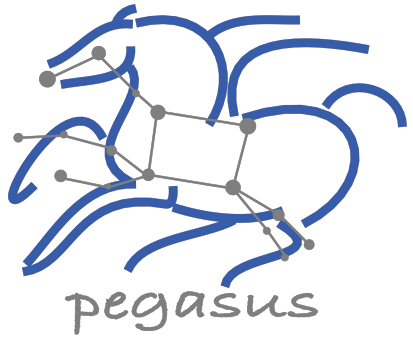
Unlock the Power of Bioinformatics Pipelines with the Pegasus Workflow Management System Workshop



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USC | Advanced Research Computing
Enabling scientific breakthroughs at scale

ACCESS | Advancing Innovation

NSF U.S. DEPARTMENT OF ENERGY NIH DARPA

Preparations and Outline

- You need to be on USC Network (USC Secure Wifi or USC VPN) and need to use your USC credentials to log in
- Use a web browser and log on to USC OnDemand Instance at https://ondemand.carc.usc.edu

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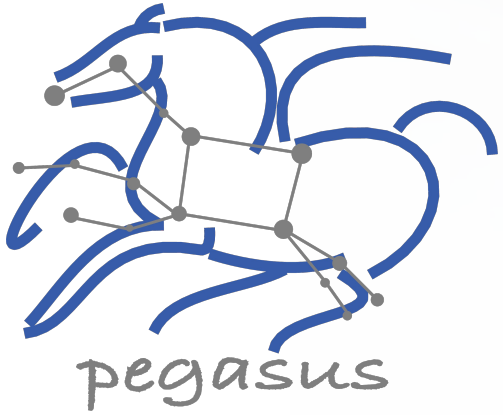
- SlideDeck: https://pegasus.isi.edu/tutorial/keck23/USC-HSC-2023-Pegasus.pdf
- Slides - Introduction to Pegasus
- Hands on (API, Debugging, Command Line)
- Variant Calling Example



1. Introduction

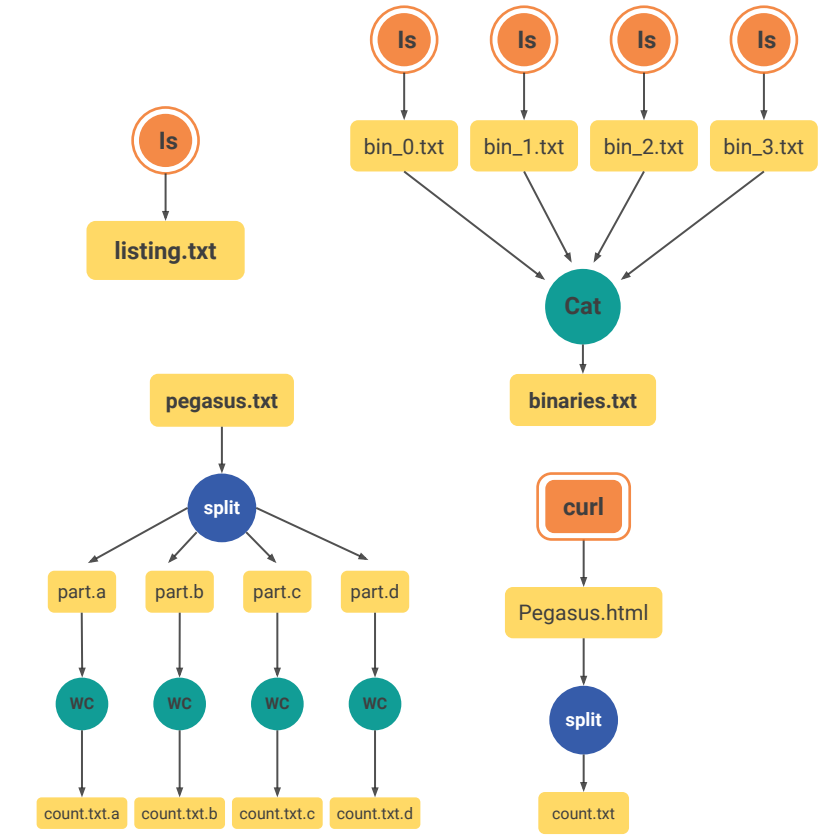
Workflow Systems and USC CARC / HPC?

- We will talk about:
  - Multiple job workloads
  - Relationship between jobs
  - Automatic data management
  - … and more
- HPC is not just parallel jobs
  - High throughput computing (HTC)

What are Scientific Workflows

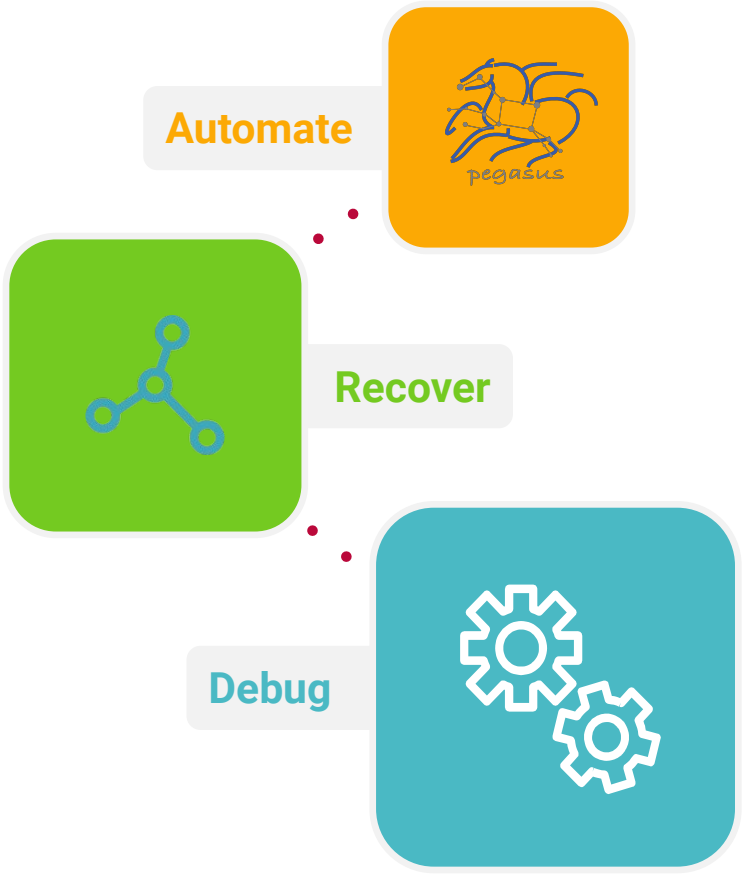
- **Conducts a series of computational tasks.**
  - Resources distributed across Internet.
- **Chaining (outputs become inputs) replaces manual hand-offs.**
  - Accelerated creation of products.
- **Ease of use - gives non-developers access to sophisticated codes.**
  - Resources distributed across Internet.
- **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

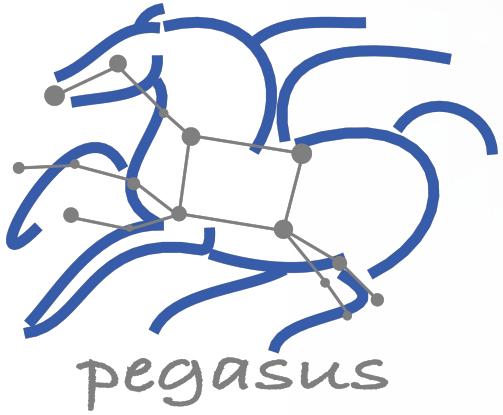
Why Pegasus?



- **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

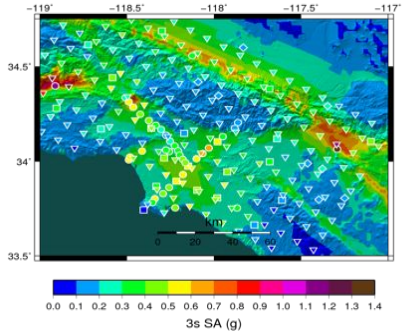
HTCondor High Throughput Computing

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



Some of The Success Stories...

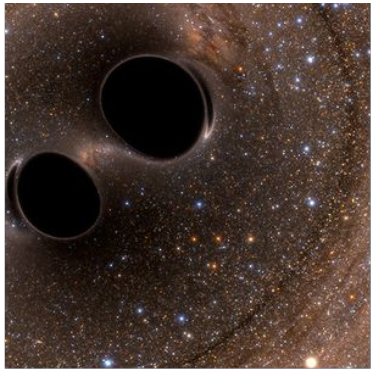
Southern California Earthquake Center's CyberShake



Mix of MPI and single-core jobs, mix of CPU, GPU codes.
Large data sets (10s of TBs), ~300 workflows with 420,000 tasks each
Supported since 2005: changing CI, x-platform execution

First Physics-Based "Shake map" of Southern California

Laser Interferometer Gravitational-Wave Observatory (LIGO)

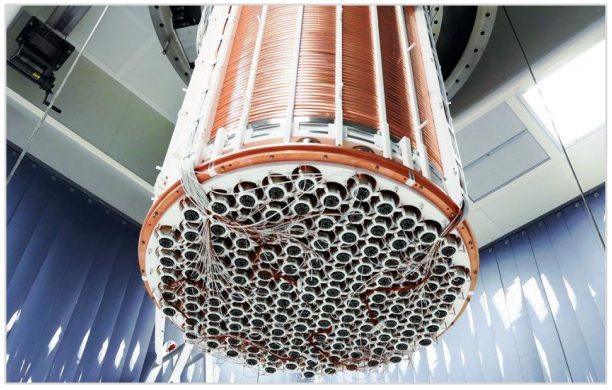


High-throughput computing workload, access to HPC resources, ~ 21K Pegasus workflows, ~ 107M tasks

Supported since 2001, distributed data, opportunistic computing resources

First direct detection of a gravitational wave (colliding black holes)

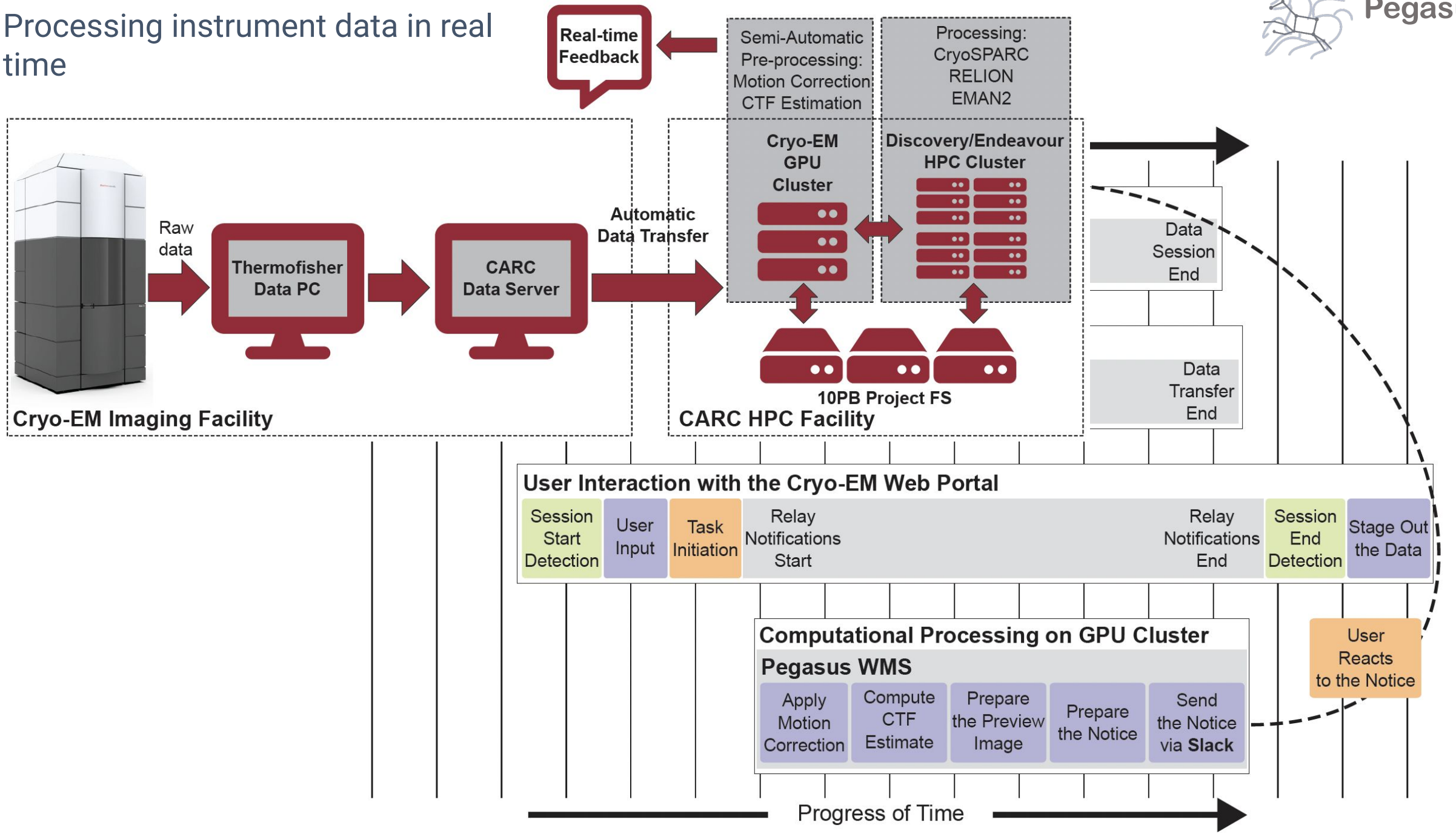
XENONnT - Dark Matter Search



- Custom data management
- Rucio for data management
- MongoDB instance to track science runs and data products.

Monte Carlo simulations and the main processing pipeline.

Processing instrument data in real time

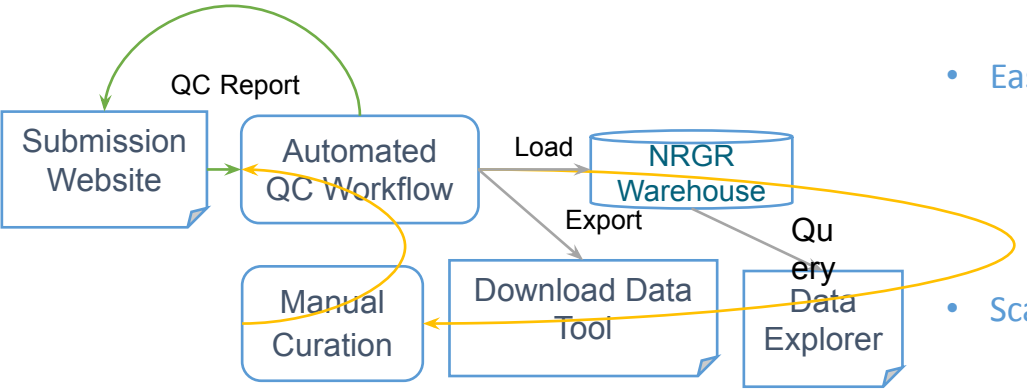


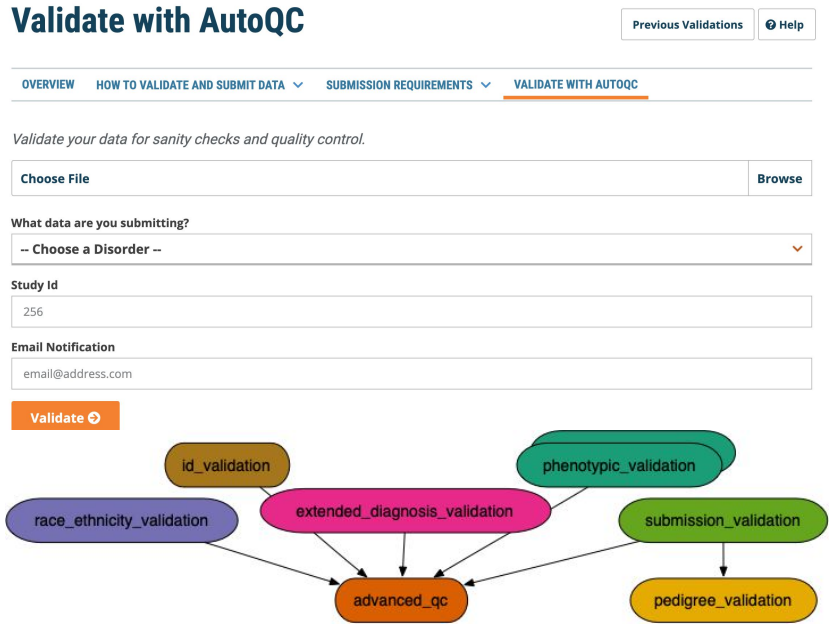
Automated Quality Control of Phenotypic Datasets

NIMH REPOSITORY & GENOMICS RESOURCE

Pegasus

The NIMH Center for Collaborative Genomic Studies on Mental Disorders, now known as the NIMH Repository and Genomics Resource (NRGR), maintains biomaterials, demographic, and phenotypic data from over 200,000 well-characterized individuals with a range of psychiatric illnesses, their family members, and unaffected controls.



