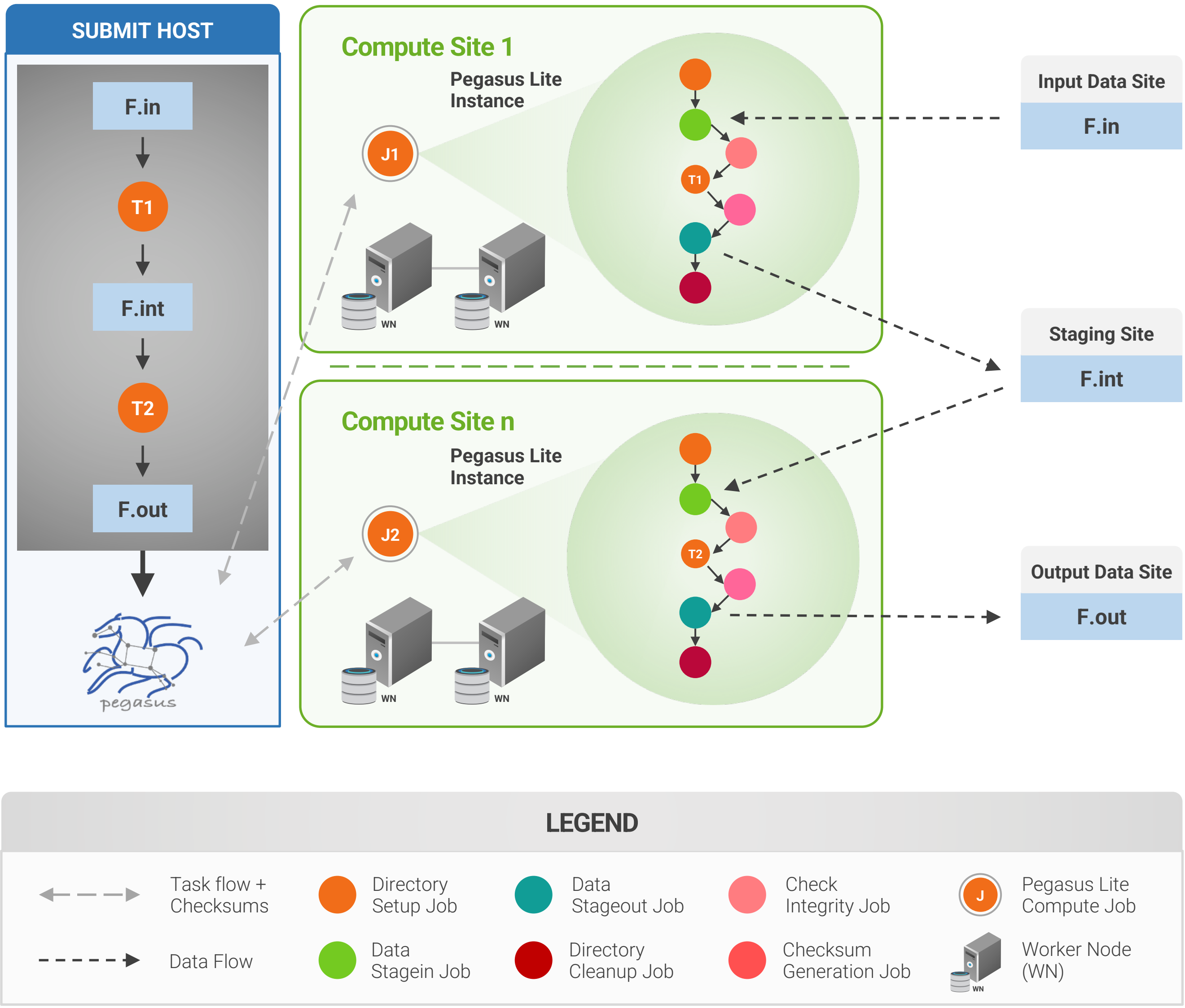
- Host Input Data

Data Staging Site

- Coordinate data movement for workflow

Output Site

- Where output data is placed



LEGEND

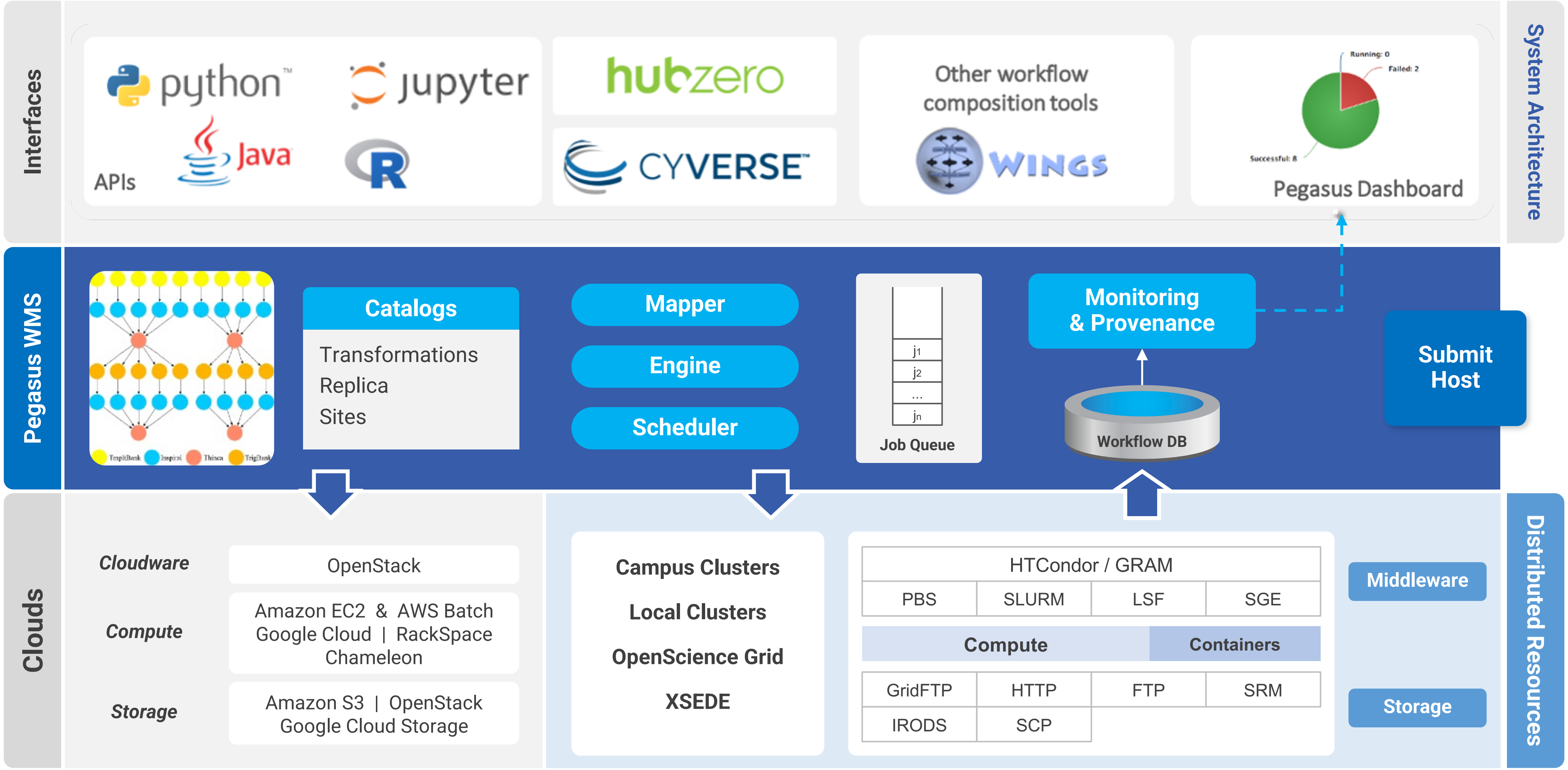
- ← - - → Task flow + Checksums
- - - - → Data Flow
- ● Directory Setup Job
- ● Data Stagein Job
- ● Data Stageout Job
- ● Directory Cleanup Job
- ● Check Integrity Job
- ● Checksum Generation Job
- J Pegasus Lite Compute Job
- WN Worker Node (WN)

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



System Architecture

Interfaces

APIs

Other workflow composition tools

Pegasus Dashboard

Pegasus WMS

Catalogs

- Transformations
- Replica
- Sites

Mapper

Engine

Scheduler

Job Queue

Monitoring & Provenance

Workflow DB

Submit Host

Clouds

Cloudware	OpenStack
Compute	Amazon EC2 & AWS Batch Google Cloud | RackSpace Chameleon
Storage	Amazon S3 | OpenStack Google Cloud Storage

Distributed Resources

Campus Clusters

Local Clusters

OpenScience Grid

XSEDE

HTCondor / GRAM

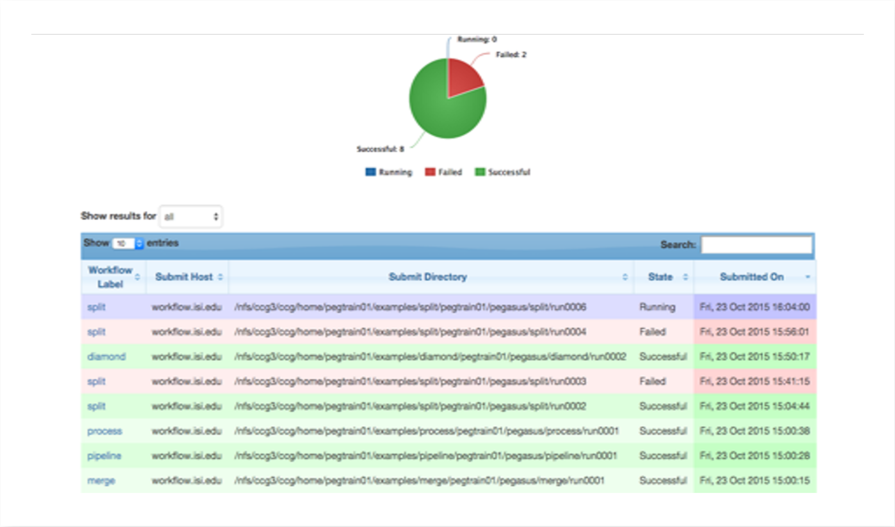
PBS	SLURM	LSF	SGE

Compute | Containers

Middleware

GridFTP	HTTP	FTP	SRM
IRODS	SCP		

Storage



Show results for all

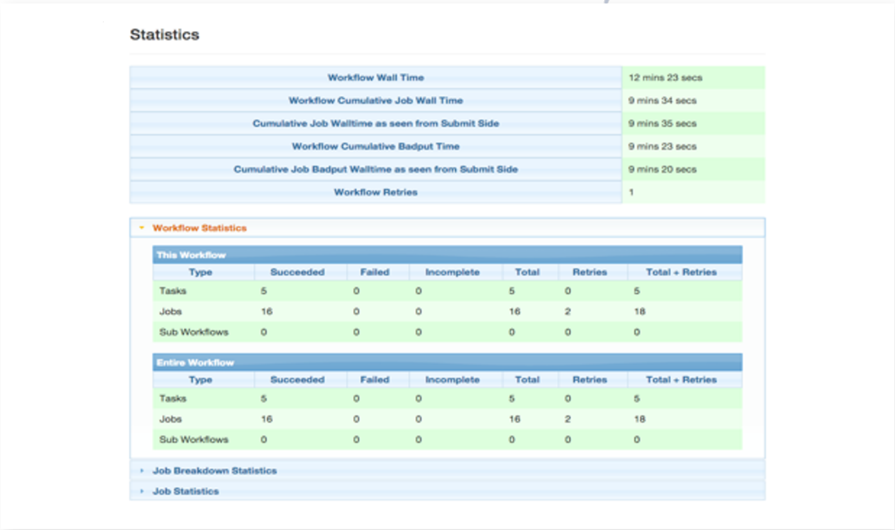
Show 10 entries Search:

Workflow Label	Submit Host	Submit Directory	State	Submitted On
split	workflow.isi.edu	/nfs/ccg3/ccg/home/pegtrain01/examples/split/pegtrain01/pegasus/split/run0006	Running	Fri, 23 Oct 2015 16:04:00
split	workflow.isi.edu	/nfs/ccg3/ccg/home/pegtrain01/examples/split/pegtrain01/pegasus/split/run0004	Failed	Fri, 23 Oct 2015 15:56:01
diamond	workflow.isi.edu	/nfs/ccg3/ccg/home/pegtrain01/examples/diamond/pegtrain01/pegasus/diamond/run0002	Successful	Fri, 23 Oct 2015 15:50:17
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 15:00:38
pipeline	workflow.isi.edu	/nfs/ccg3/ccg/home/pegtrain01/examples/pipeline/pegtrain01/pegasus/pipeline/run0001	Successful	Fri, 23 Oct 2015 15:00:28
merge	workflow.isi.edu	/nfs/ccg3/ccg/home/pegtrain01/examples/merge/pegtrain01/pegasus/merge/run0001	Successful	Fri, 23 Oct 2015 15:00:15

pegasus

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

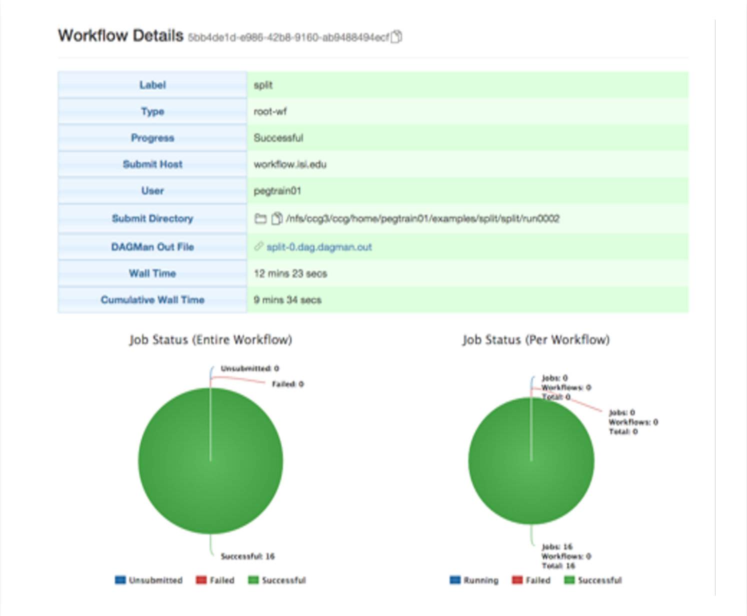
Type	Succeeded	Failed	Incomplete	Total	Retries	Total + Retries
Tasks	5	0	0	5	0	5
Jobs	16	0	0	16	2	18
Sub Workflows	0	0	0	0	0	0

▸ 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 5bb4de1d-e986-42b8-9160-ab9488494ecf

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

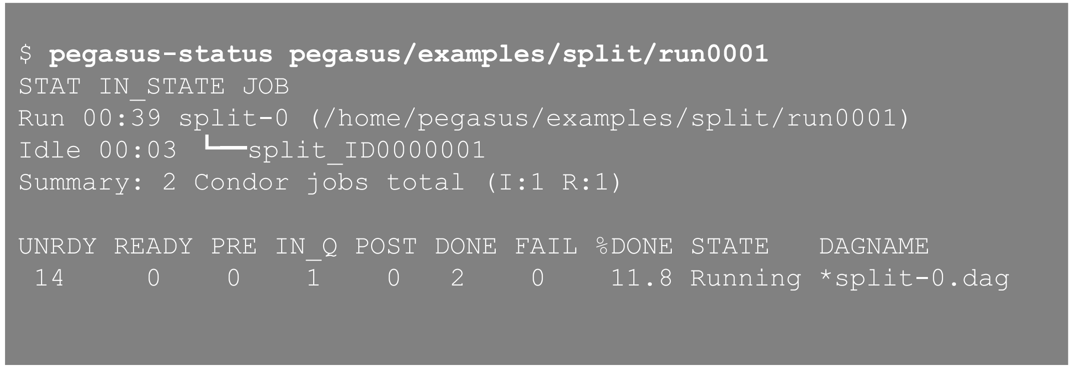
Job Status (Entire Workflow)

Job Status (Per Workflow)

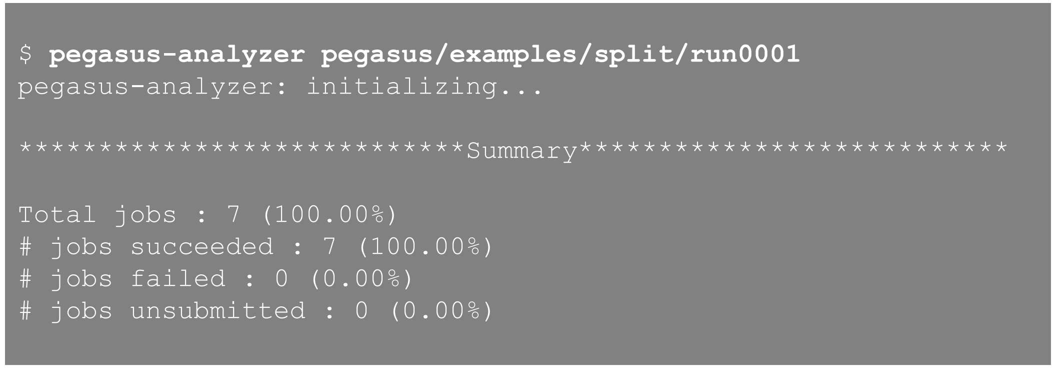
- **Real-time Monitoring**
- **Reporting**
- **Debugging**
- **Troubleshooting**
- **RESTful API**

https://pegasus.isi.edu

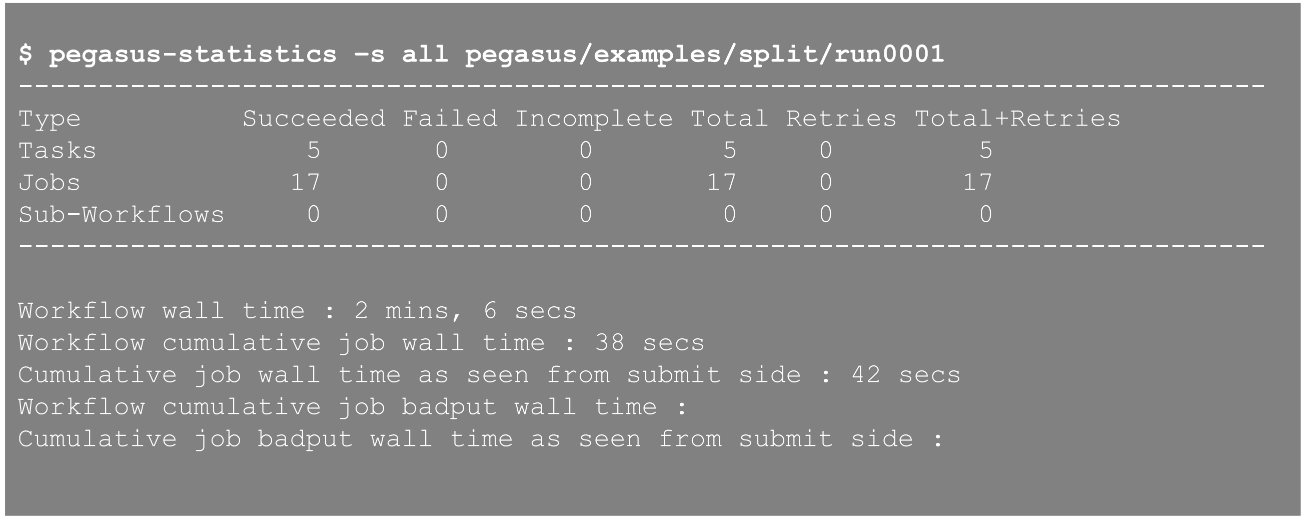
command-line…



```
$ 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
```



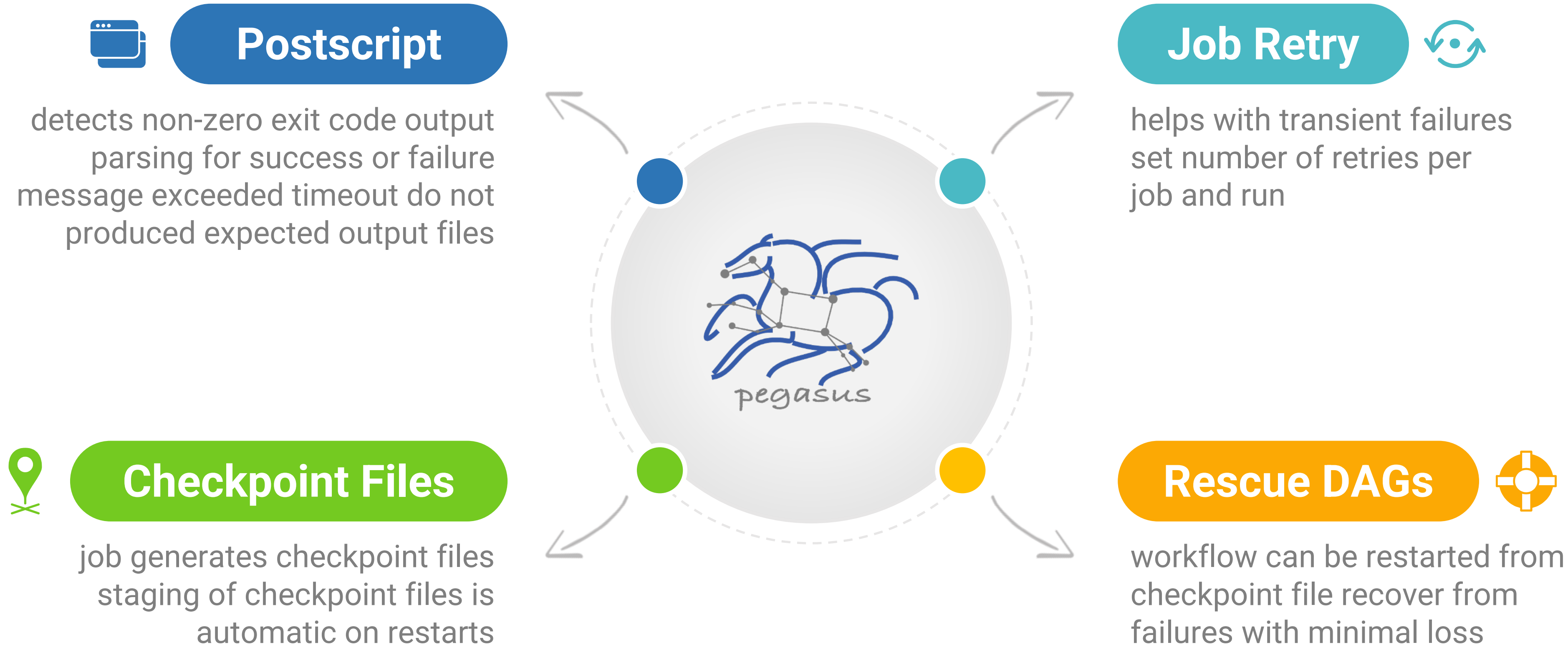
```
$ pegasus-analyzer pegasus/examples/split/run0001
pegasus-analyzer: initializing...

****************************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

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

Pegasus 5.0

Released Nov, 2020

- **New and fresh Python3 API to compose, submit and monitor workflows, and configure catalogs**
- **New Catalog Formats**
- **Python 3 Support**

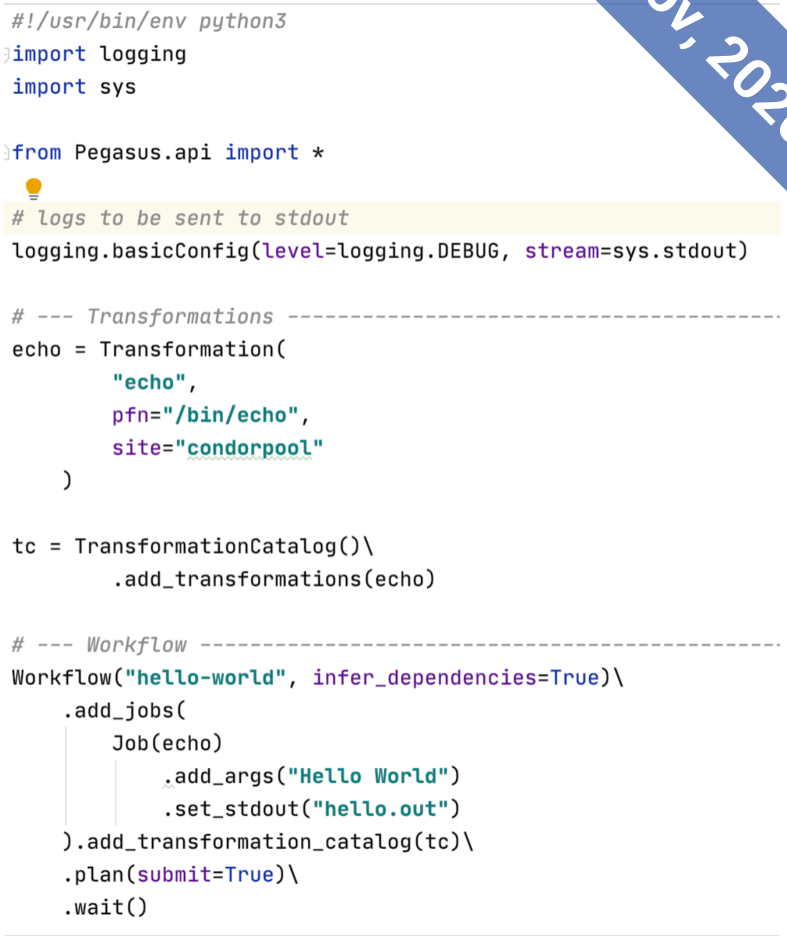
  All Pegasus tools are Python 3 compliant

  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/