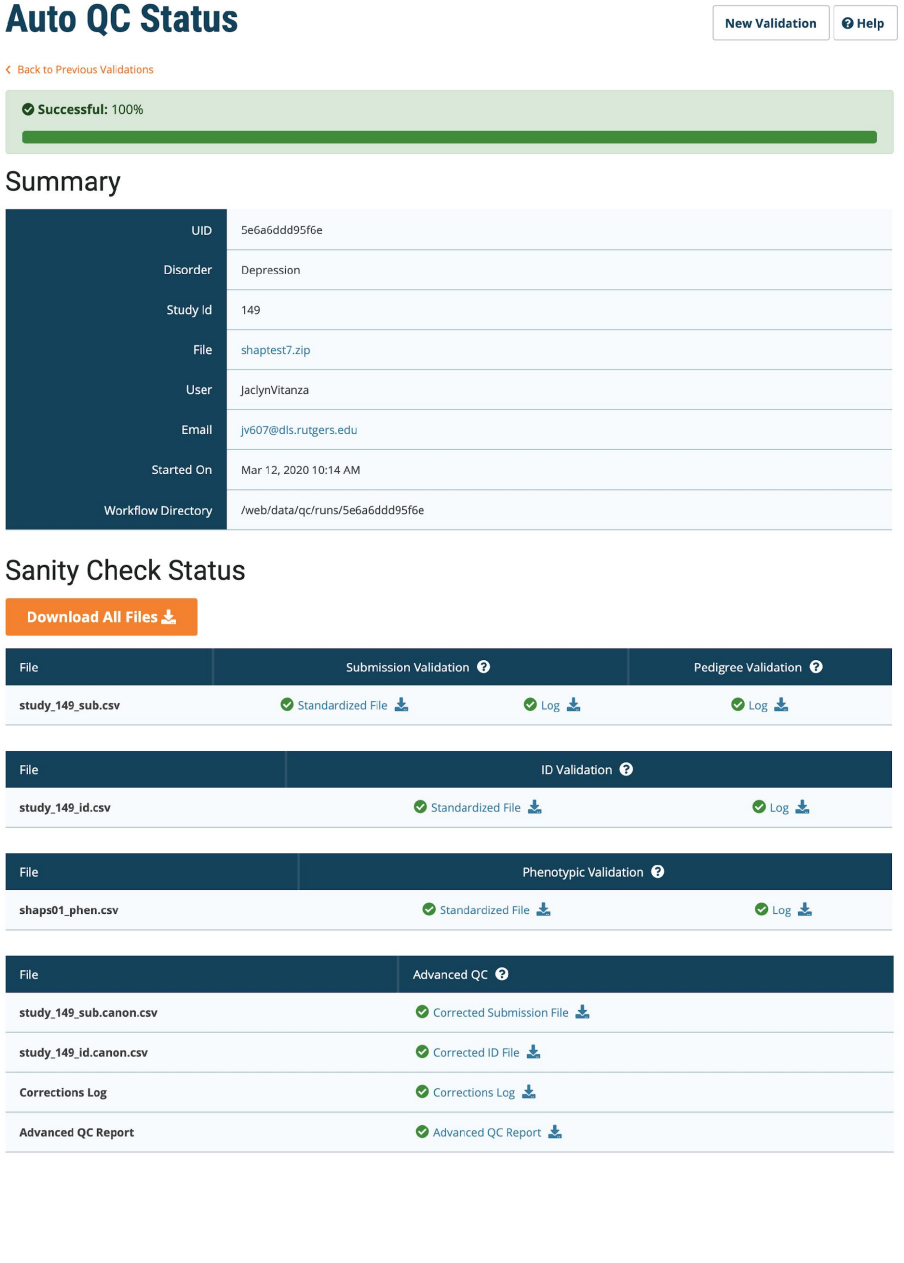


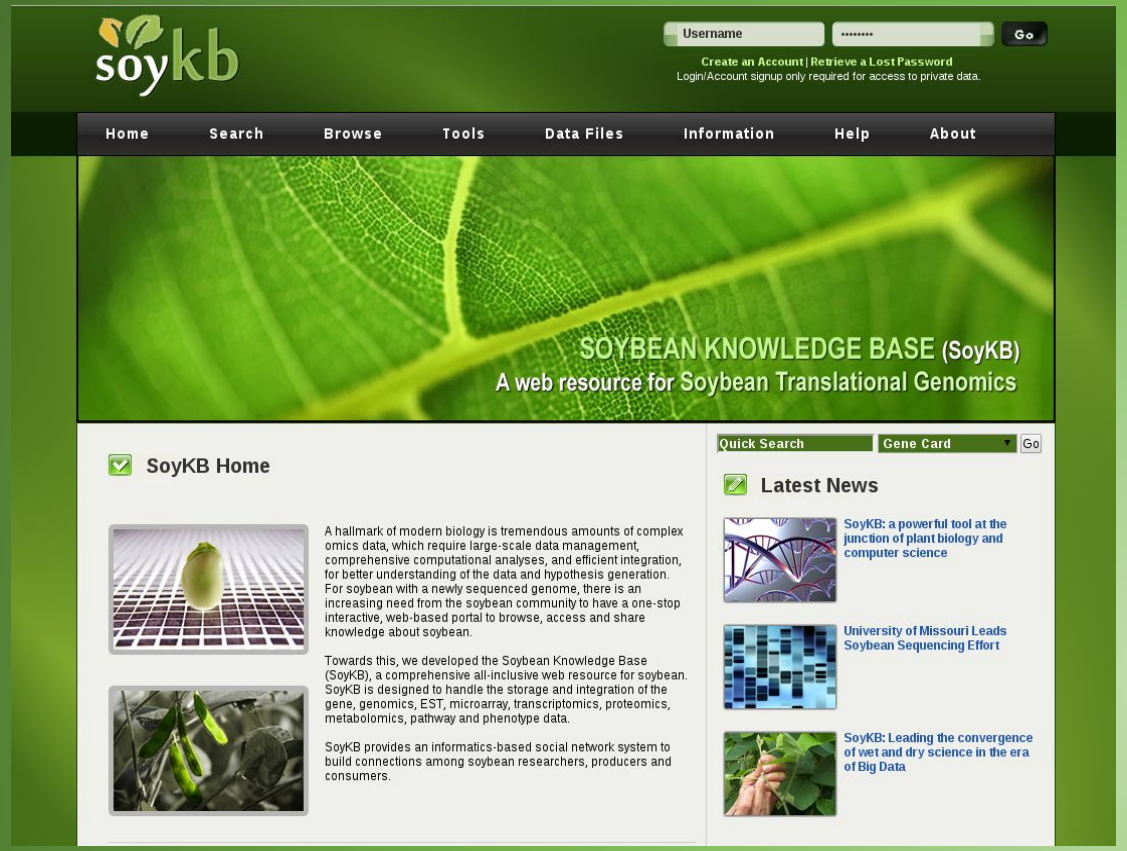
- Easy to Use Web-Based Interface
  - Simple Submission
  - Real-time Monitoring and Error Reports
  - After automated QC, submit corrected files for expert curation
- Scalable
  - Workflow based architecture using Pegasus WMS
- Extensible Design
  - Easily add new QC steps, and checks
- Enables Complex checks
  - Pedigree Checks
  - QC Checks validating data with external sources
  - QC Checks can correlate data across multiple files and across multiple fields within files

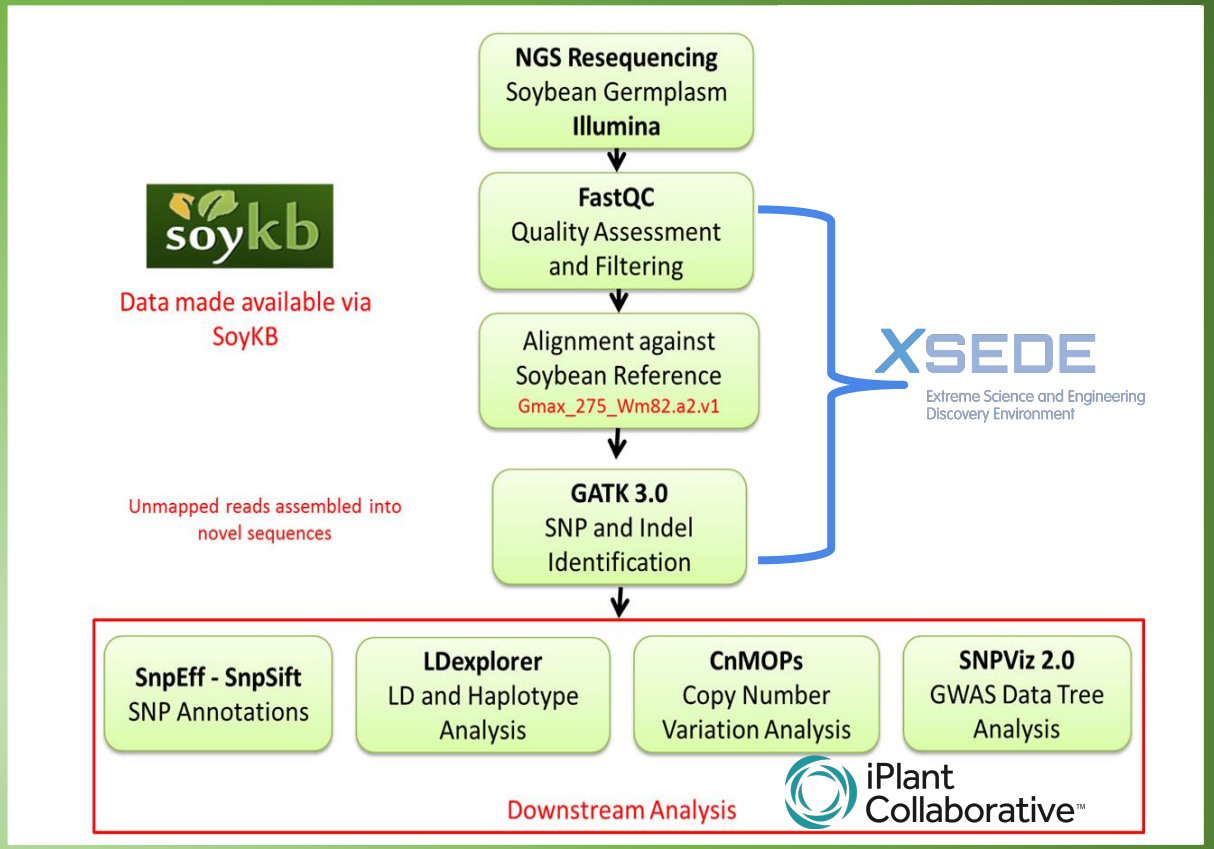
○ Ensures high-quality uniform data deposited at NRGR

○ Better resource utilization: solve most QC problems automatically, use expert curation for hard cases

https://pegasus.isi.edu





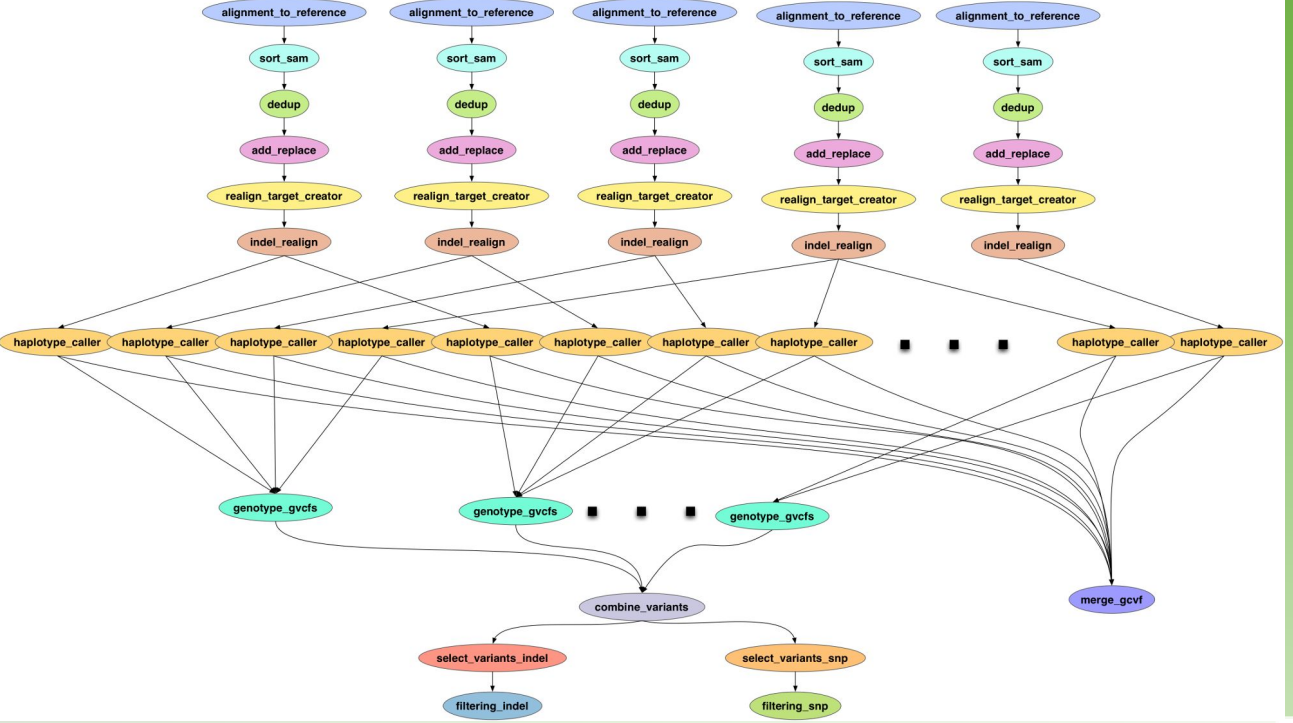


http://soykb.org

XSEDE Allocation

PI: Dong Xu

Trupti Joshi, Saad Kahn, Yang Liu, Juexin Wang, Badu Valliyodan, Jiaojiao Wang



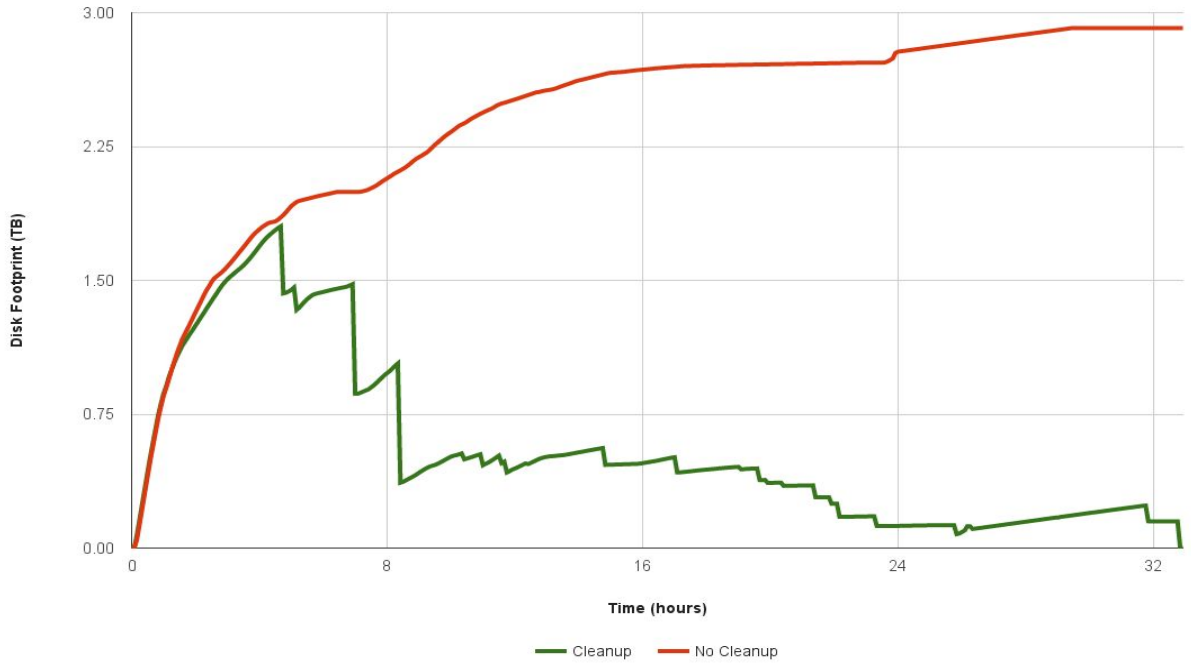
Task	Base Code	Cores (Threads)	Memory (GB)
Alignment_to_reference	BWA	7	8
Sort_sam	Picard	1	21
Dedup	Picard	1	21
Add_replace	Picard	1	21
Realign_target_creator	GATK	15	10
Indel_realign	GATK	1	10
Haplotype_caller	GATK	1	3
Genotype_gvcfs	GATK	1	10
Merge_gvcf	GATK	10	20
Combine_variants	GATK	1	10
Select_variants	GATK	14	10
Filtering	GATK	1	10