```
#!/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()
```

2. Hands on Exercises

Hands on Tutorial Exercises: Setup

It is the same (but hosted) as the self-guided tutorial available in the Pegasus documentation: https://pegasus.isi.edu/documentation/user-guide/tutorial.html

Please claim an instance by putting you name next to an unused instance in: shorturl.at/oxIO6 (see Zoom chat for clickable link!)

Follow the link next to your name.

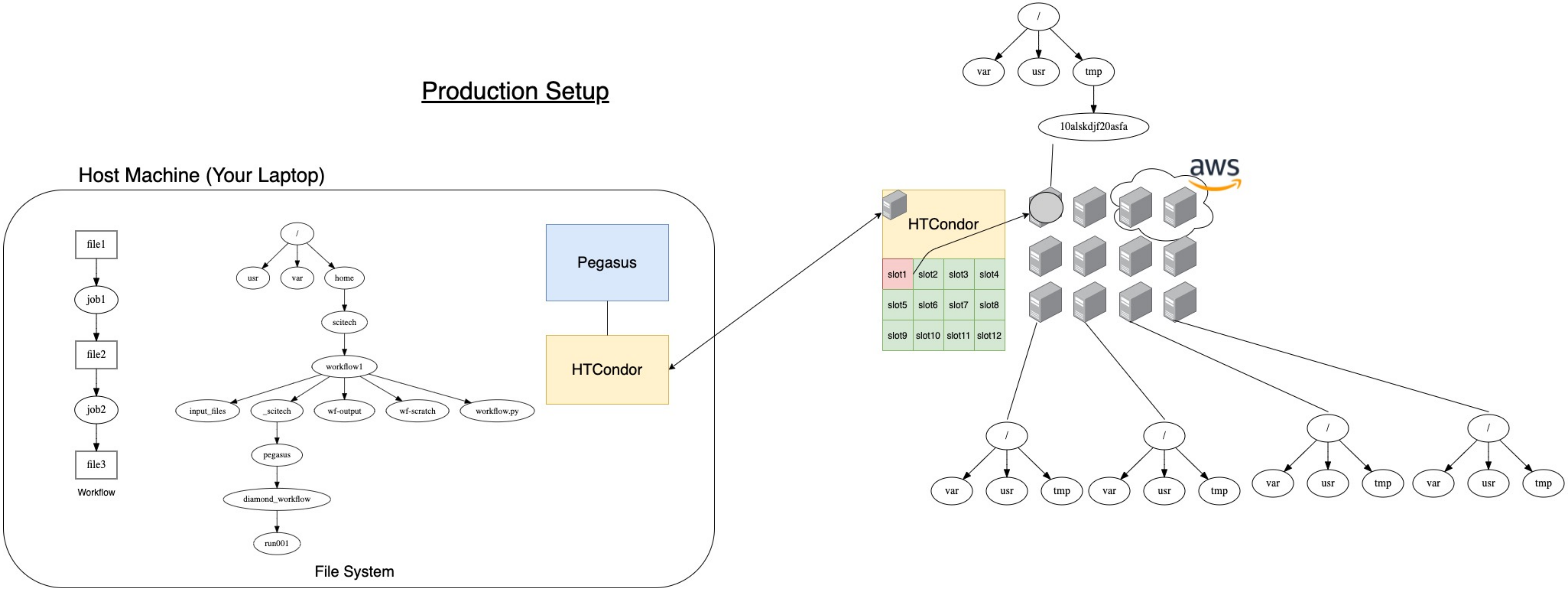
Docker Container / Jupyter Notebook

Container is for tutorial purposes - most production workflows have dedicated submit hosts

Jupyter is optional. You can choose to use just the workflow abstraction API, the full workflow management API, inside or outside Jupyter.

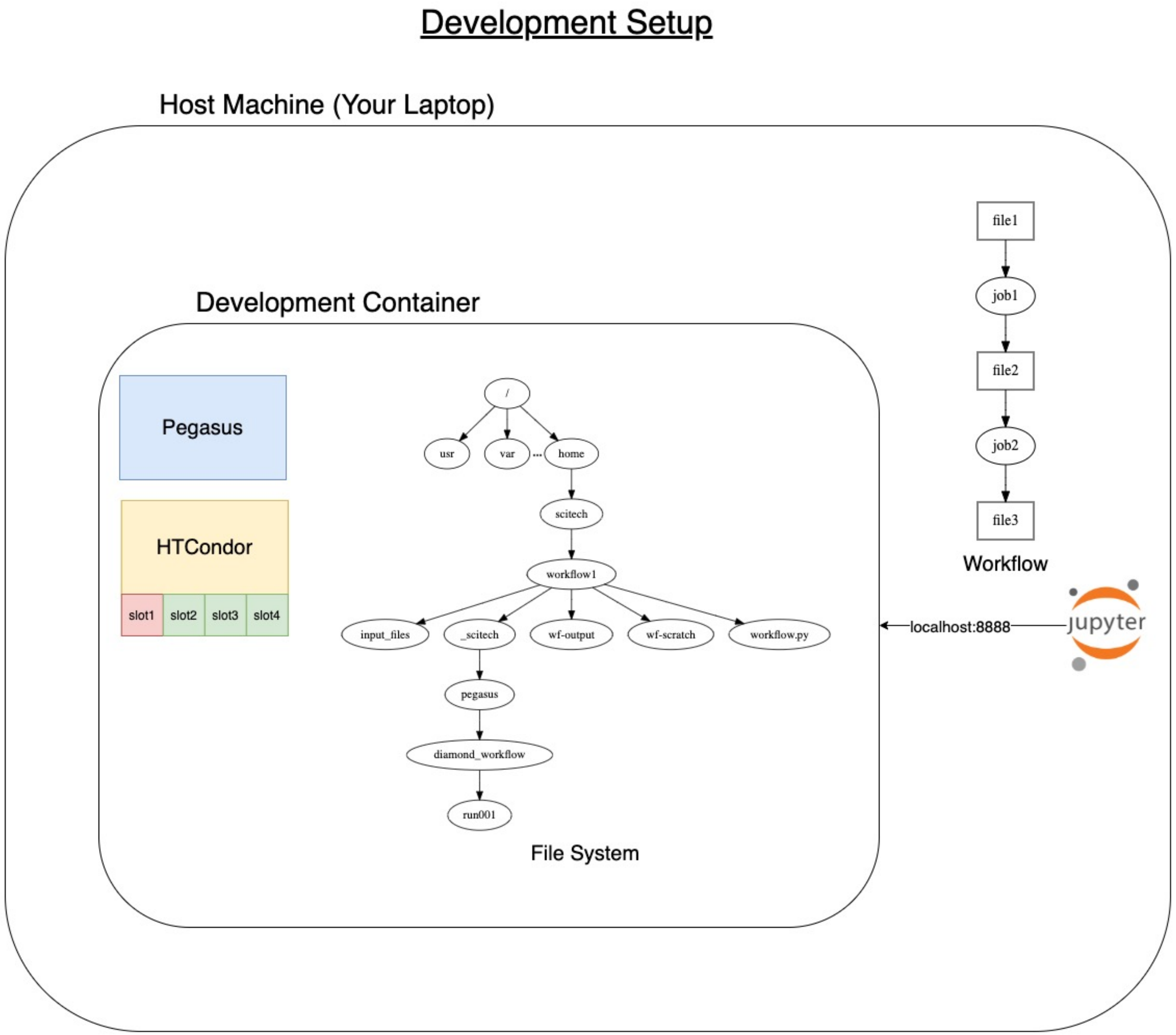
Docker Container / Jupyter Notebook

Production Setup



slot1	slot2	slot3	slot4
slot5	slot6	slot7	slot8
slot9	slot10	slot11	slot12

Docker Container / Jupyter Notebook



2.1 API

Key Pegasus Concepts