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 in the submit host - Workflow runs at a finer granularity

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



Pegasus

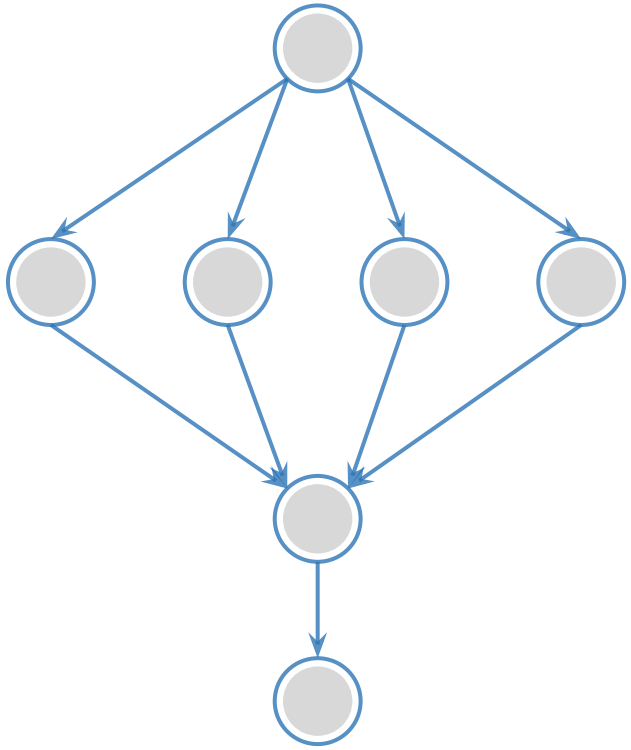
Key Pegasus Concepts

- **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

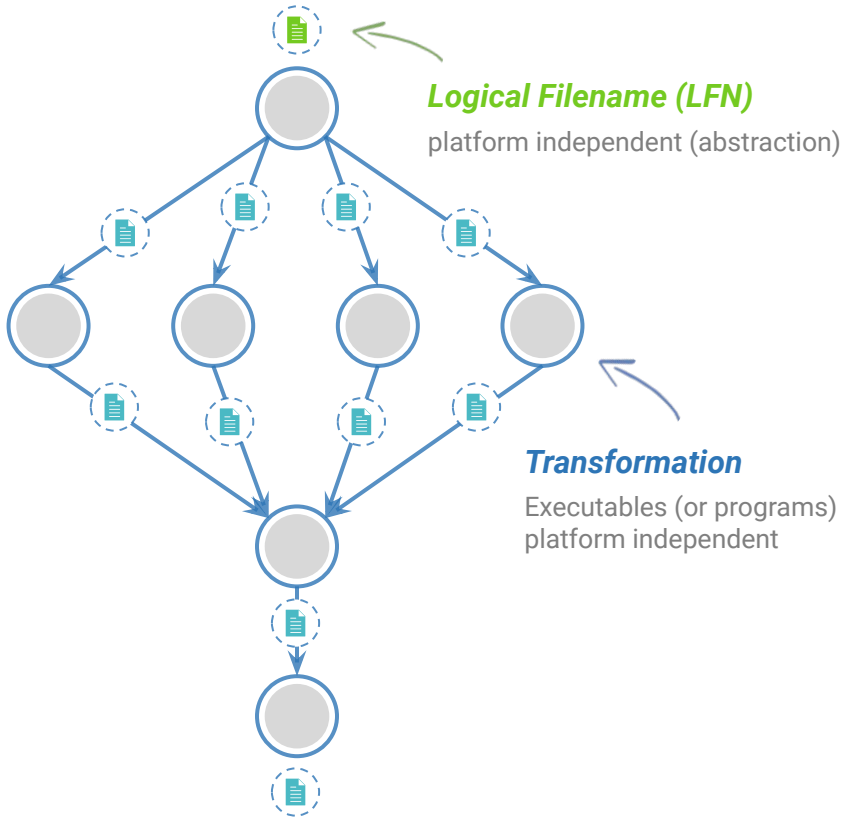
directed-acyclic graphs

Output Workflow

Portable Description

Users do not worry about low level execution details

ABSTRACT WORKFLOW

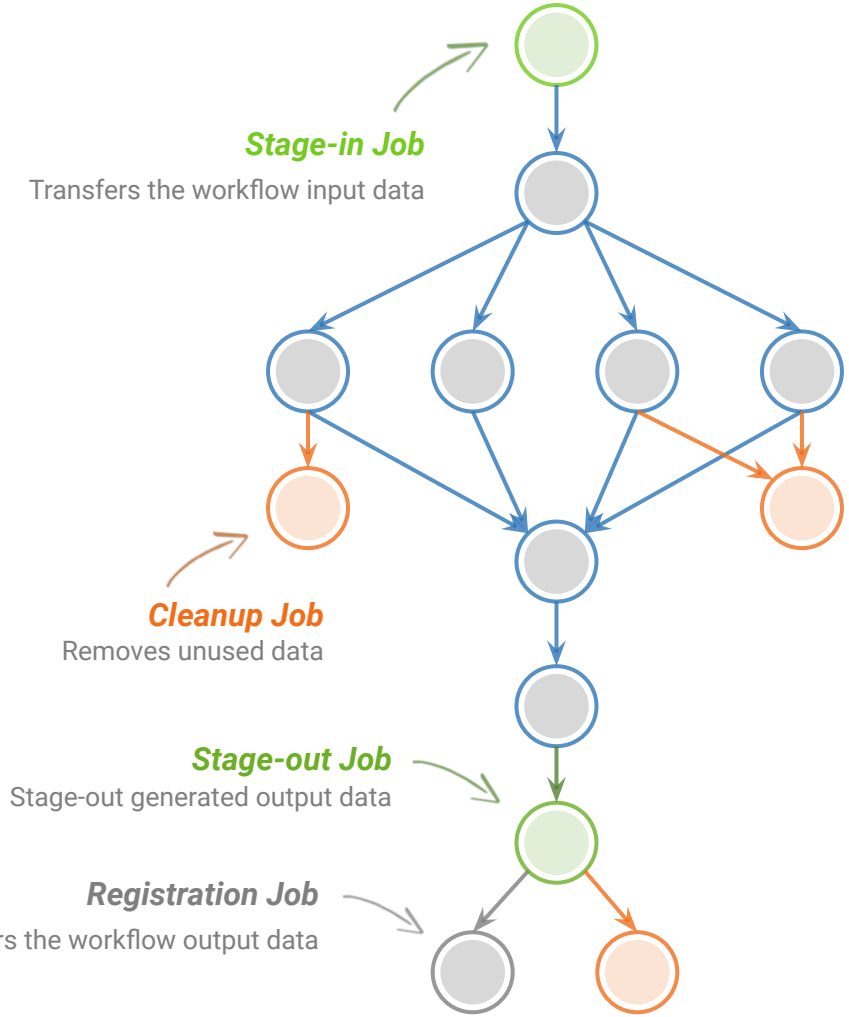


Logical Filename (LFN)

platform independent (abstraction)