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- **Workflows are DAGs**
  - Nodes: jobs, edges: dependencies
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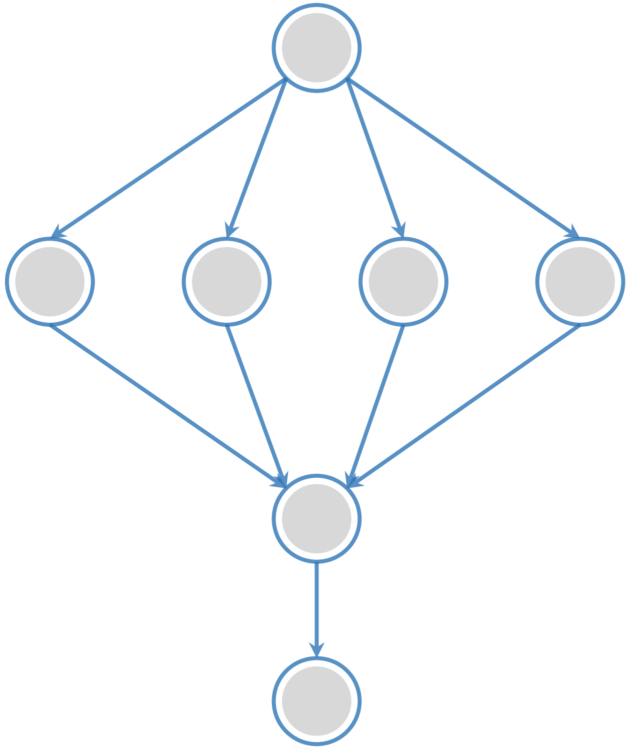
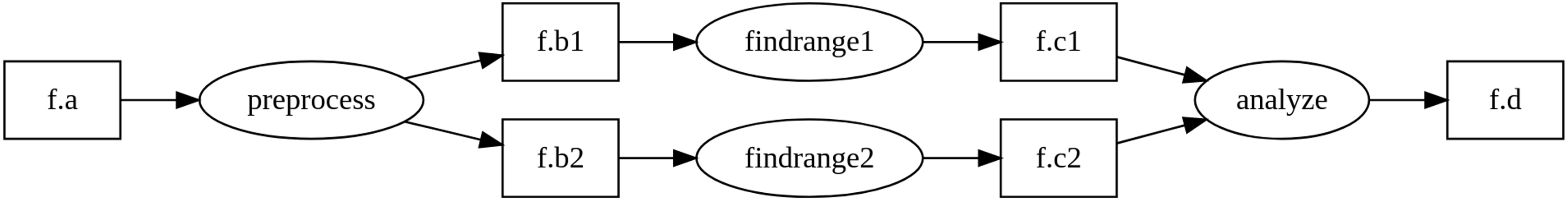
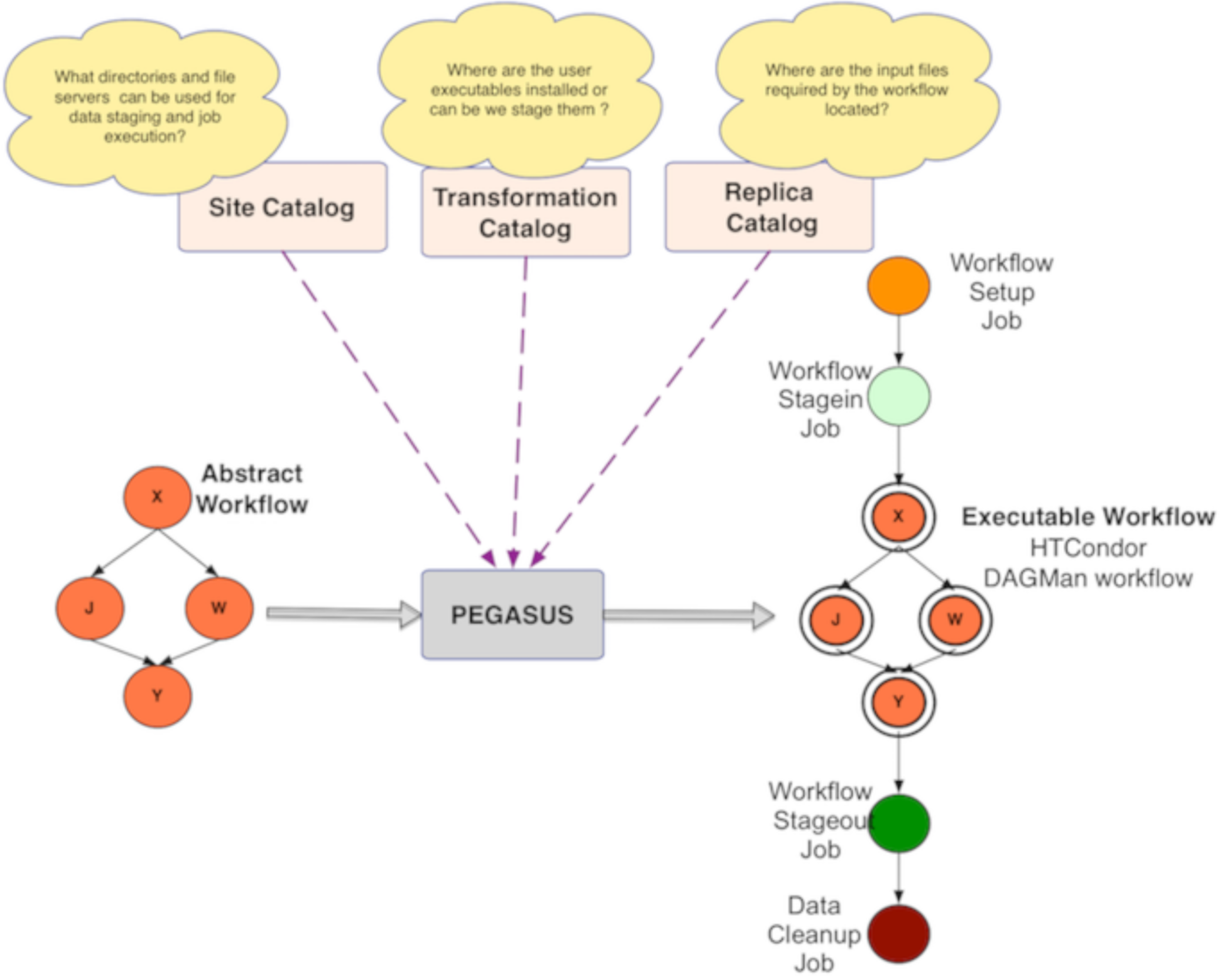
- **Planning occurs ahead of execution**

- **Planning converts an abstract workflow into a concrete, executable workflow**
  - Planner is like a compiler

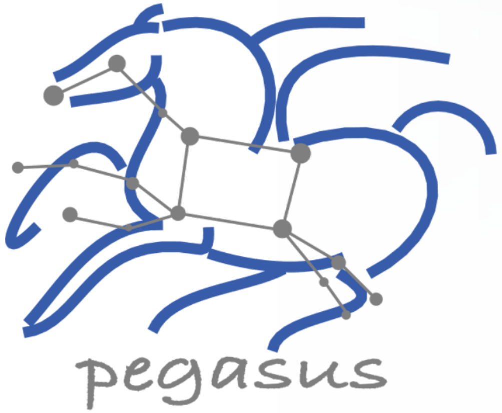



f.a
preprocess
f.b1
f.b2
findrange1
findrange2
f.c1
f.c2
analyze
f.d


What directories and file servers can be used for data staging and job execution?
Where are the user executables installed or can be we stage them ?
Where are the input files required by the workflow located?
Site Catalog
Transformation Catalog
Replica Catalog
Workflow Setup Job
Workflow Stagein Job
Abstract Workflow
X
J
W
Y
PEGASUS
Executable Workflow
HTCondor DAGMan workflow
X
J
W
Y
Workflow Stageout Job
Data Cleanup Job

2.2 Debugging

2.3 Command Line Tools



2.4 Summary