Transformation

Executables (or programs)
platform independent



Stage-in Job

Transfers the workflow input data

Cleanup Job

Removes unused data

Stage-out Job

Stage-out generated output data

Registration Job

Registers the workflow output data

EXECUTABLE WORKFLOW

Pegasus Deployment

Workflow Submit Node

- Pegasus WMS
- HTCondor

One or more Compute Sites

- Compute Clusters
- Cloud
- OSG

Input Sites

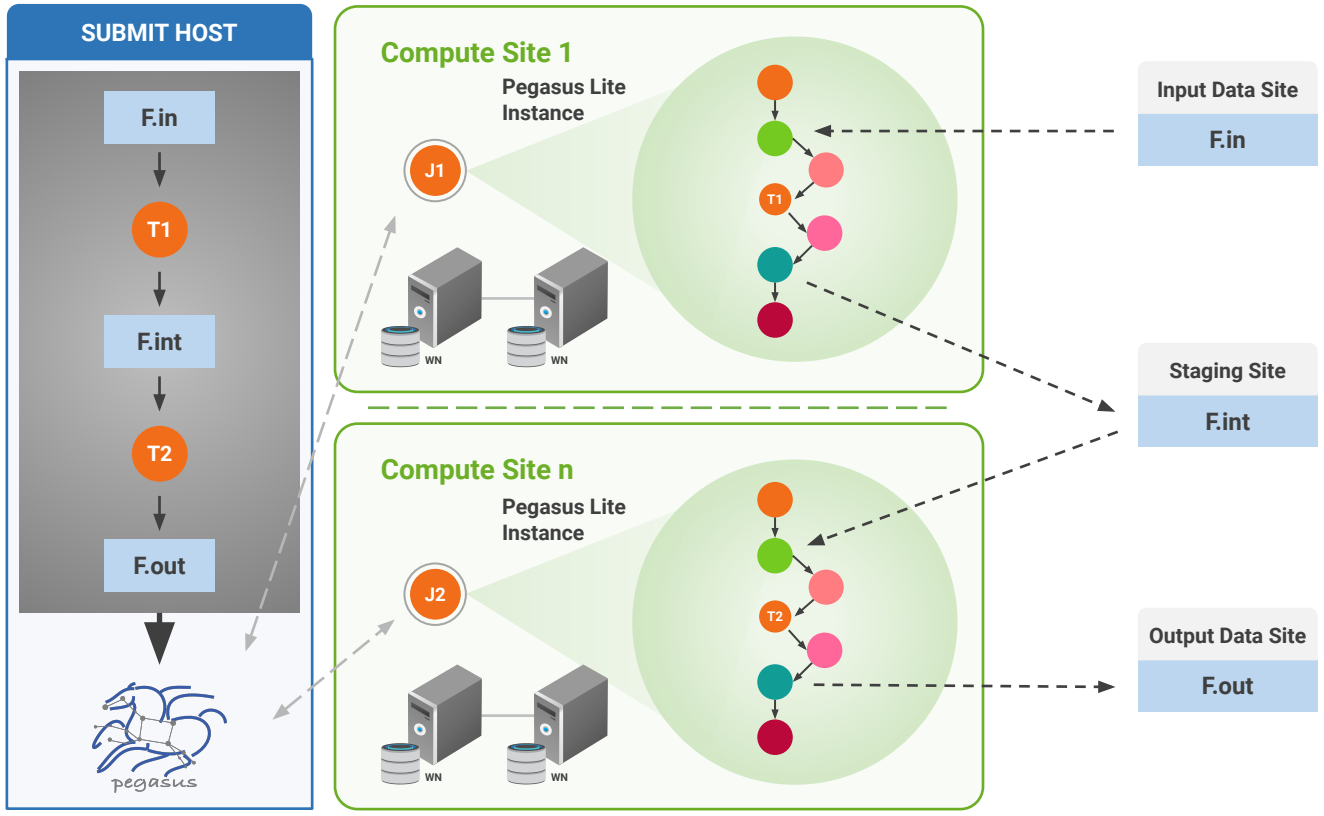
- Host Input Data

Data Staging Site

- Coordinate data movement for workflow

Output Site

- Where output data is placed

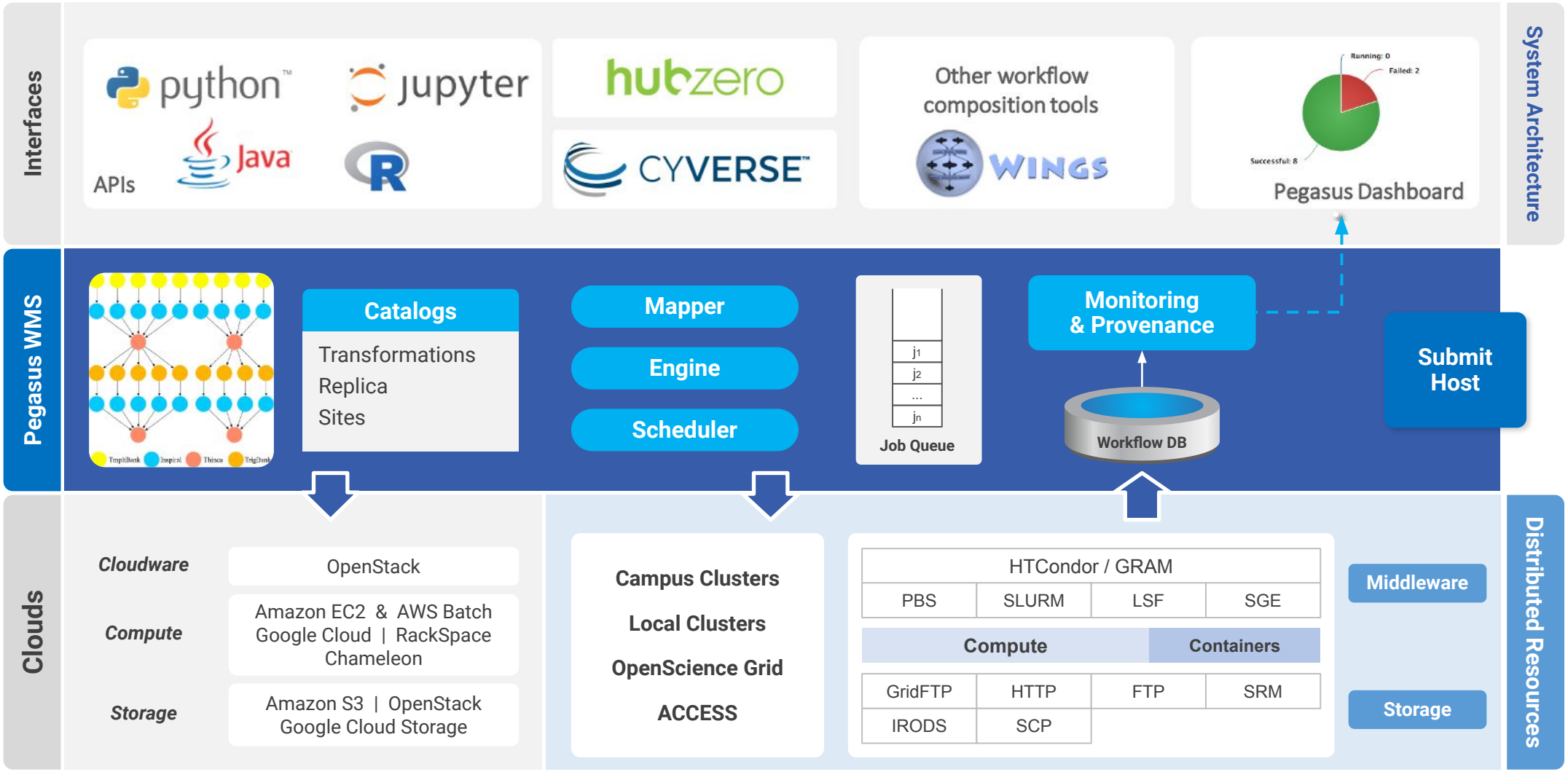


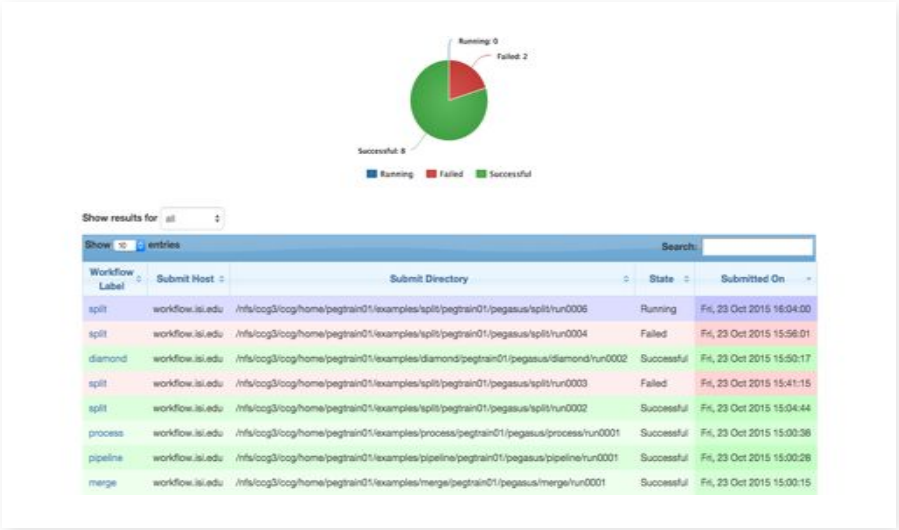
Pegasus-transfer

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
```


Interfaces
python
jupyter
APIs
Java
R
hubzero
CYVERSE
Other workflow composition tools
WINGS
Running: 0
Failed: 2
Successful: 8
Pegasus Dashboard
System Architecture
Pegasus WMS
Catalogs
Transformations
Replica
Sites
Mapper
Engine
Scheduler
j1
j2
...
jn
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
Campus Clusters
Local Clusters
OpenScience Grid
ACCESS
HTCondor / GRAM
PBS
SLURM
LSF
SGE
Compute
Containers
GridFTP
HTTP
FTP
SRM
IRODS
SCP
Middleware
Storage
Distributed Resources

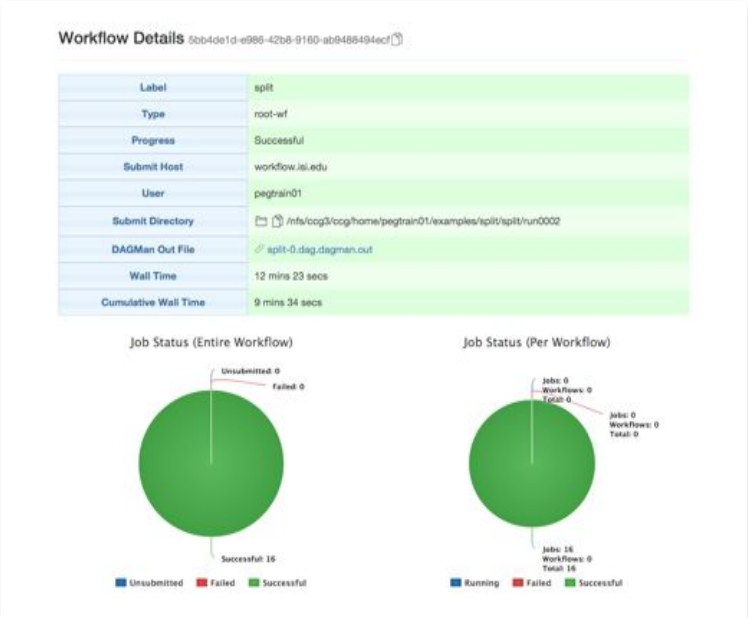


PEGASUS DASHBOARD

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

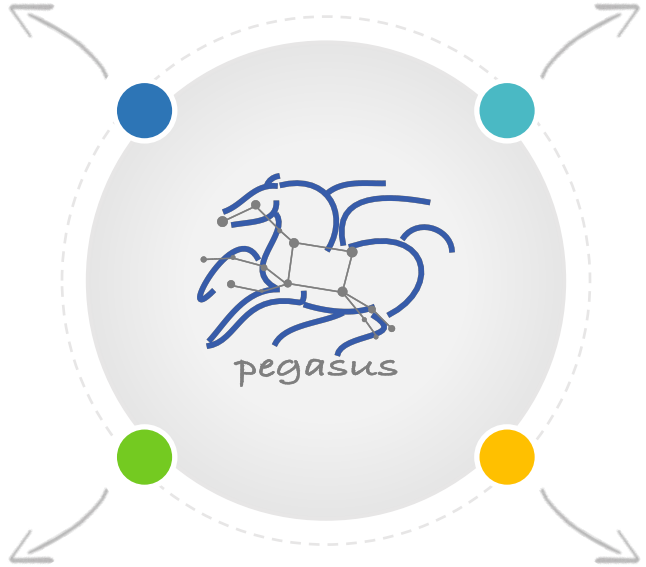
And if a job fails?

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



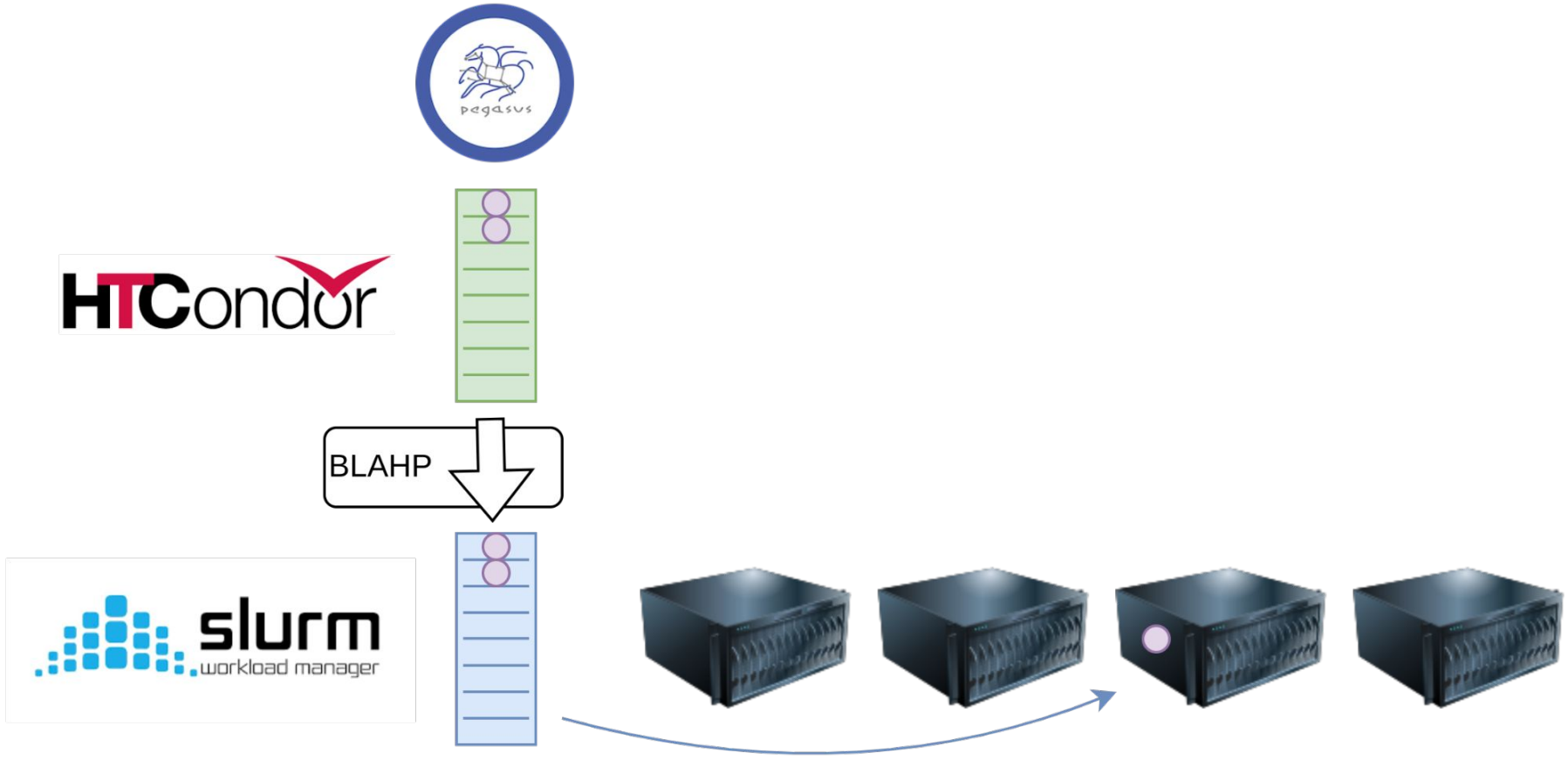
Checkpoint Files

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

HTCondor with BLAHP translation layer

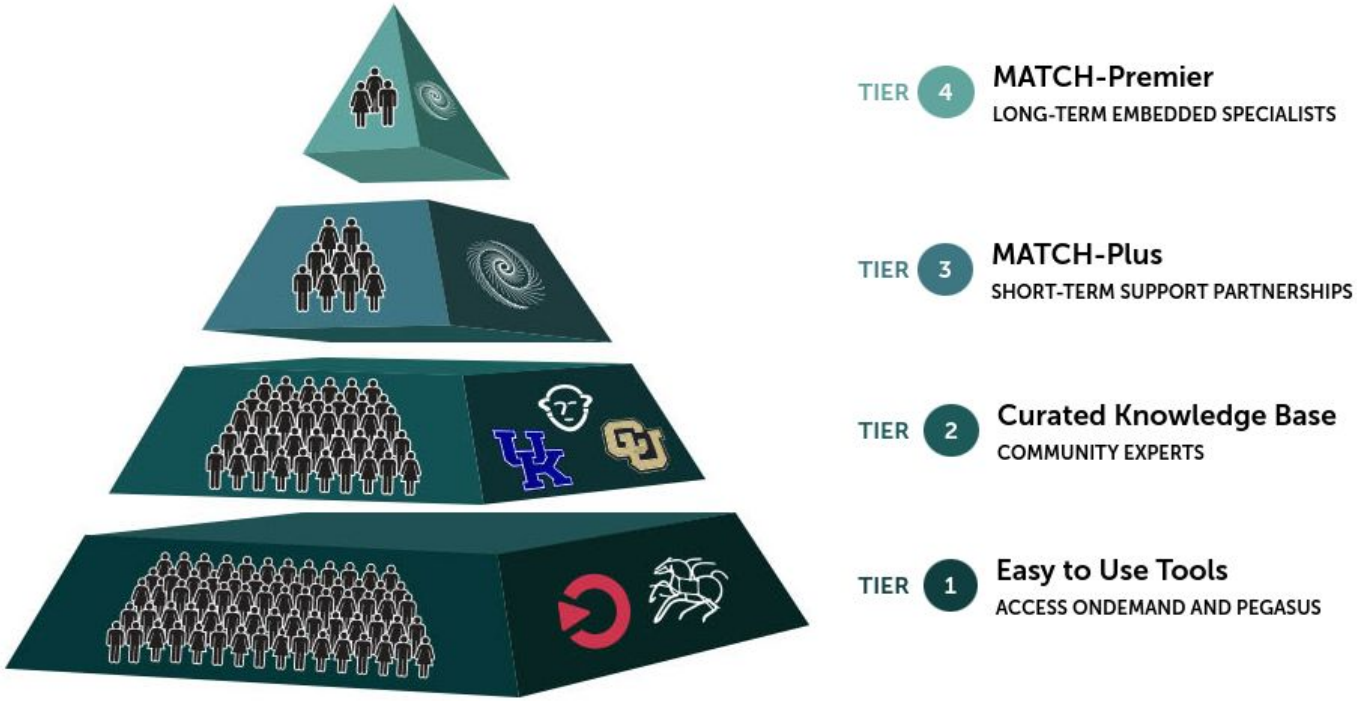