NSF U.S. DEPARTMENT OF ENERGY NIH DARPA

15 Minute Break

3. Advanced Topics

Data Staging Configurations

HTCondor I/O (HTCondor pools, OSG, …)

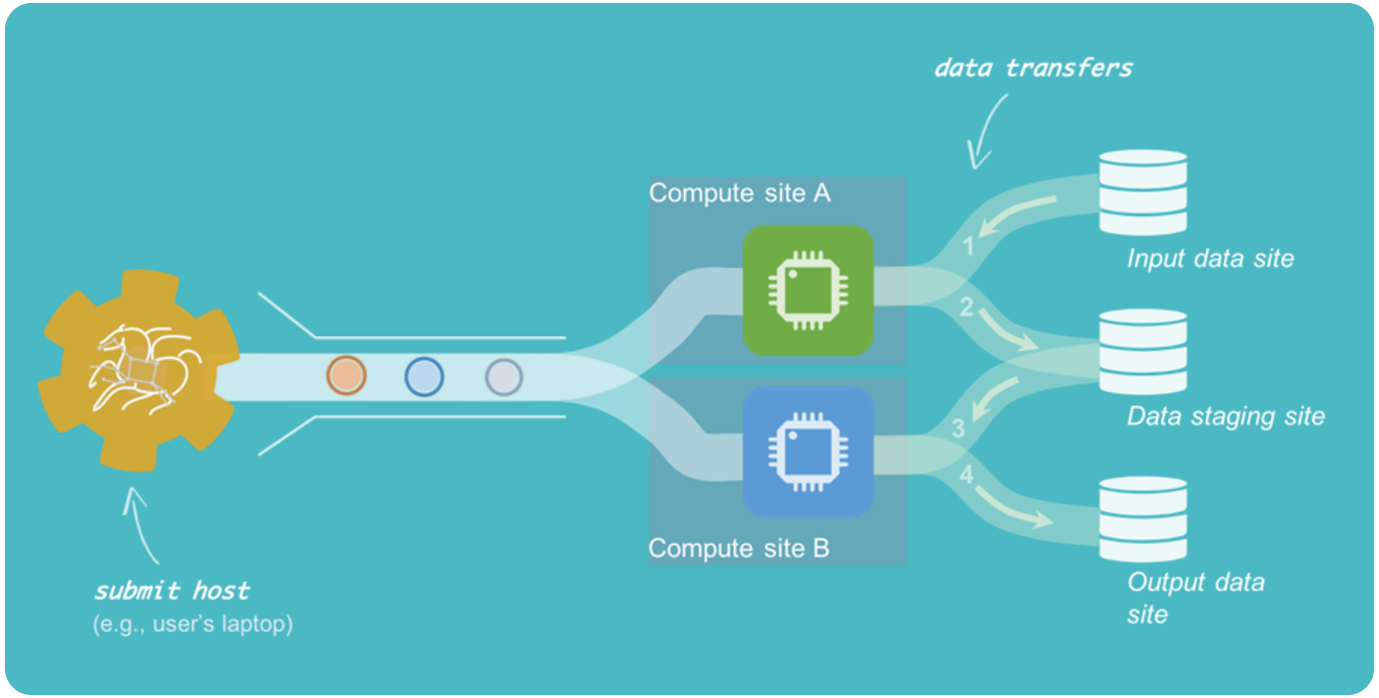
- Worker nodes do not share a file system
- Data is pulled from / pushed to the submit host via HTCondor file transfers
- Staging site is the submit host

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

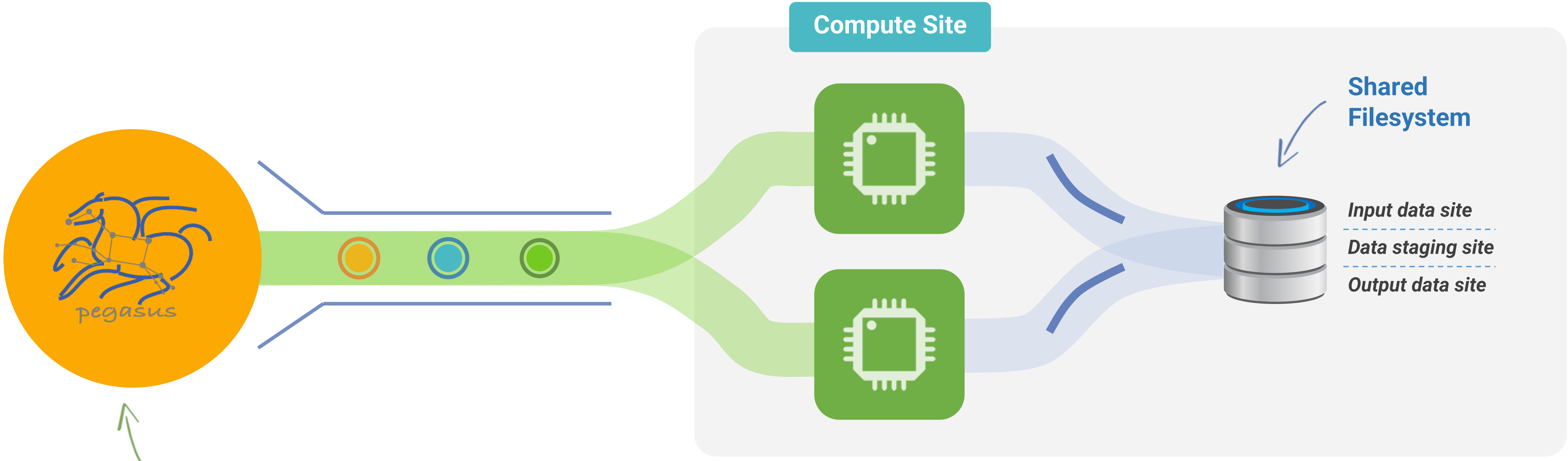
Shared File System (HPC sites, XSEDE, Campus clusters, …)

- I/O is directly against the shared file system



High Performance Computing

There are several possible configurations…

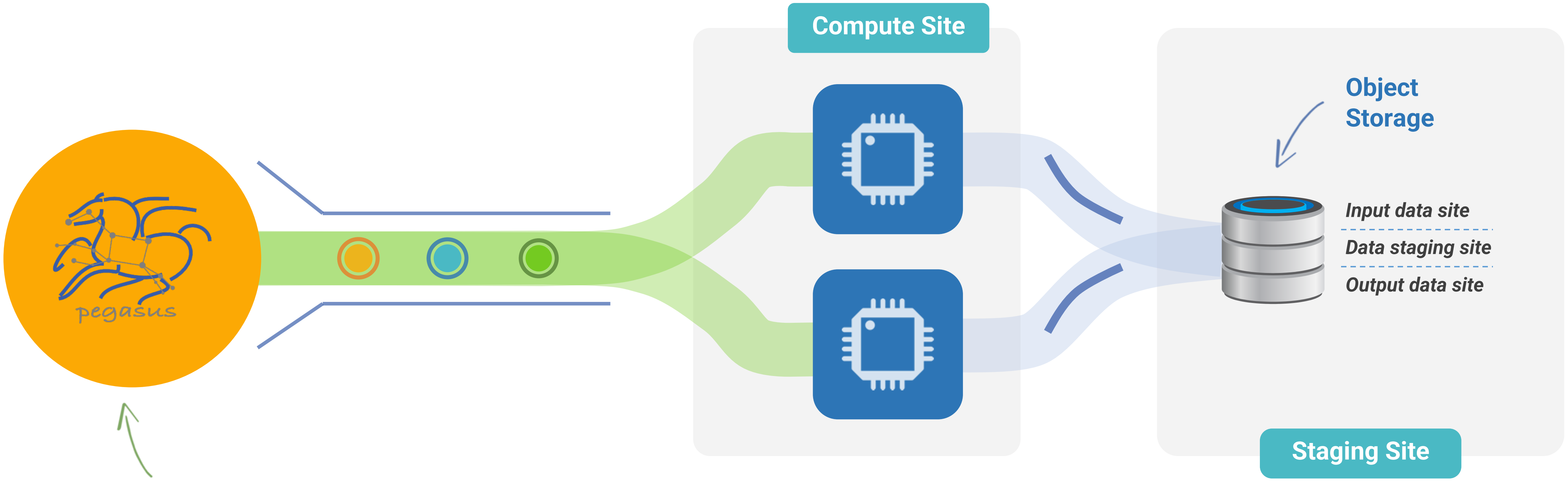


Submit Host

Typically Most HPC Sites

Cloud Computing

High-scalable object storages

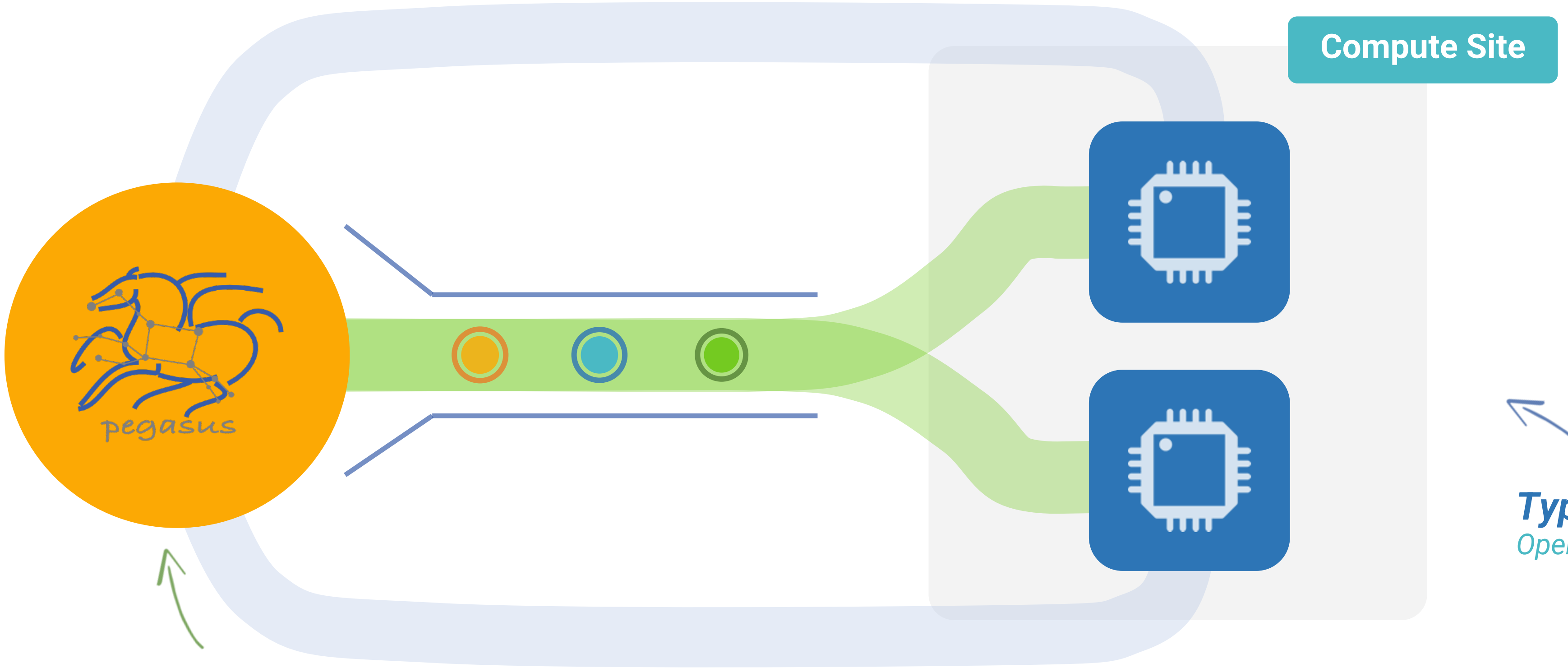


Submit Host

Typical cloud computing deployment (Amazon S3, Google Storage)

Grid Computing

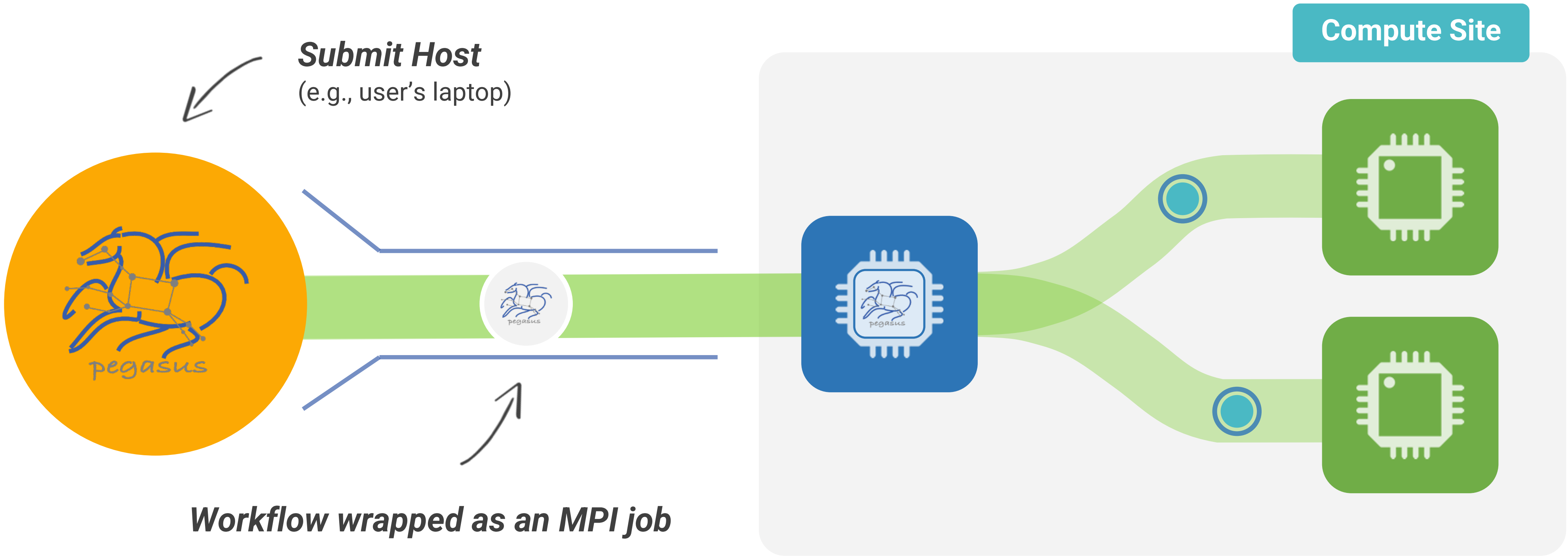
Local data management



Submit Host

Typical OSG sites
Open Science Grid

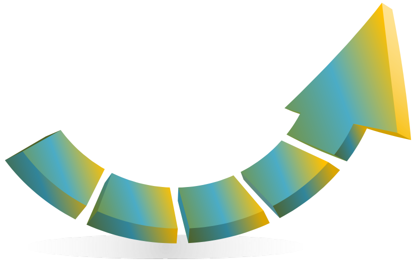