Pegasus is part of the ACCESS support strategy

Pegasus is be used as a tier 1 tool

Central Open OnDemand instance with Pegasus, HTCondor and Jupyter

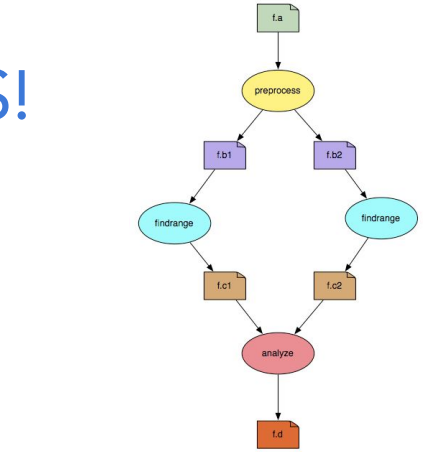
It is be easy to run HTC workflows across ACCESS sites

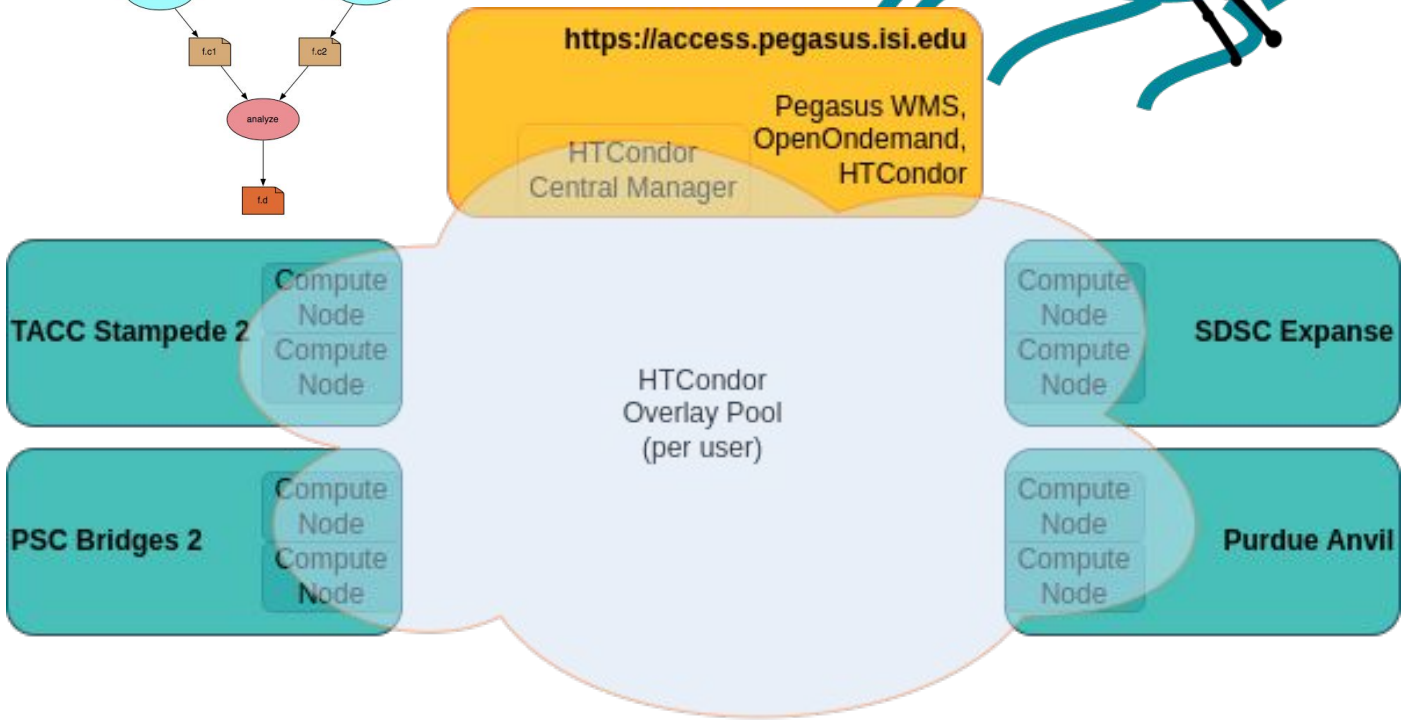


ACCESS Pegasus

Bring your workflows to ACCESS!

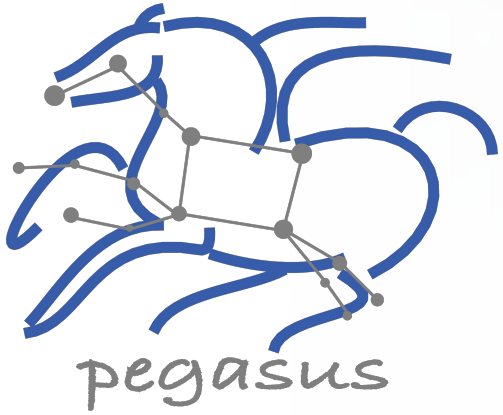
- **Execute scientific workflows across ACCESS resources**
- OpenOnDemand Portal: **has all you need**: Jupyter Notebooks, ACCESS authentication, Pegasus workflow management, and HTCondor job management
- **Bring your own ACCESS capacity**: HTCondor Annex - pilot jobs automatically create a virtual HTCondor pool





https://access.pegasus.isi.edu

More at: support.access-ci.org/pegasus



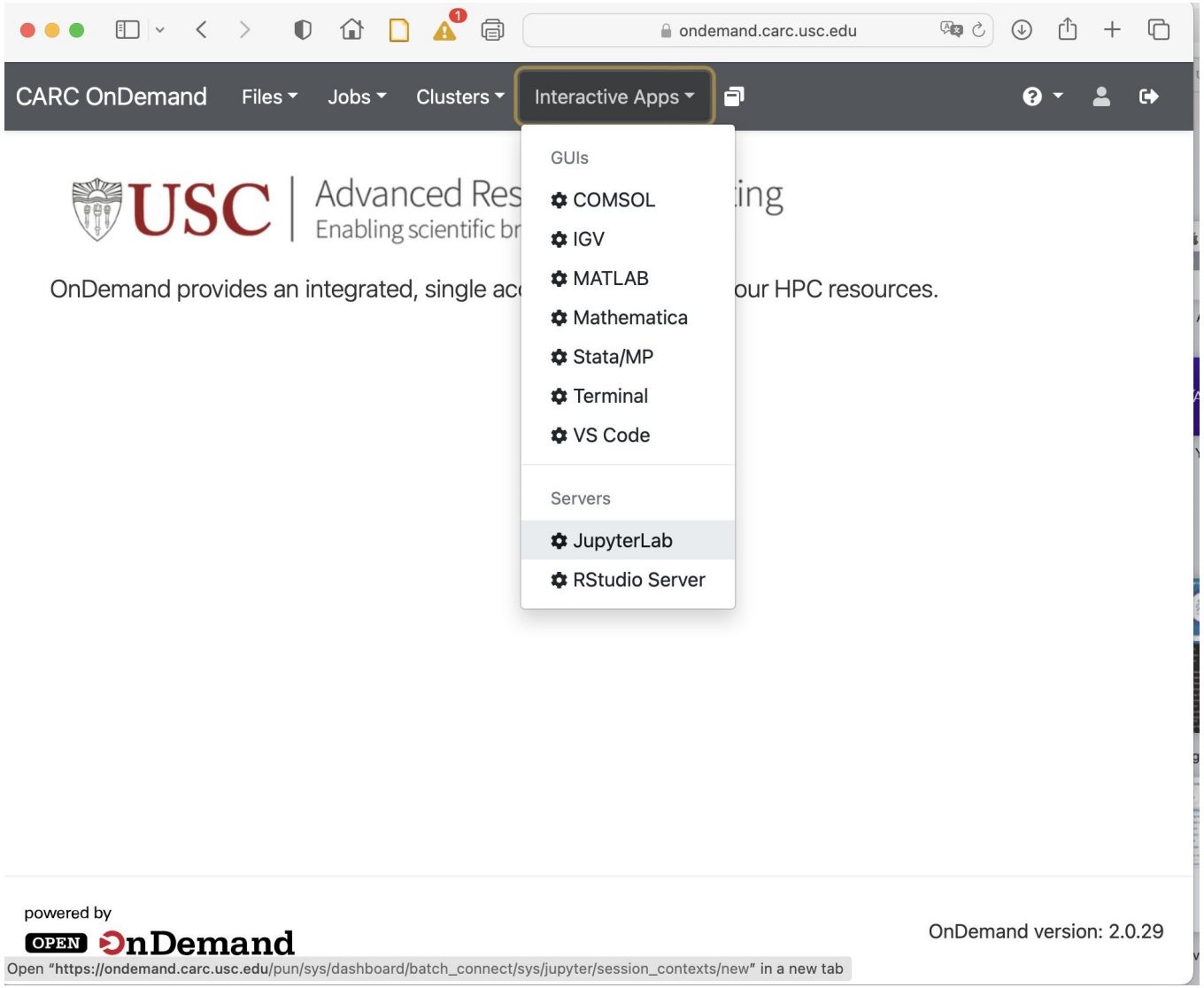
2. Hands on Exercises

Hands on Tutorial Exercises: Login to Open OnDemand

- You need to be on USC Network (USC Secure Wifi or USC VPN) and need to use your USC credentials to log in
- Use a web browser and log on to USC OnDemand Instance at https://ondemand.carc.usc.edu .

Hands on Tutorial Exercises: Start a Jupyter Server

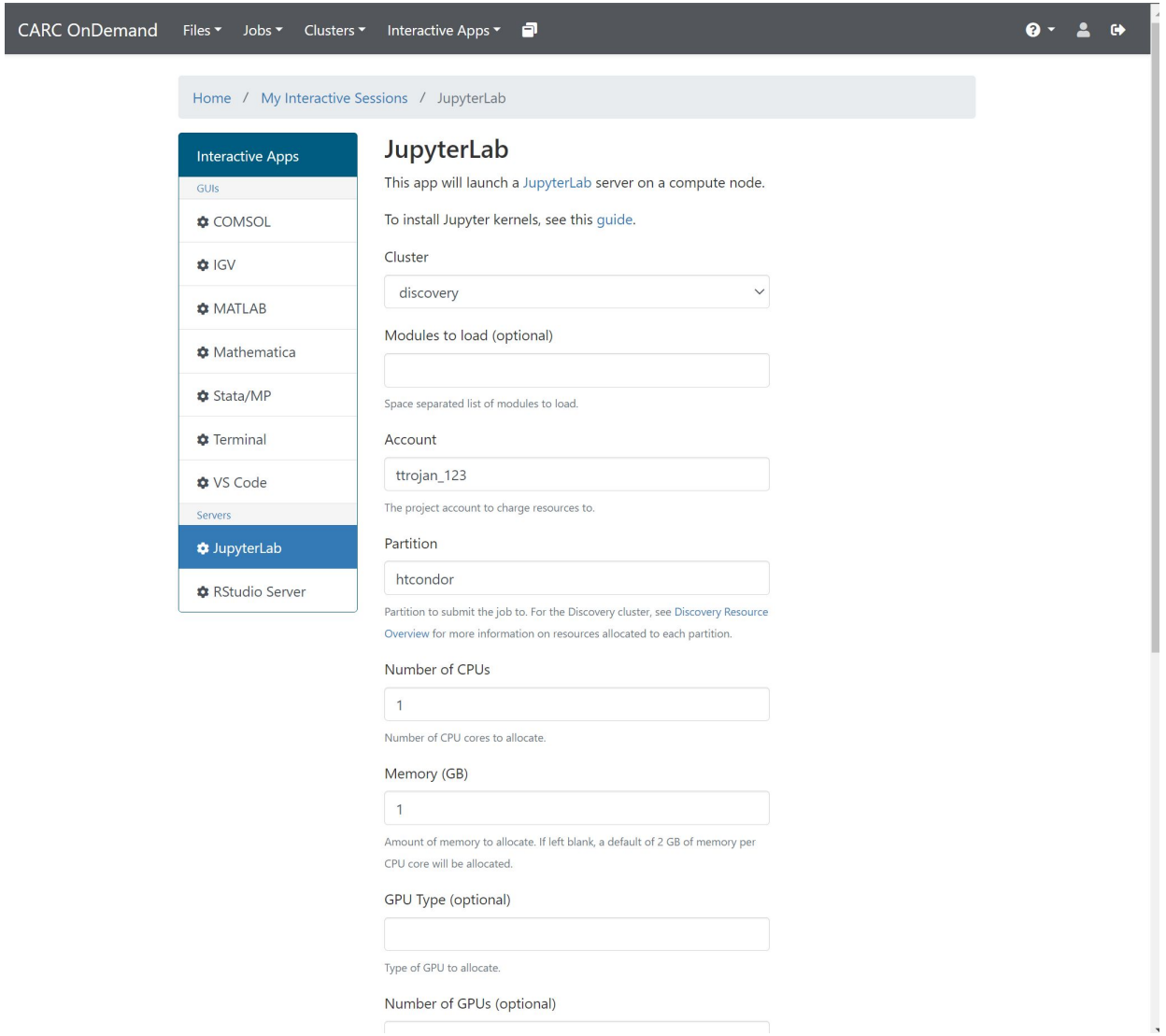
- Start a Jupyter notebook server, Click on Interactive Apps and then select JupyterLab



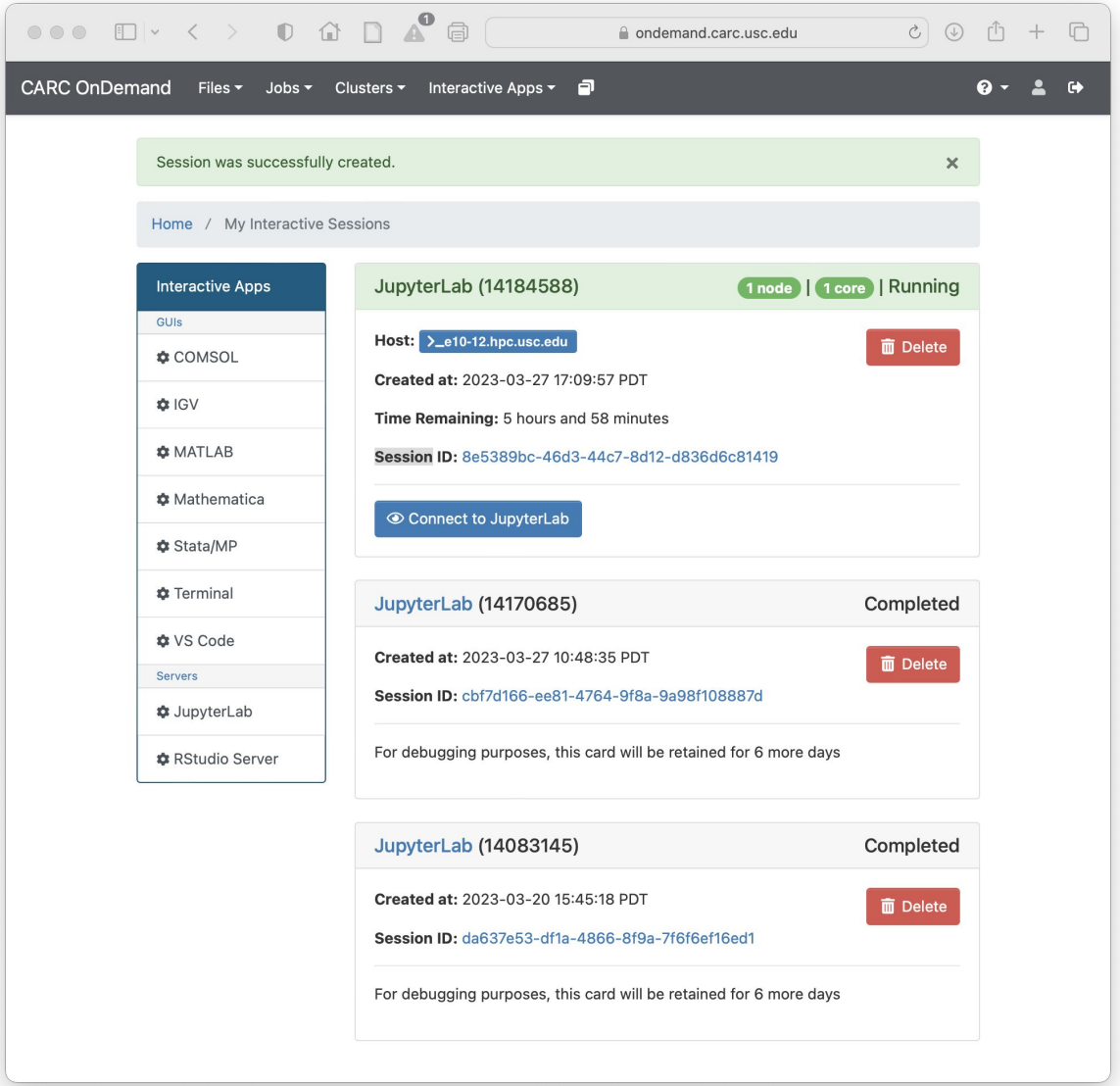
Hands on Tutorial Exercises: Jupyter Lab Configuration

- When launching the Jupyter Lab, it is important to select the following
- For Cluster: specify Discovery
- For Account: specify the account osinski_982 *
- For Partition specify htcondor

*The account is workshop specific and will be active for **7 days** after the workshop

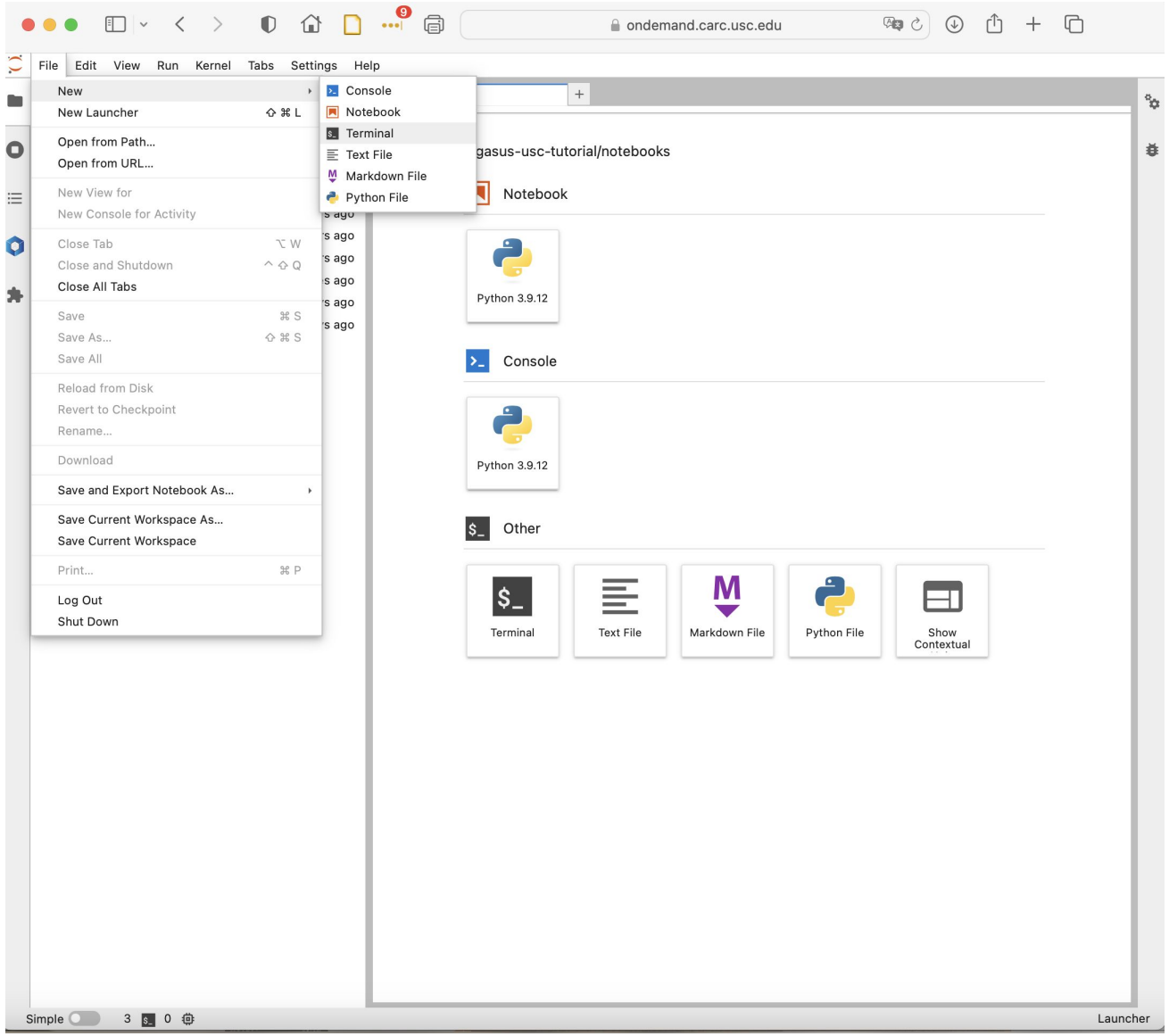