Running fine-grained workflows on HPC systems…



Submit Host
(e.g., user's laptop)

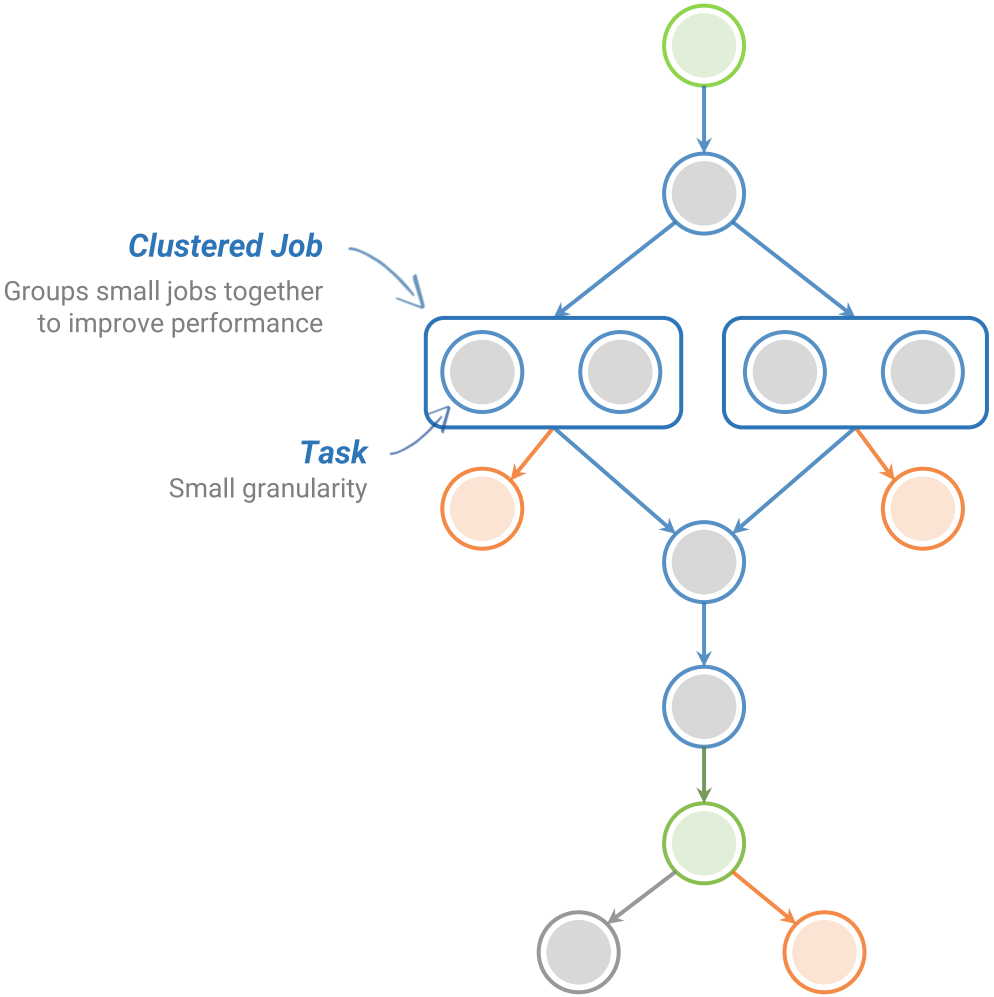
Workflow wrapped as an MPI job

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



Performance.

Why not improve it?



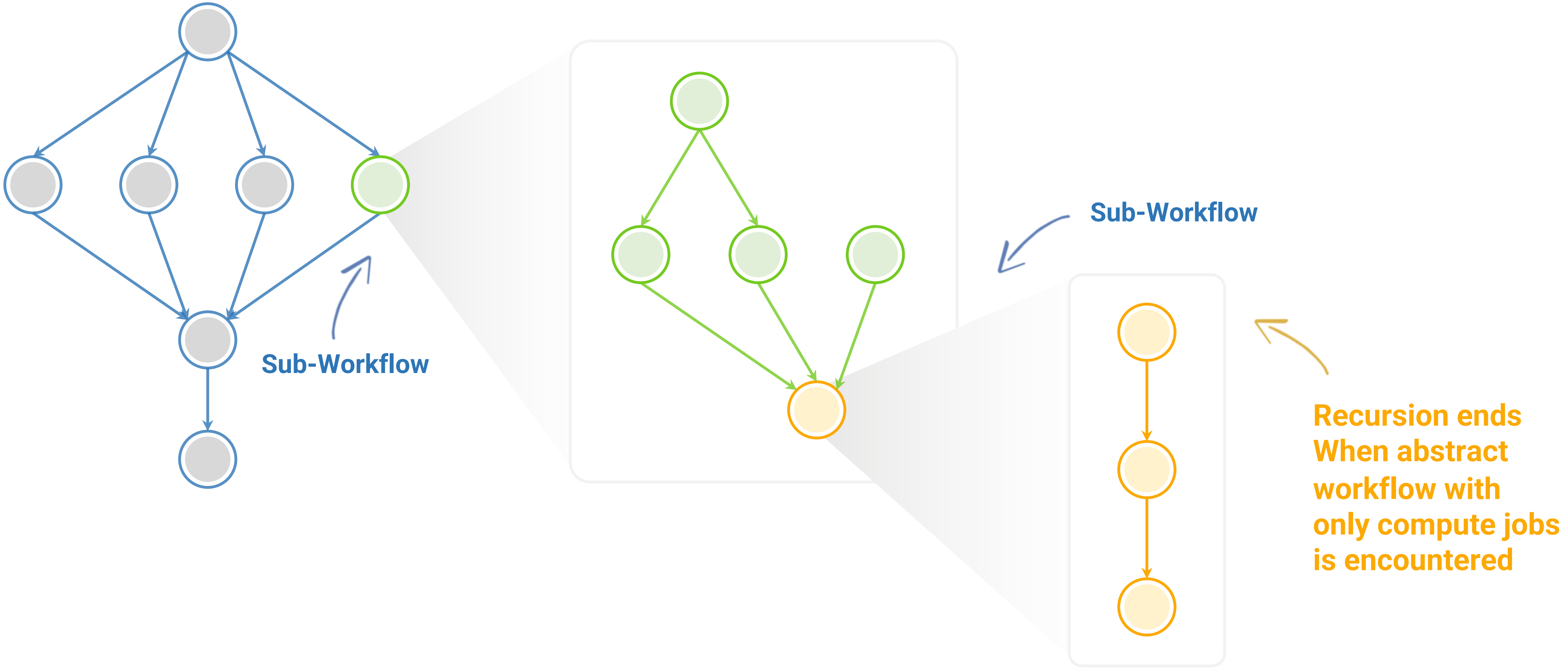
Clustered Job

Groups small jobs together
to improve performance

Task

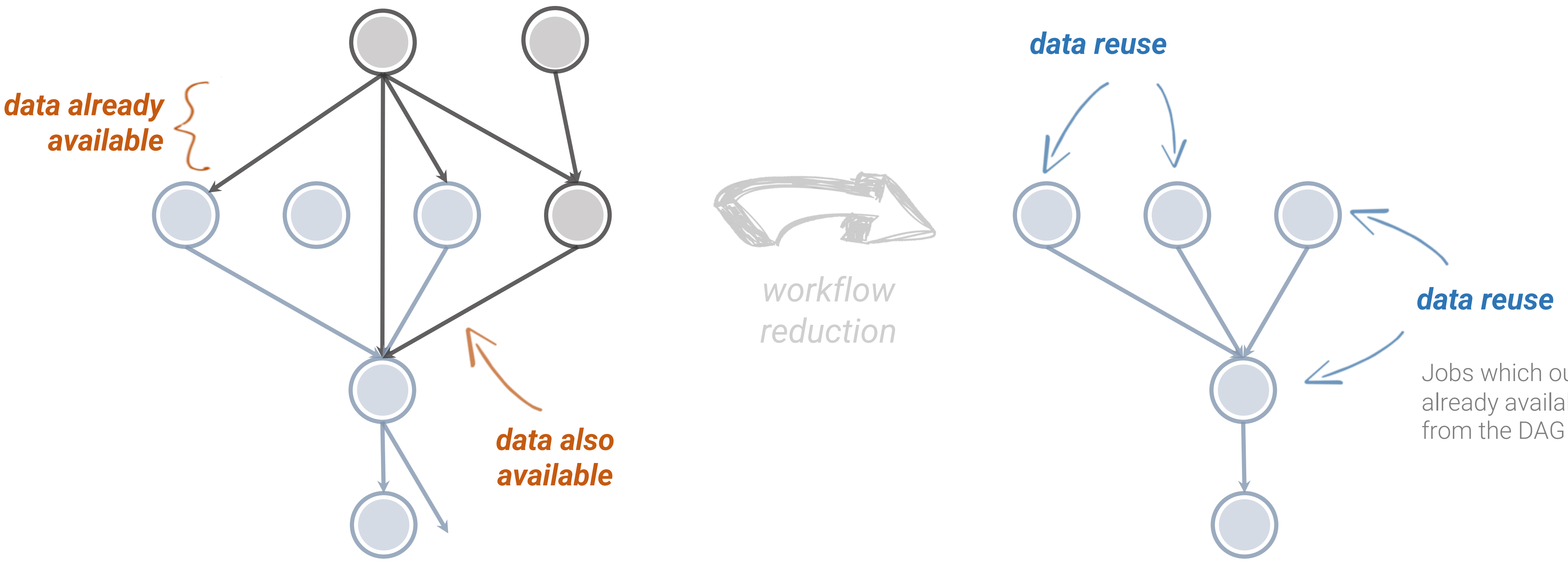
Small granularity

Pegasus also handles large-scale workflows



Recursion ends When abstract workflow with only compute jobs is encountered

Data Reuse prune jobs if output data already exists



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

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

Metadata

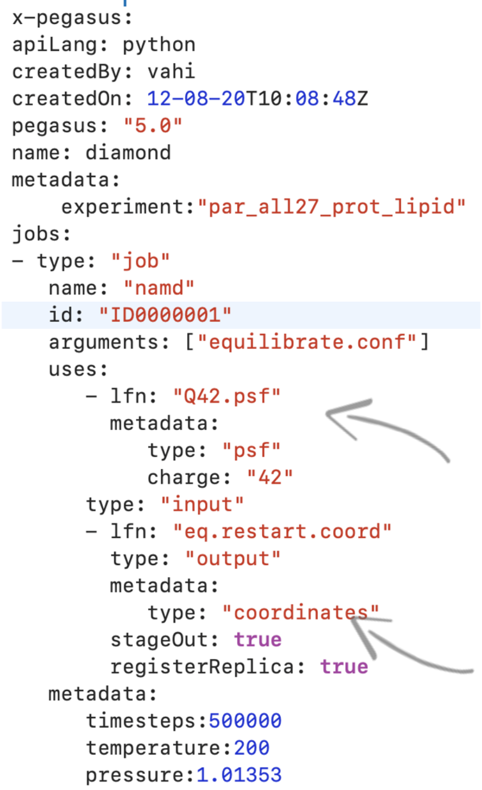
Can associate arbitrary key-value pairs with workflows, jobs, and files

Data Registration

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

Static and Runtime Metadata

Static: application parameters
Runtime: performance metrics

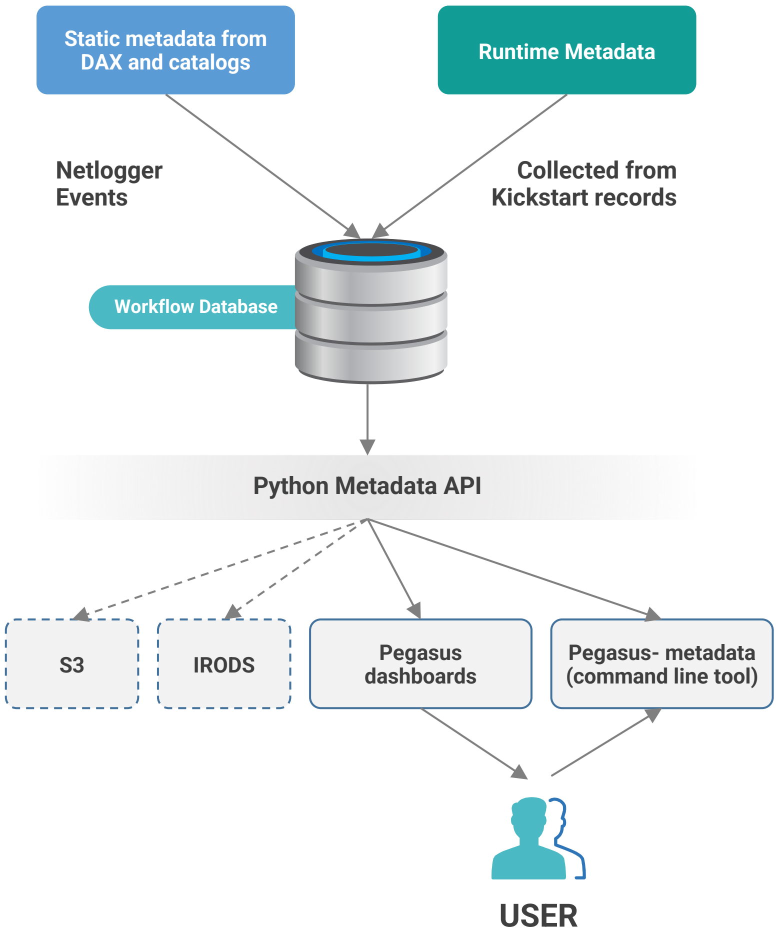