Hands on Tutorial Exercises: Connect to JupyterLab



Hands on Tutorial Exercises: Start a Terminal

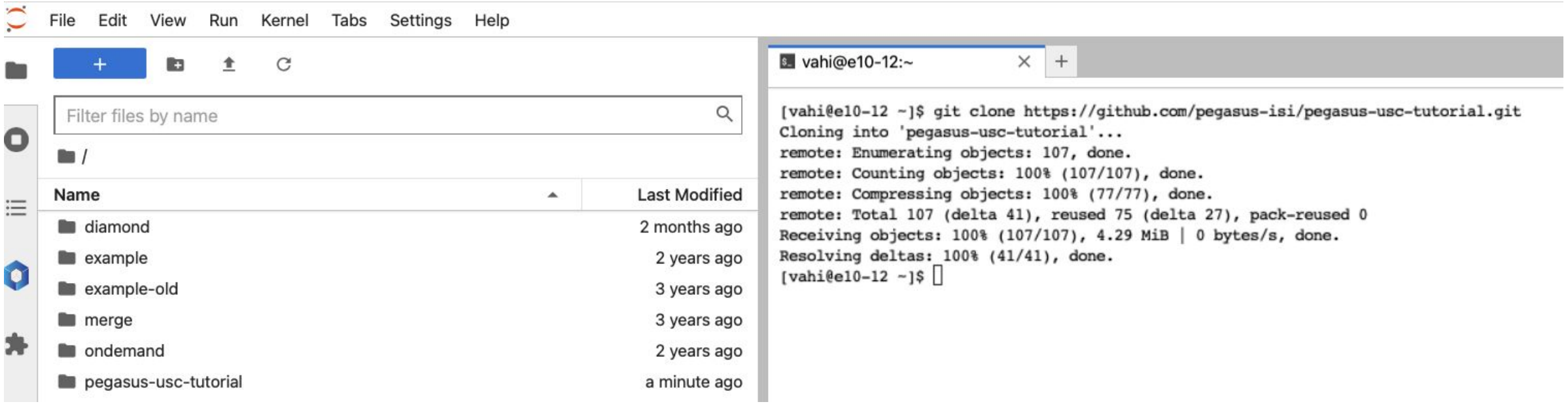
- In JupyterLab, Click on File -> New and then click on Terminal to get the terminal
-



Hands on Tutorial Exercises: Clone Repository

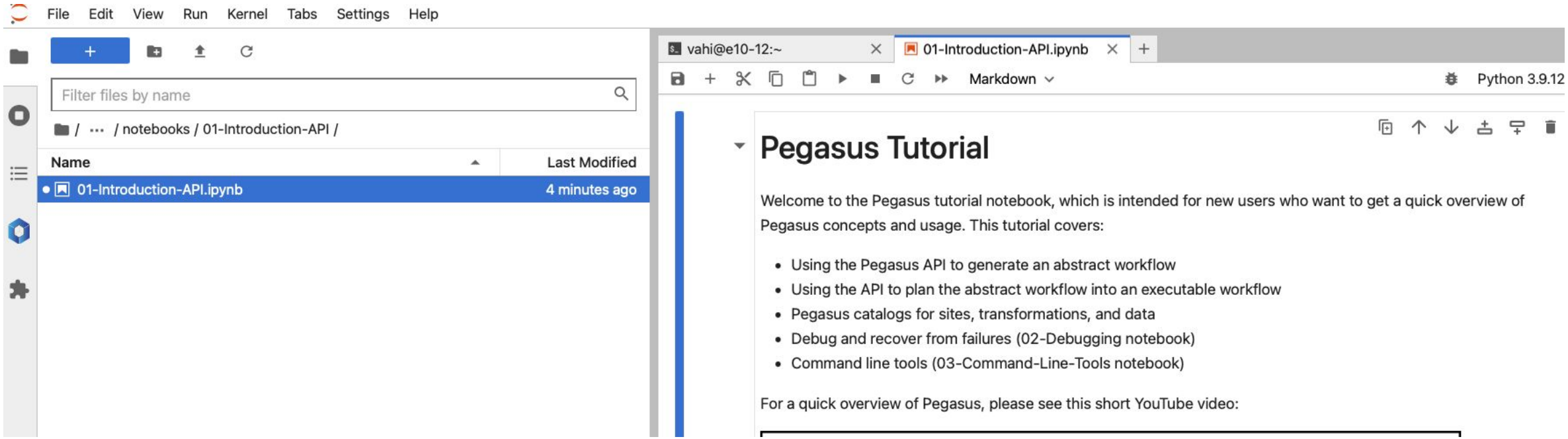
- Clone Tutorial Repository in the terminal

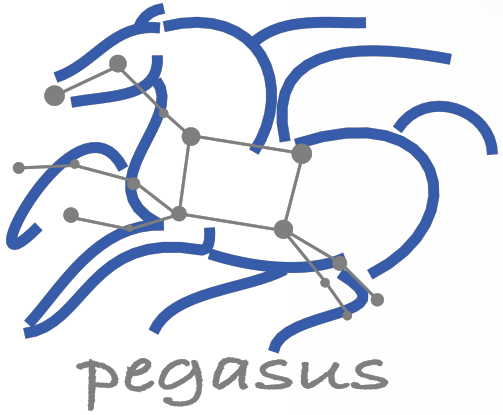
  git clone https://github.com/pegasus-isi/pegasus-usc-tutorial.git



Hands on Tutorial Exercises: Navigate to Notebooks

- In Jupyter, navigate to the example you are interested in, and step through the notebook.
- For first time users, we highly recommend to do the notebooks in order, as they build up on concepts in the previous notebooks.

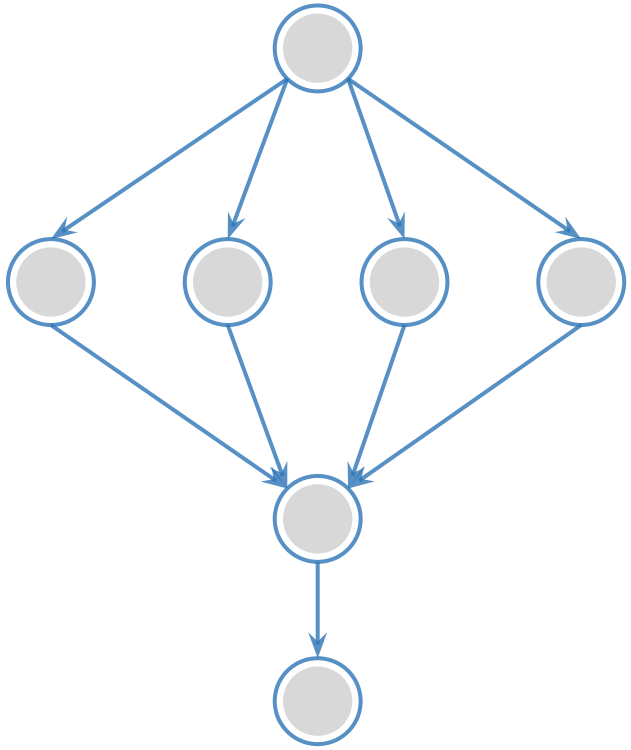




2.1 API

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



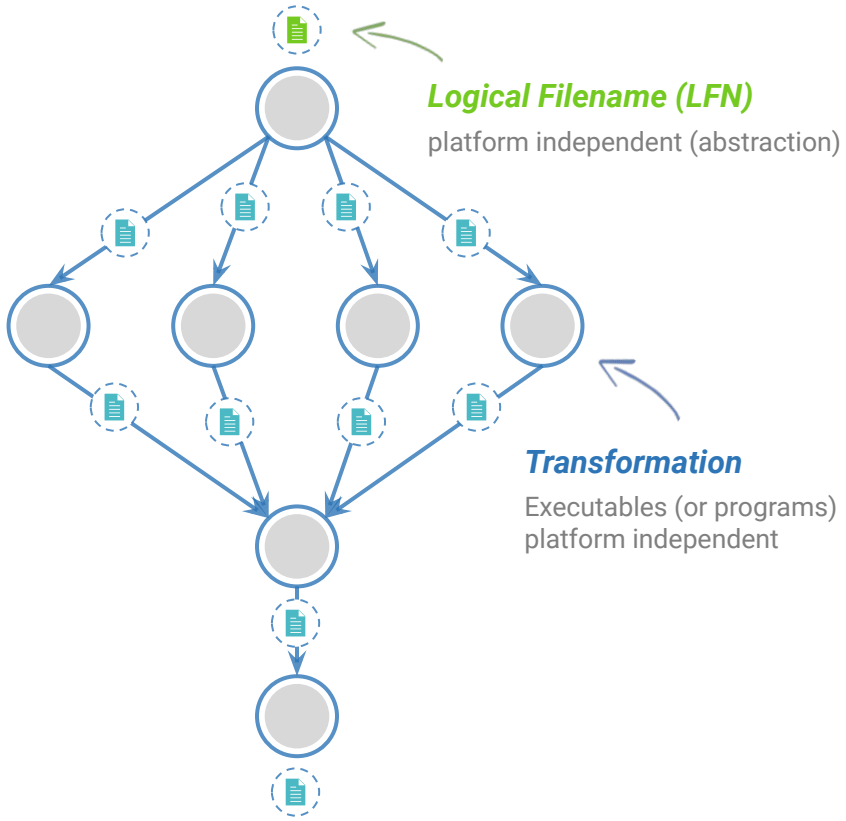
Input Workflow Specification YAML formatted

directed-acyclic graphs Output Workflow

Portable Description

Users do not worry about low level execution details

ABSTRACT WORKFLOW

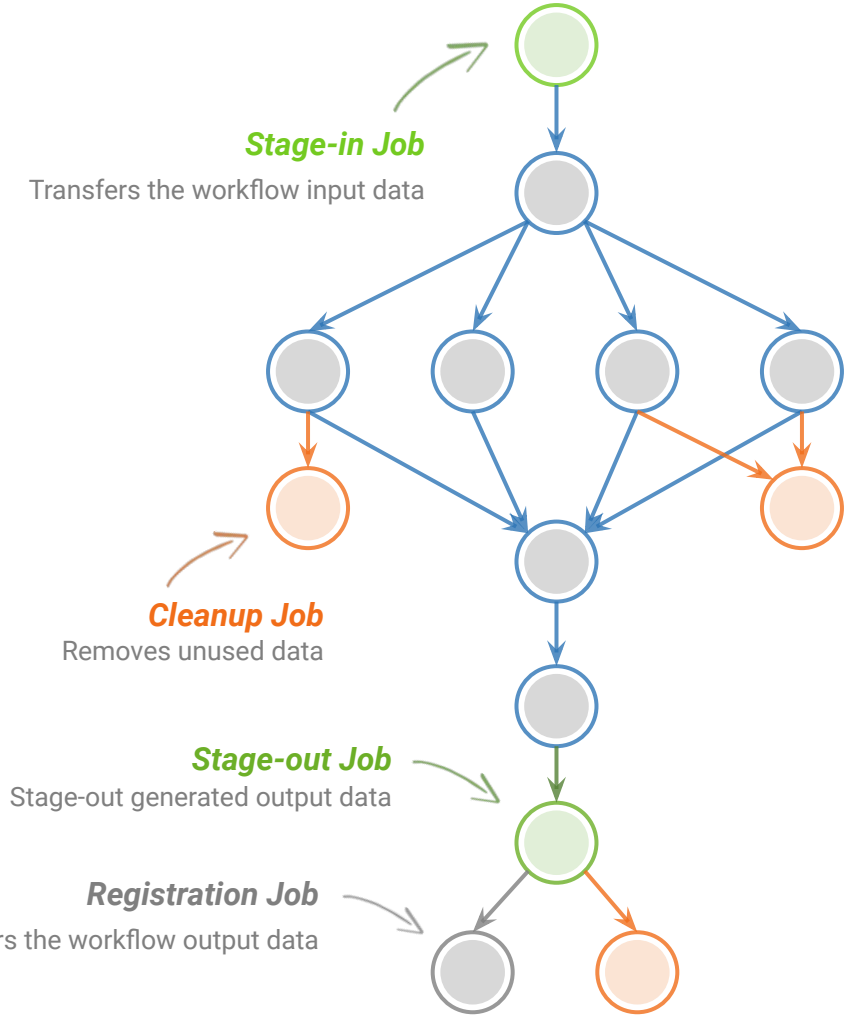


Logical Filename (LFN)

platform independent (abstraction)

Transformation

Executables (or programs)
platform independent



Stage-in Job

Transfers the workflow input data

Cleanup Job

Removes unused data

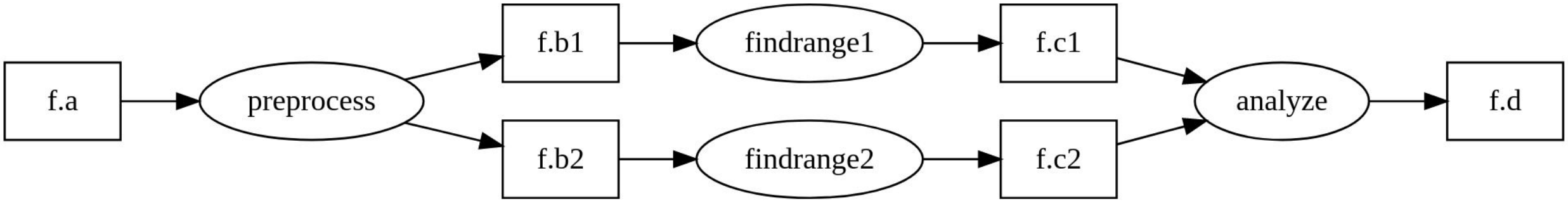
Stage-out Job

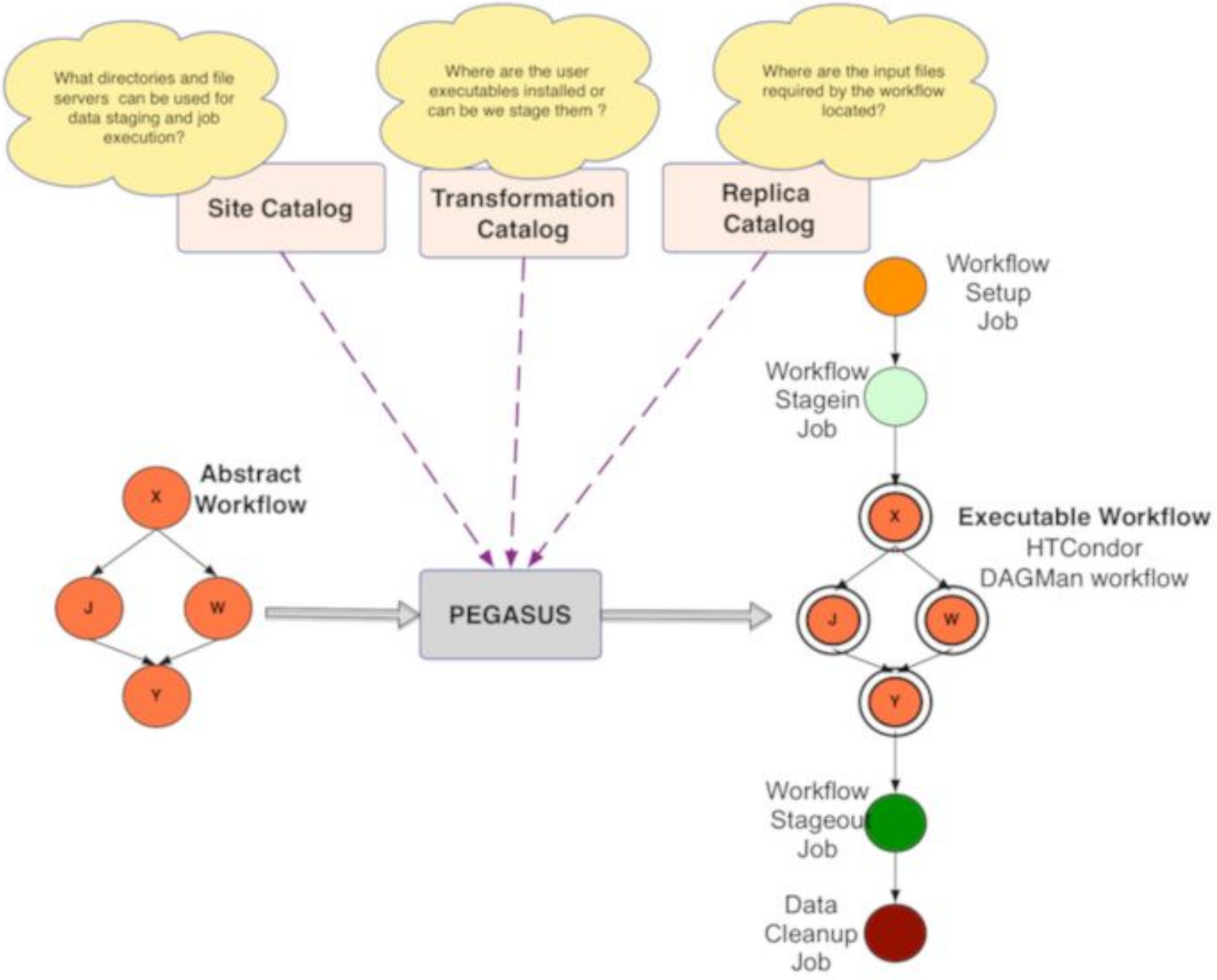
Stage-out generated output data

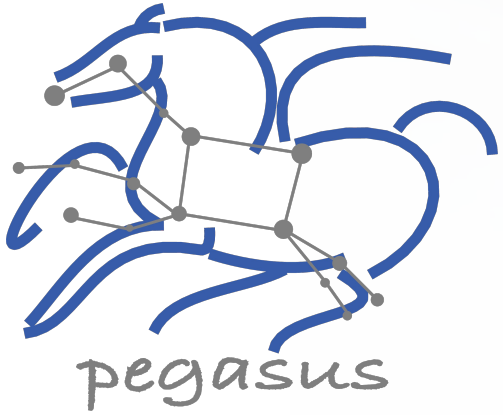
Registration Job

Registers the workflow output data

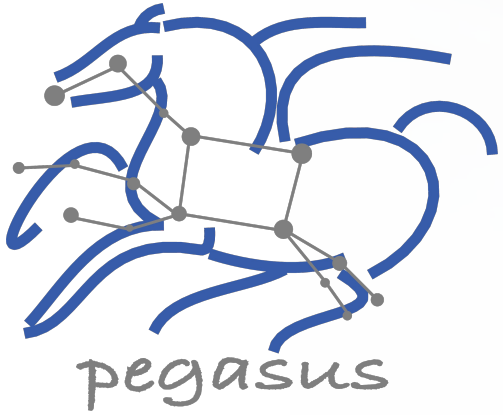
EXECUTABLE WORKFLOW


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
Workflow Stageout Job