```
x-pegasus:
apiLang: python
createdBy: vahi
createdOn: 12-08-20T10:08:48Z
pegasus: "5.0"
name: diamond
metadata:
    experiment:"par_all27_prot_lipid"
jobs:
- type: "job"
   name: "namd"
   id: "ID0000001"
   arguments: ["equilibrate.conf"]
   uses:
      - lfn: "Q42.psf"
        metadata:
           type: "psf"
           charge: "42"
      type: "input"
      - lfn: "eq.restart.coord"
        type: "output"
        metadata:
           type: "coordinates"
        stageOut: true
        registerReplica: true
   metadata:
      timesteps:500000
      temperature:200
      pressure:1.01353
```

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 dashboards
Pegasus- metadata (command line tool)
USER

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

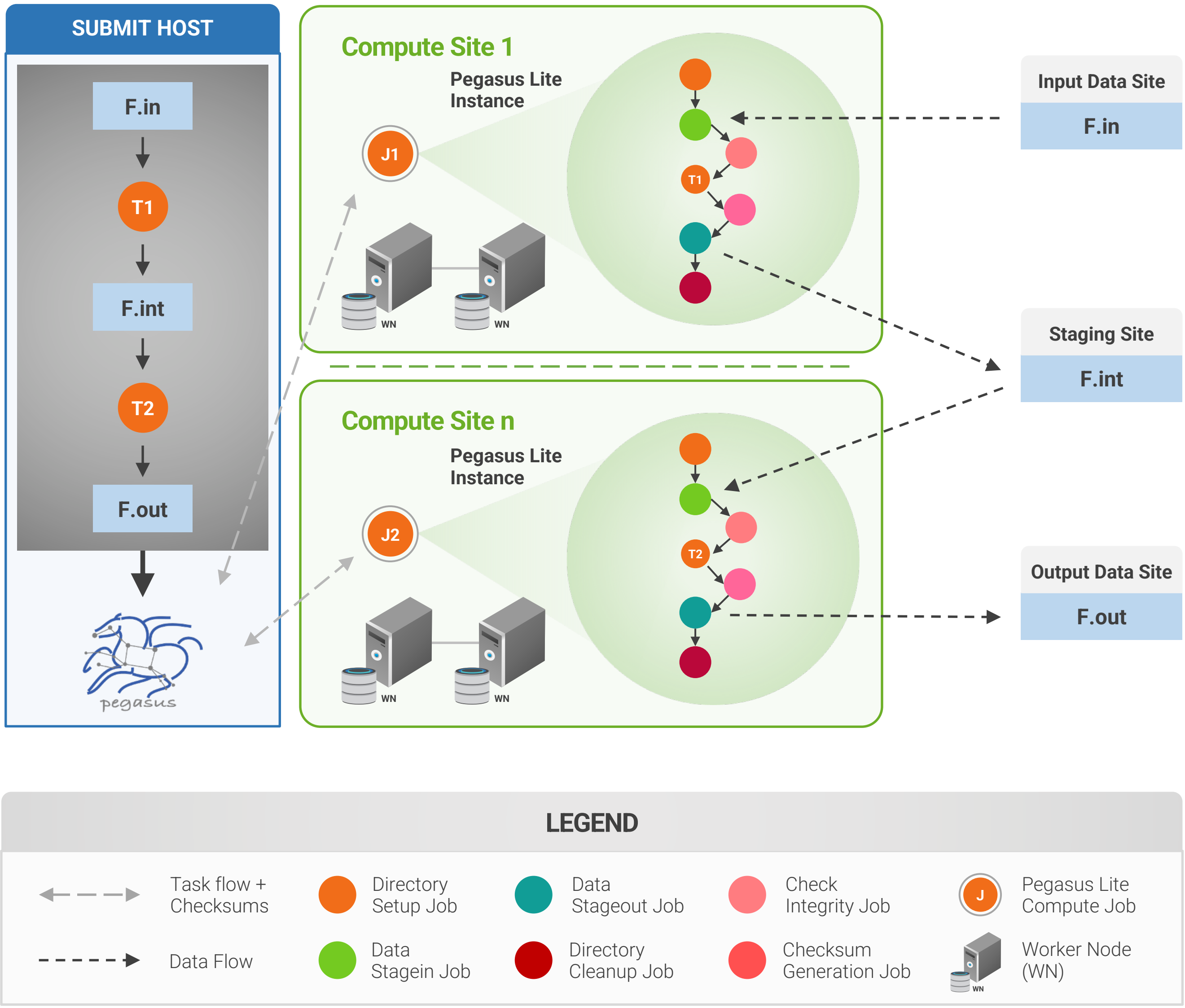
Pegasus performs integrity checksums on input files right before a job starts on the remote node.

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

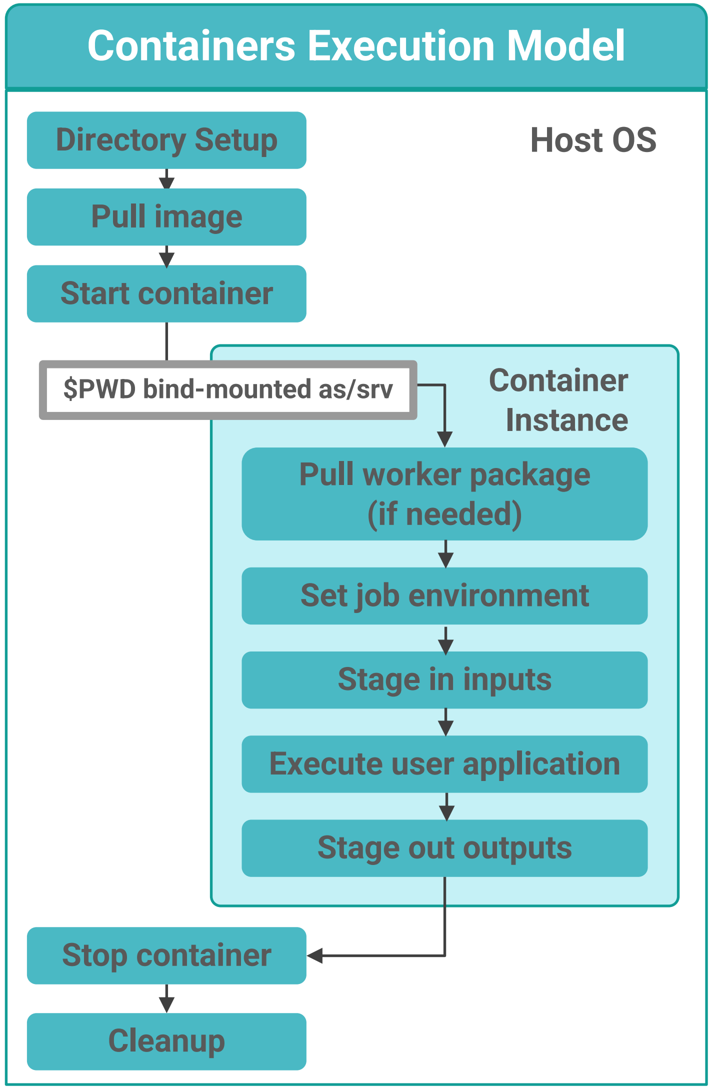
Users can refer to **containers** in the **Transformation Catalog** with their executable preinstalled

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*



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 file system such as **CVMFS**
- The exported tar file is then shipped with the workflow and made available to the jobs

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

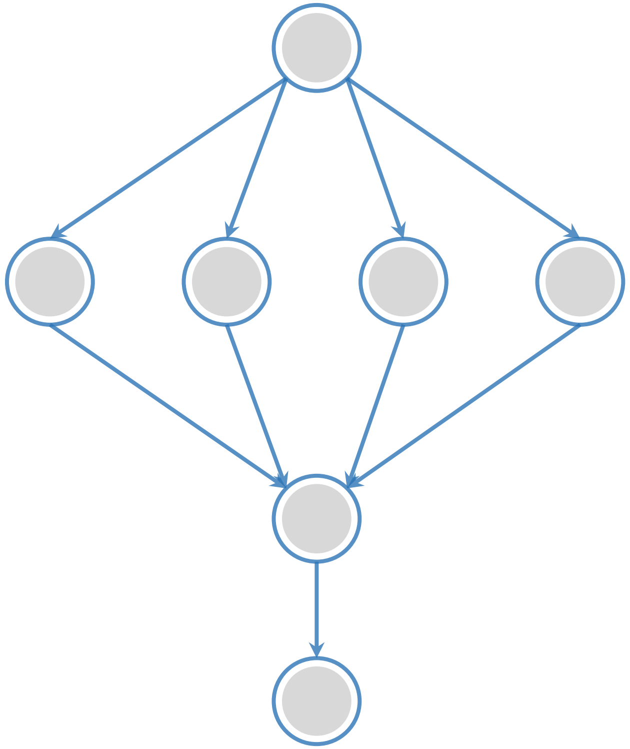
- Users can specify credentials in a **generic credentials file** on submit host
- Associate credentials with sites in site catalog

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



Amazon AWS Batch

AWS Batch

Container based, dynamically scaled and efficient batch computing service

Automatically launches compute nodes in Amazon based on demand in the associated job queue

Users can specify compute environment that dictates what type of VM's are launched

Pegasus will **allow clusters of jobs** to be run on **Amazon EC2** using **AWS Batch Service**

New command line tool: **pegasus-aws-batch**

Automates most of the batch setup programmatically

- **Sets up and Deprovisions**
  - Compute Environment
  - Job Queues
- **Follows AWS Batch HTTP specification**

Ensemble Manager

Allow users to submit a collection of workflows (ensembles)

Automatically **spawn** and **manage** collections of workflows

Trigger submission of workflows

Properties

Workflows within an ensemble may have **different priorities**

> *Priorities can also be changed at runtime*

Ensembles may limit the number of **concurrent** planned and running workflows

Additional Actions

Ensembles can be **paused, resumed, removed, re-planned**, and **re-executed**
A **debugging** mechanism is also provided to investigate failures in workflow runs
Actions can be performed both to ensembles and single workflows within ensembles

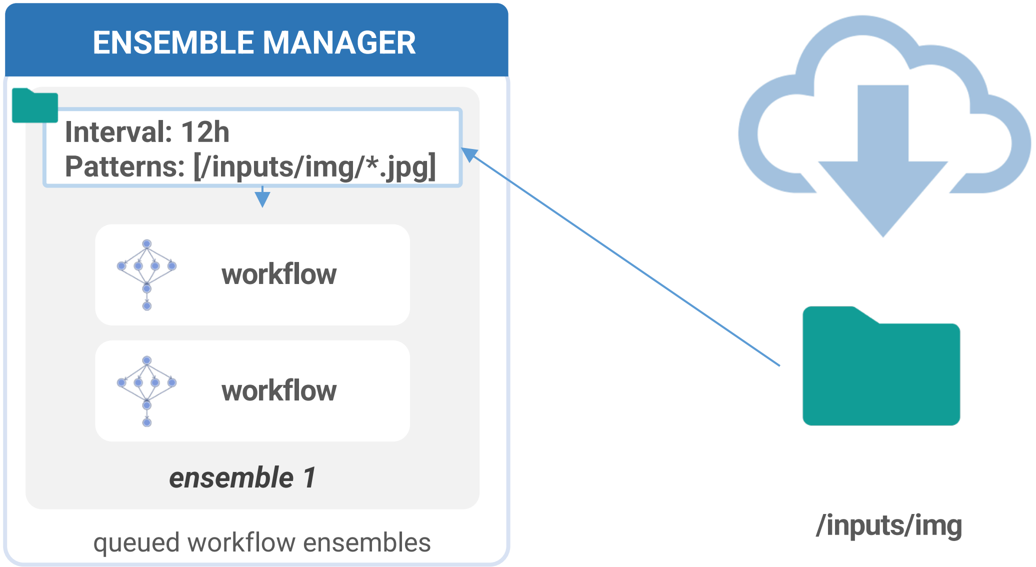
Ensemble Manager Triggers

Cron workflow trigger

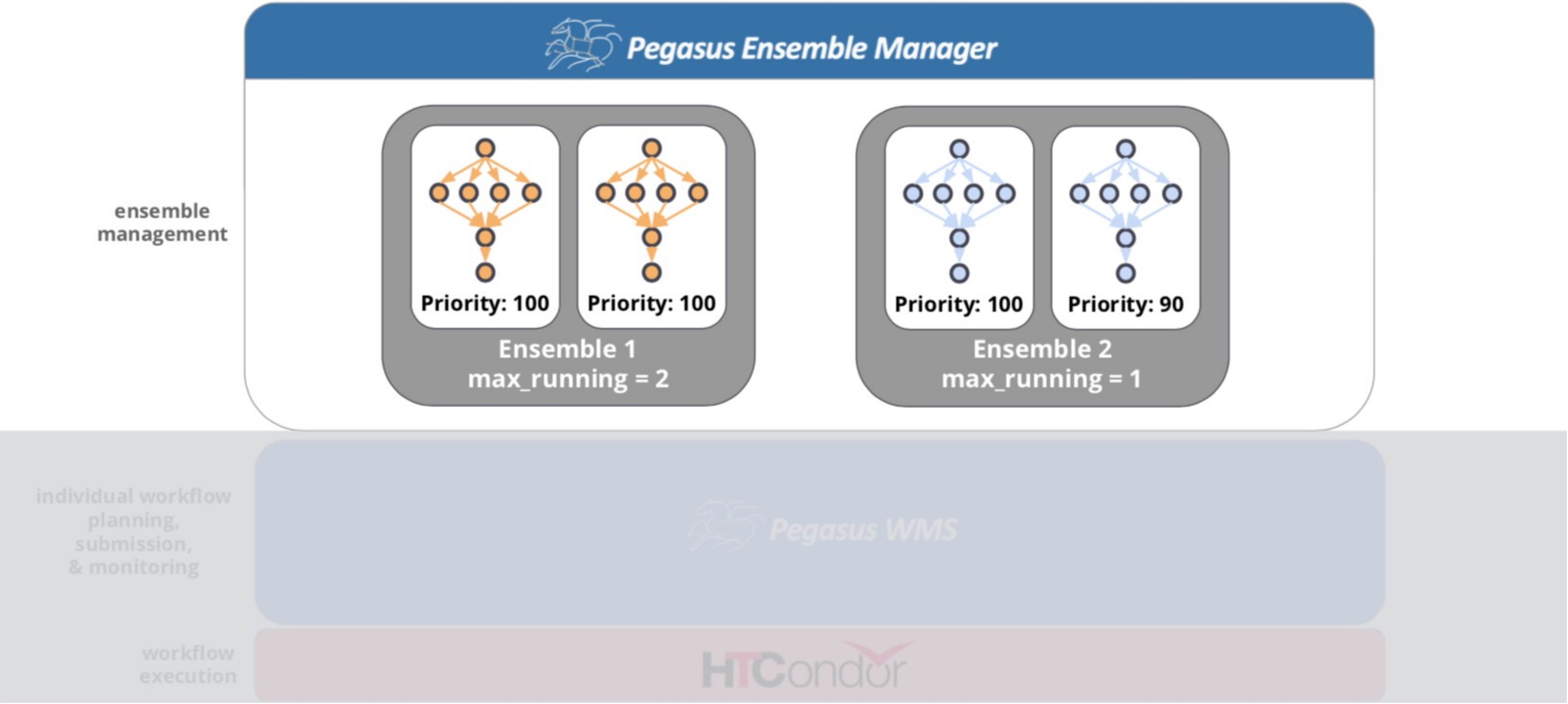
Automatically submit workflows to the ensemble manager at **regularly occurring time intervals**

File pattern workflow trigger

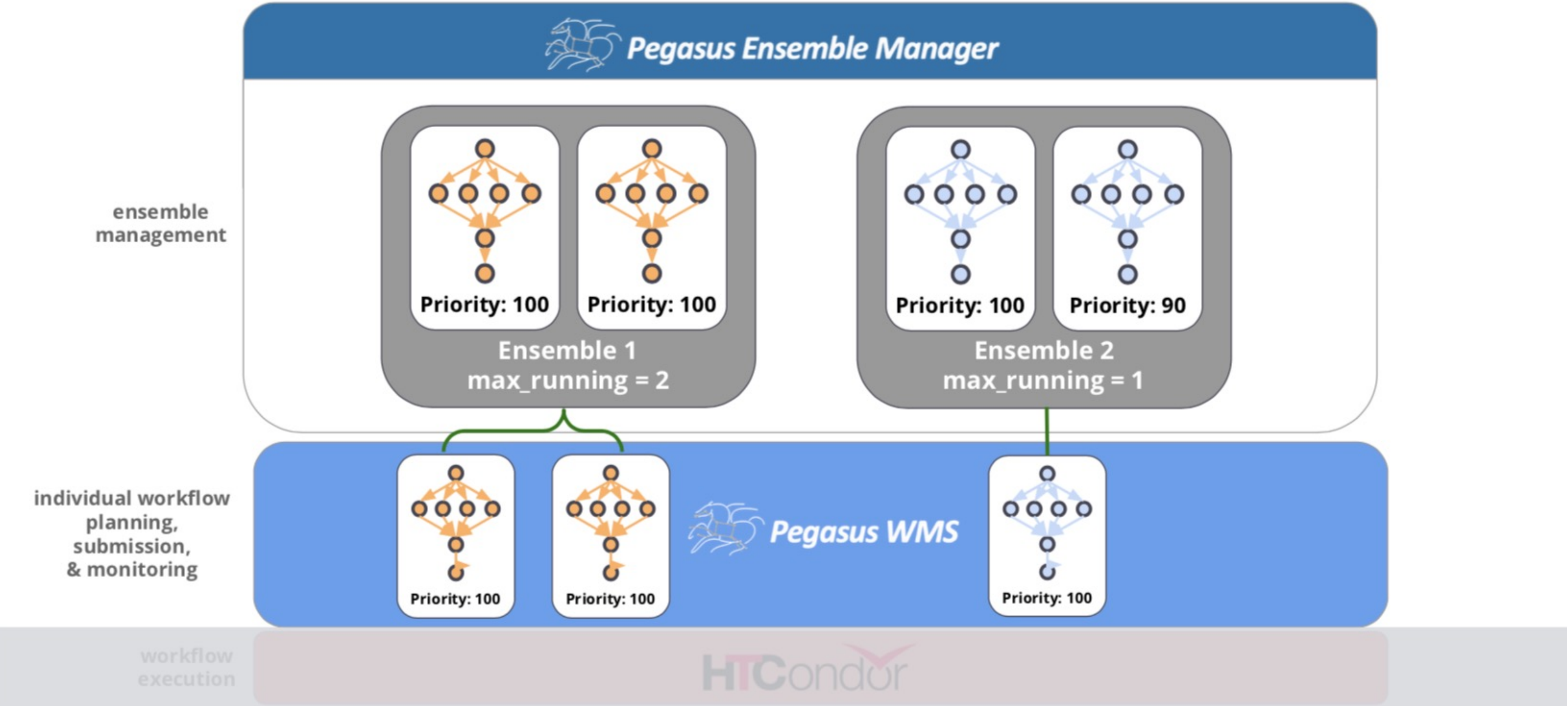
Cron trigger functionality
New **input files matching a given file pattern(s) will be passed** as input
Ideal for **regular batch processing** of data as it arrives in one or more given directories



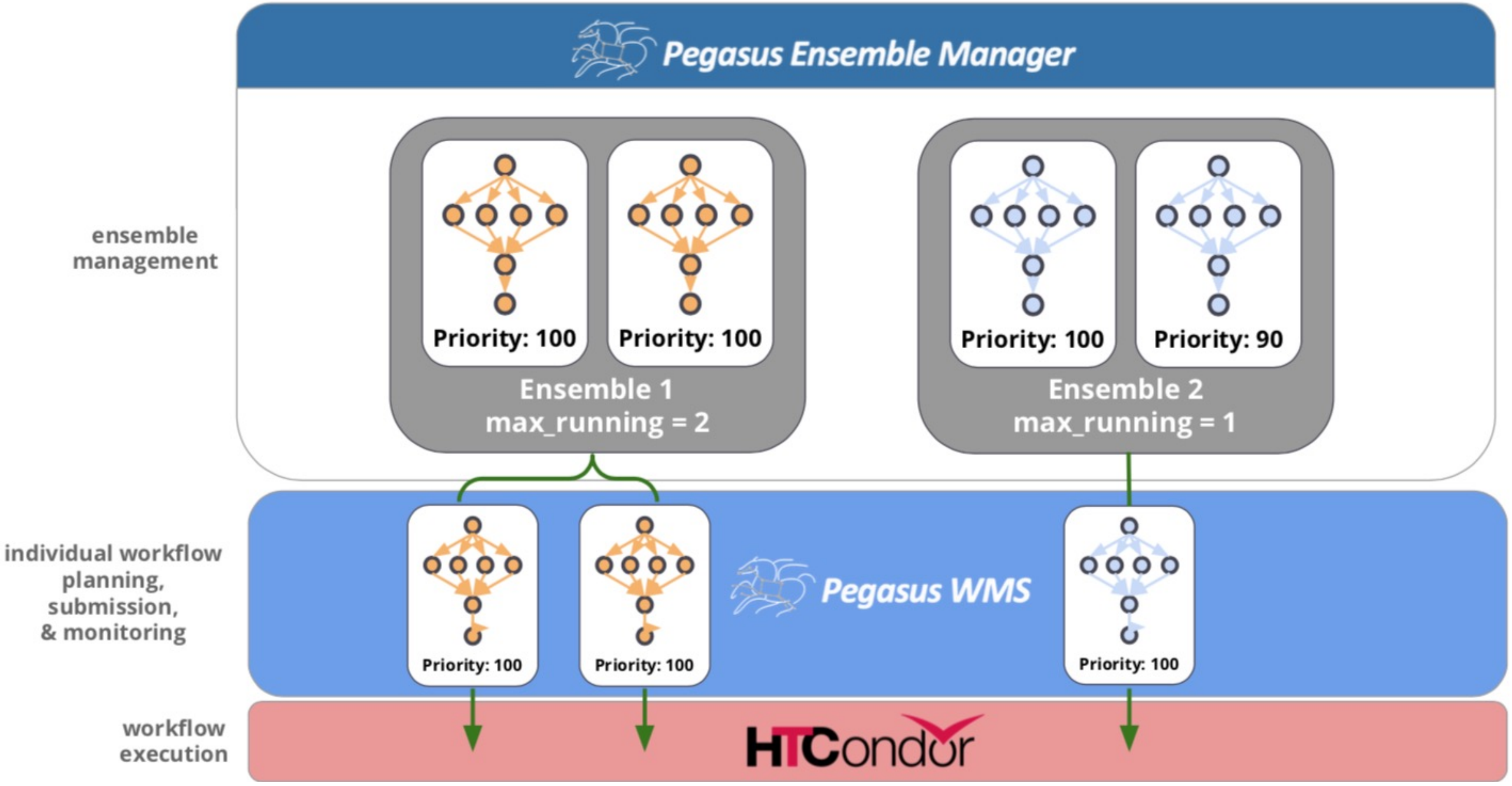
Ensemble Manager Overview



Ensemble Manager Overview



Ensemble Manager Overview



Pegasus est. 2001

Automate, recover, and debug scientific computations.

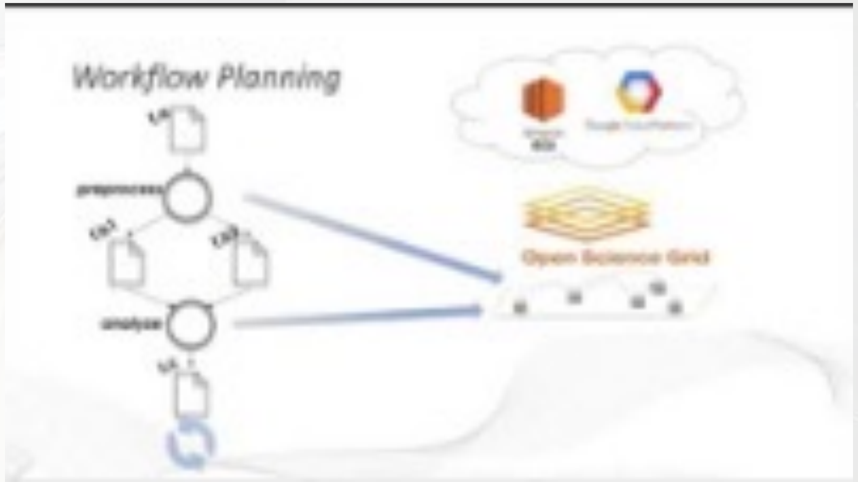
Get Started

- **Pegasus Website**
  https://pegasus.isi.edu
- **Users Mailing List**
  pegasus-users@isi.edu
- **Support**
  pegasus-support@isi.edu
- **Slack**
  Ask for an invite by trying to join pegasus-users.slack.com in the Slack app
- **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

YouTube Channel

https://www.youtube.com/channel/UCwJQln1CqBvTJqiNr9X9F1Q/featured



Pegasus in 5 Minutes