Data Cleanup Job



2.2 Debugging



2.3 Command Line Tools

Pegasus Container Support

Pegasus

docker SHIFTER

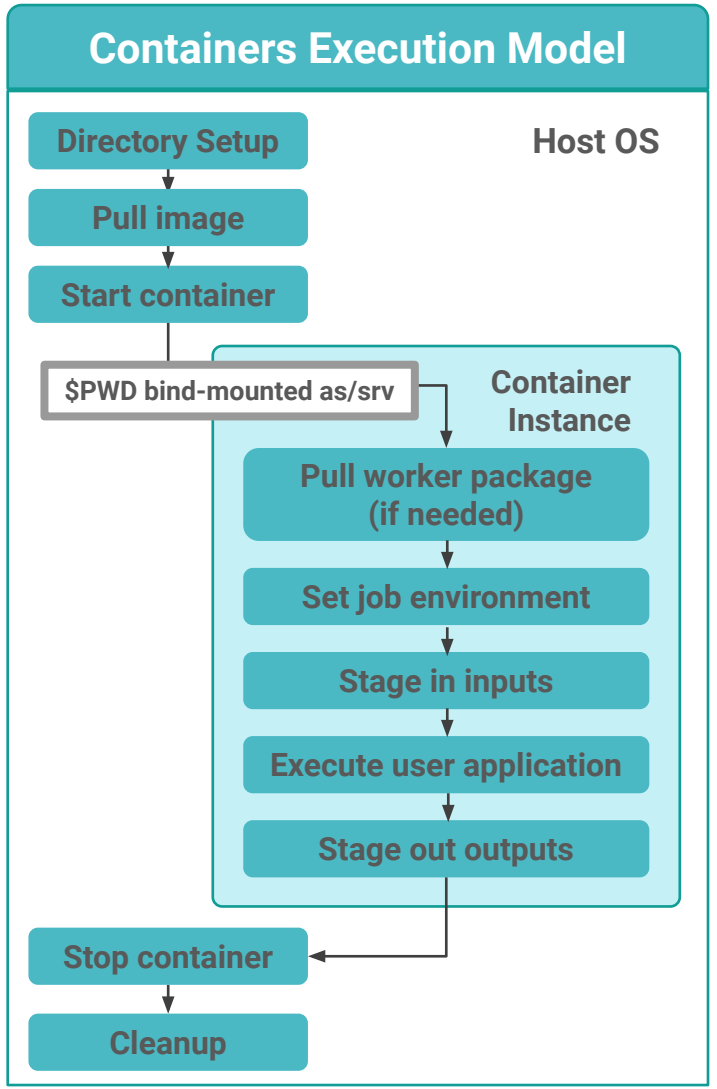
Users can refer to **containers** in the **Transformation Catalog** with their executable preinstalled

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

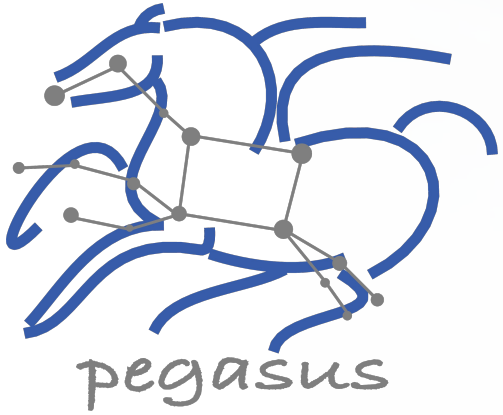
- Staged to compute node if not present
- Docker or Singularity Hub URL's
- Docker Image exported as a TAR file and available at a server, just like any other input dataset

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



2.4 Variant Calling Workflow

Genomics Analysis on HPC cluster

Not only GUI applications

Three reasons why a lot of genomics analysis is done using command-line tools:

- a large number of files - the command-line allows you to automate repetitive tasks,
- more compute power than is available on your local computer - remote computers require a command-line interface
- custom analyses - command-line tools often enable more customization than the corresponding GUI tools (if in fact a GUI tool even exists)

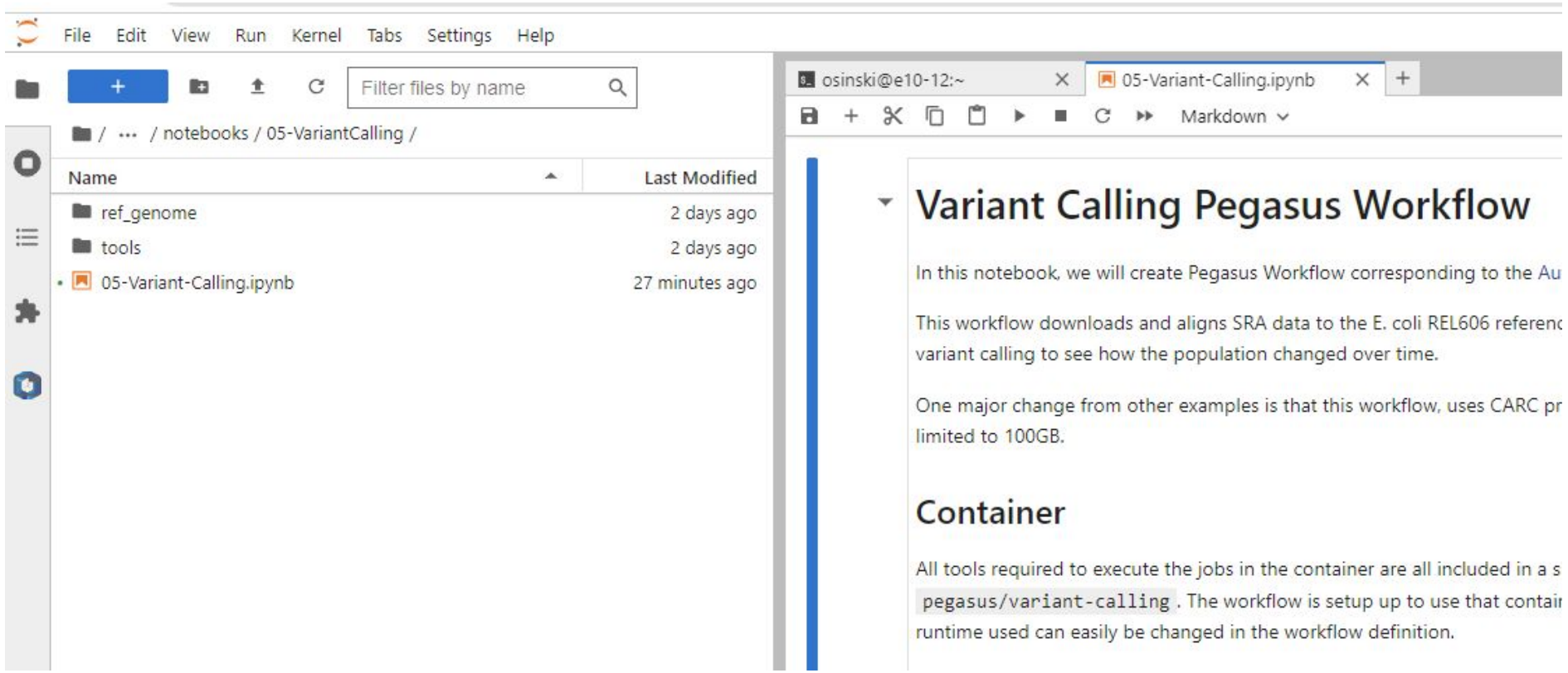
The tools used in example:

- Burrows-Wheeler Aligner (BWA) 0.7.17
- SamTools 1.15.1
- Bcftools 1.15.1
- HTSlib 1.15.1
- SRA Tools 3.0.0

Genomics Analysis on HPC cluster

Example: Variant Calling

Navigate in the file manager on the left and double-click the notebook to start:



Genomics Analysis on HPC cluster

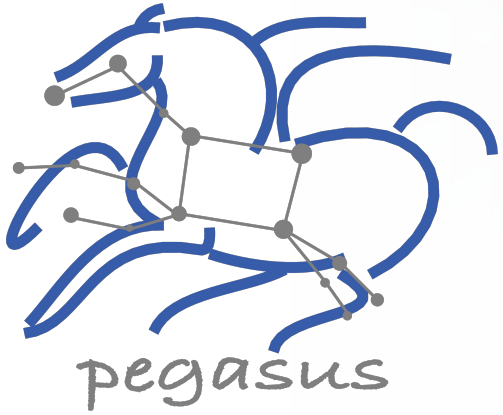
Example: Variant Calling

Reference genome: Escherichia coli B strains REL606 (ecoli_rel606)

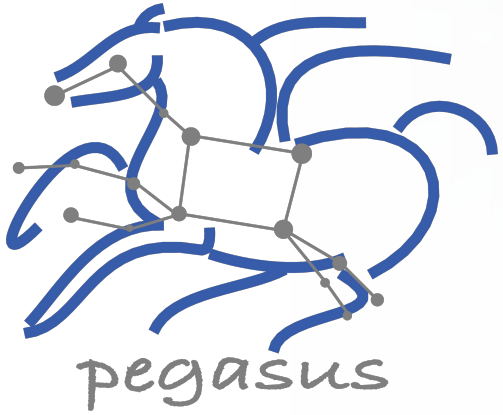
SRA data: SRR2584866, SRR2589044

Tasks performed:

```
fasterq-dump –split-files sra_id
bwa mem genome fastq_1 fastq_2 > sam_file
samtools view -S -b sam_file> > bam_file
samtools sort -o sorted_bam bam_file
samtools index sorted_bam
bcftools mpileup -O b -o raw_bcf -f genome sorted_bam
bcftools call --ploidy 1 -m -v -o variants raw_bcf
vcfutils.pl varFilter variants > final_variants
```



2.5 Summary



3. Advanced Topics

Data Staging Configurations

HTCondor I/O (HTCondor pools, OSG, …)

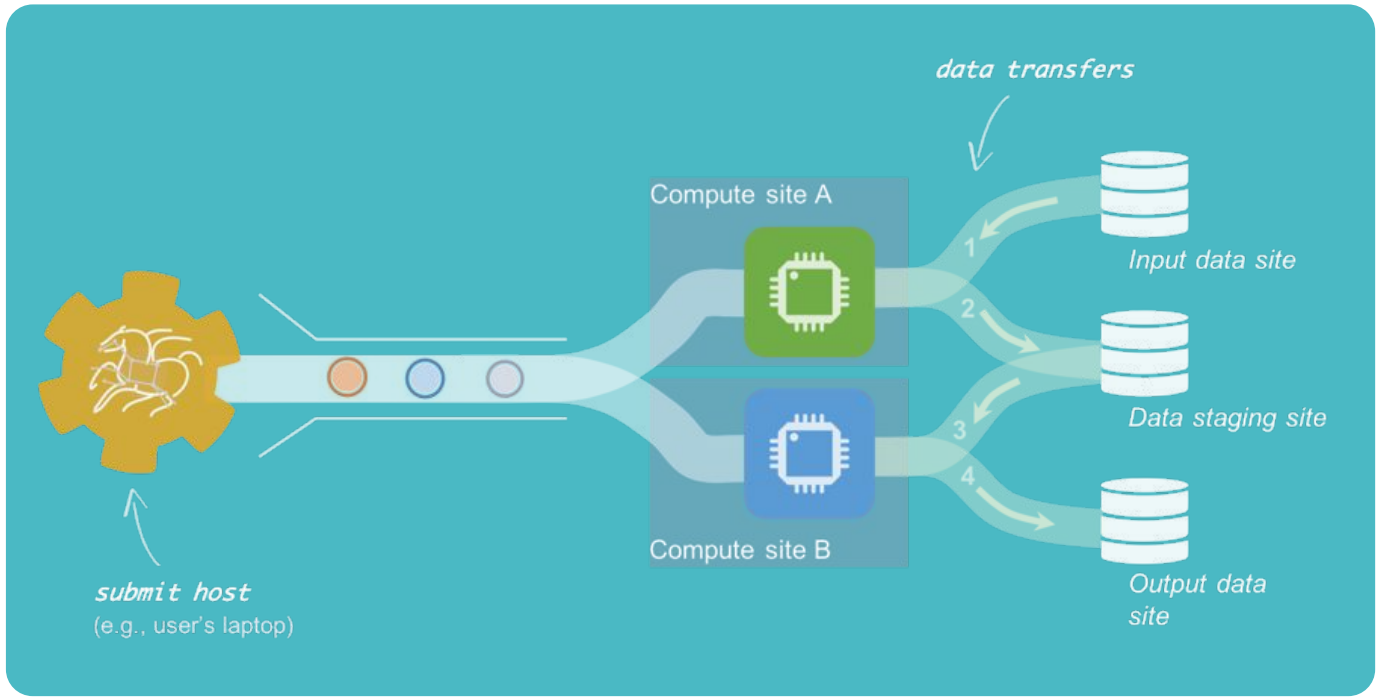
- Worker nodes do not share a file system
- Data is pulled from / pushed to the submit host via HTCondor file transfers
- Staging site is the submit host

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

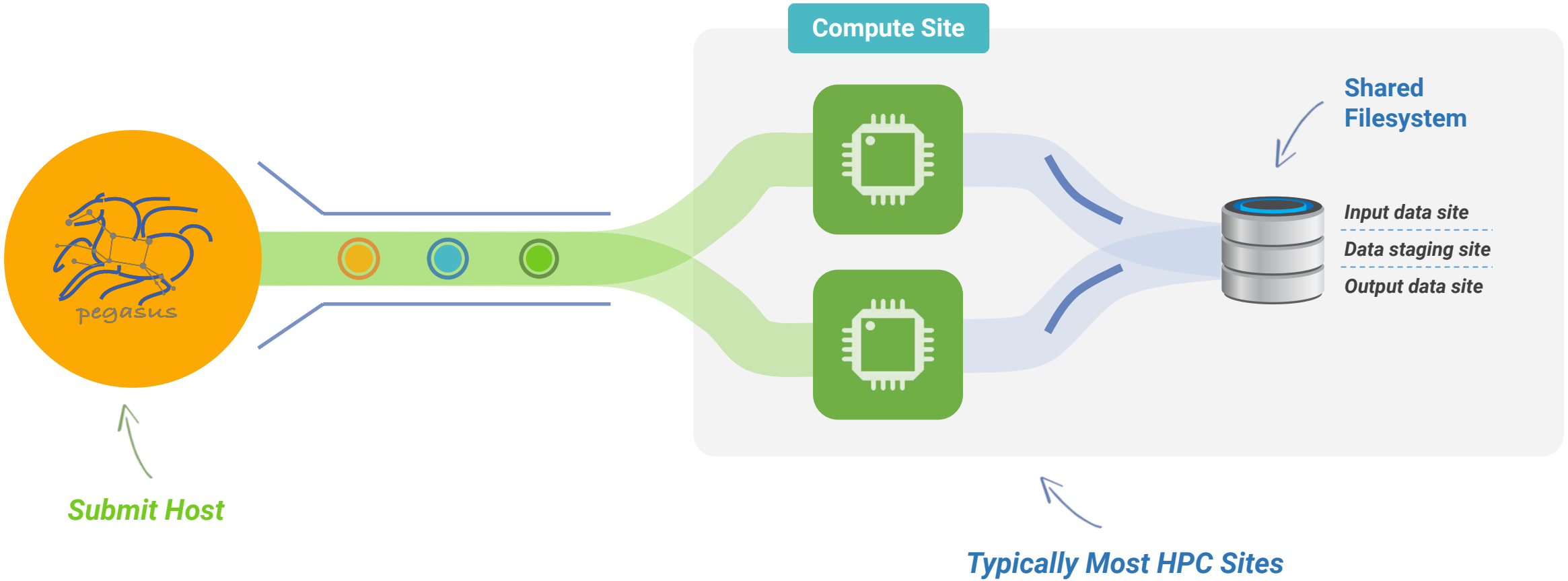
Shared File System (HPC sites, XSEDE, Campus clusters, …)

- I/O is directly against the shared file system



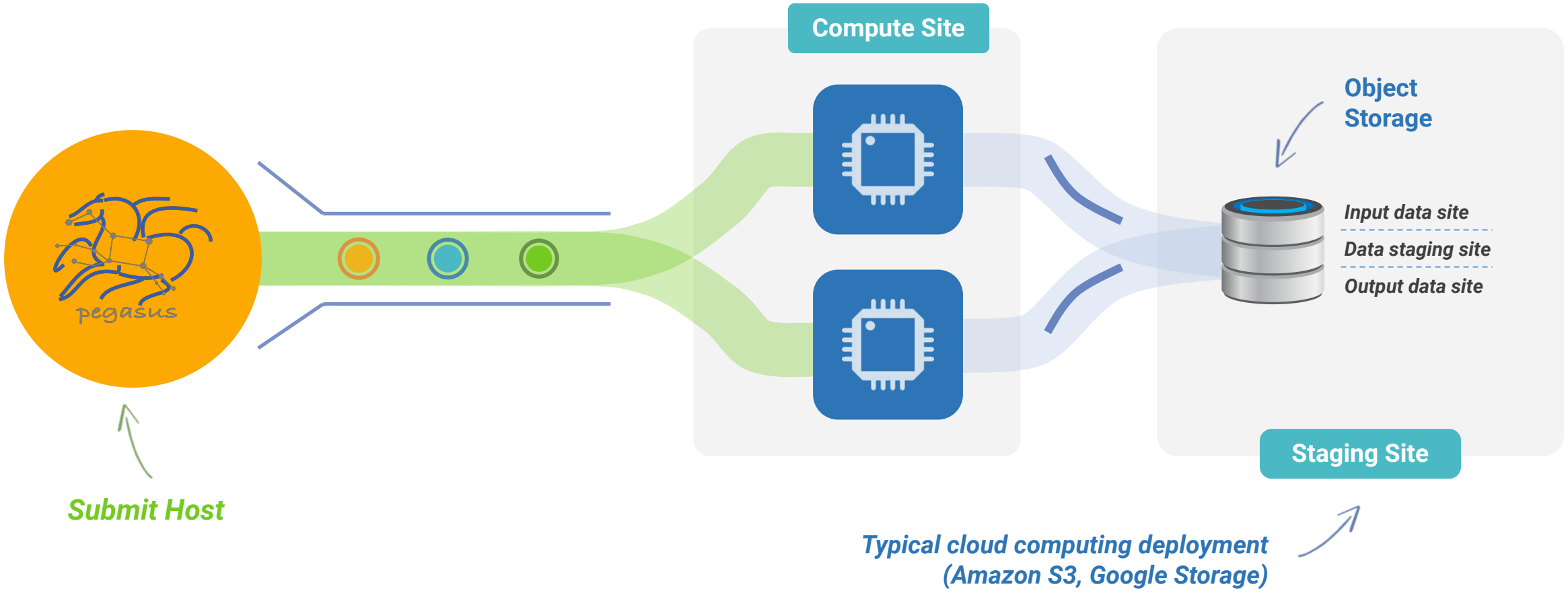
High Performance Computing

There are several possible configurations…



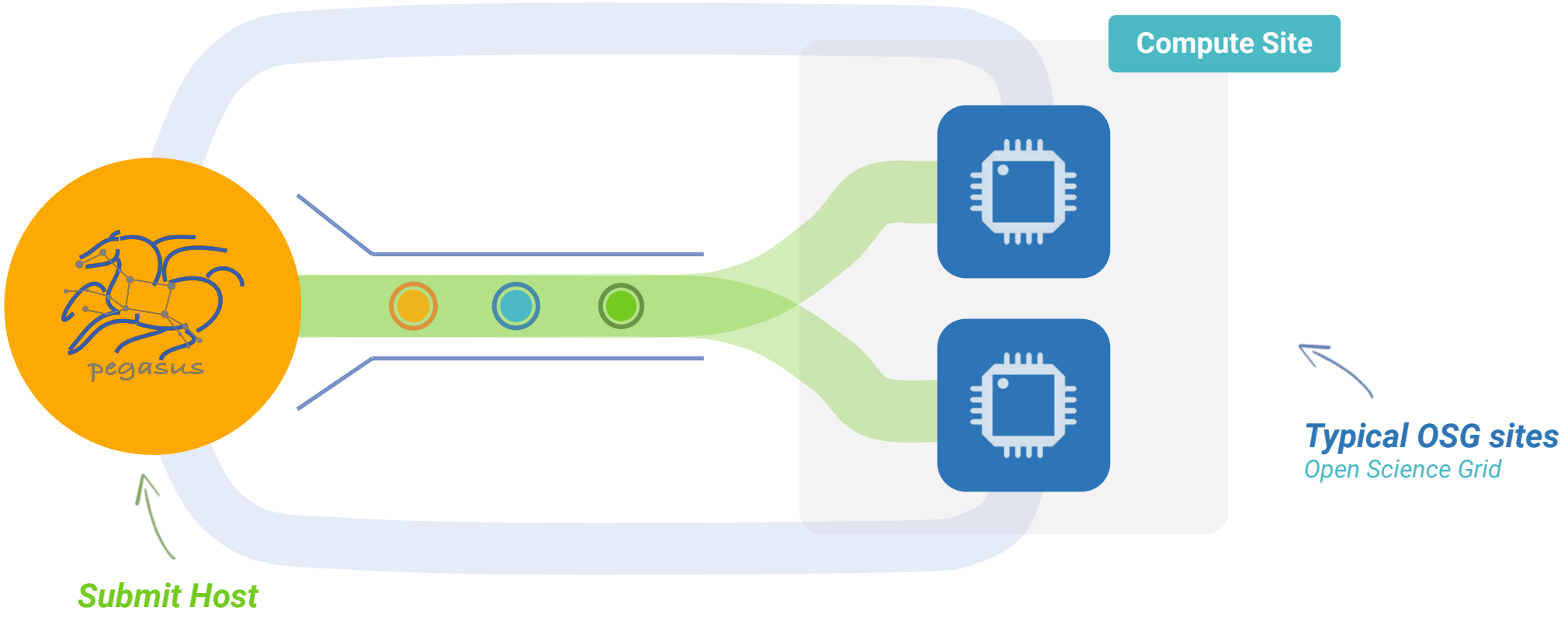
Cloud Computing

High-scalable object storages

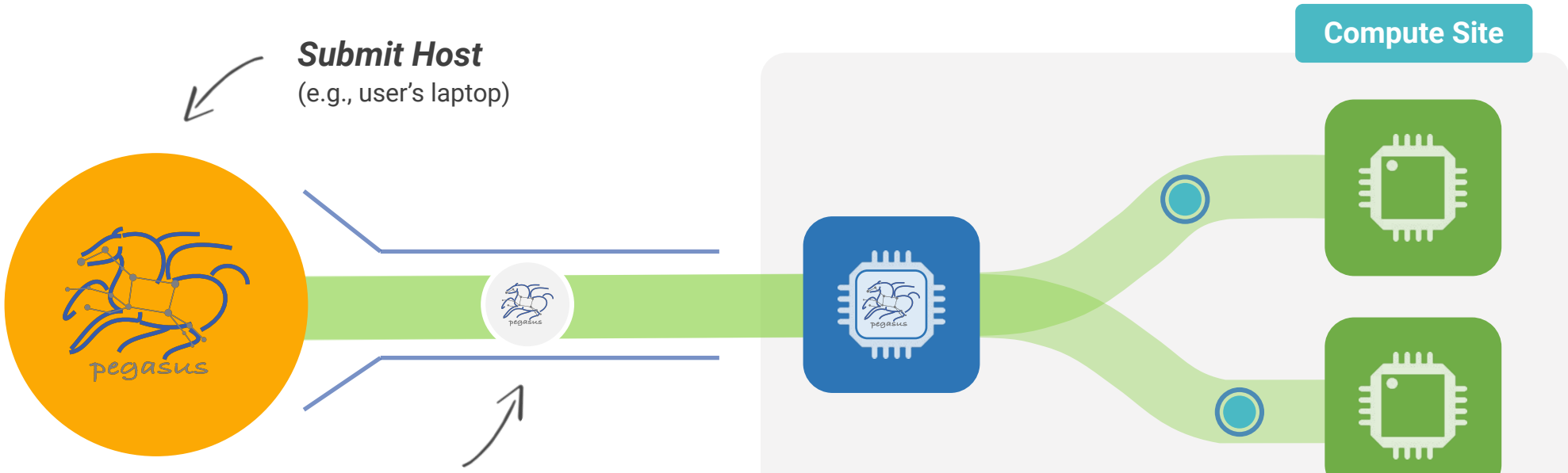


Grid Computing

Local data management

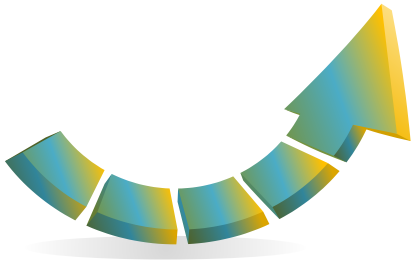


Running fine-grained workflows on HPC systems…

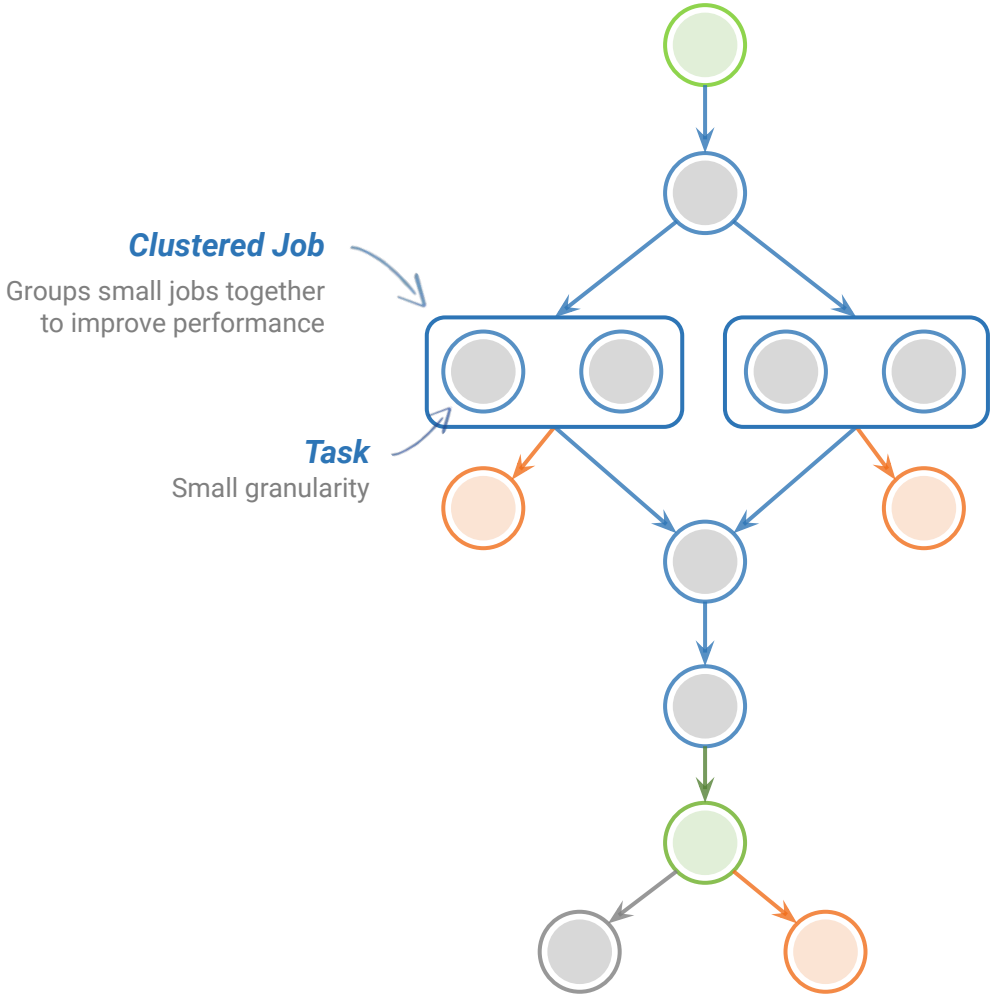


Workflow wrapped as an MPI job

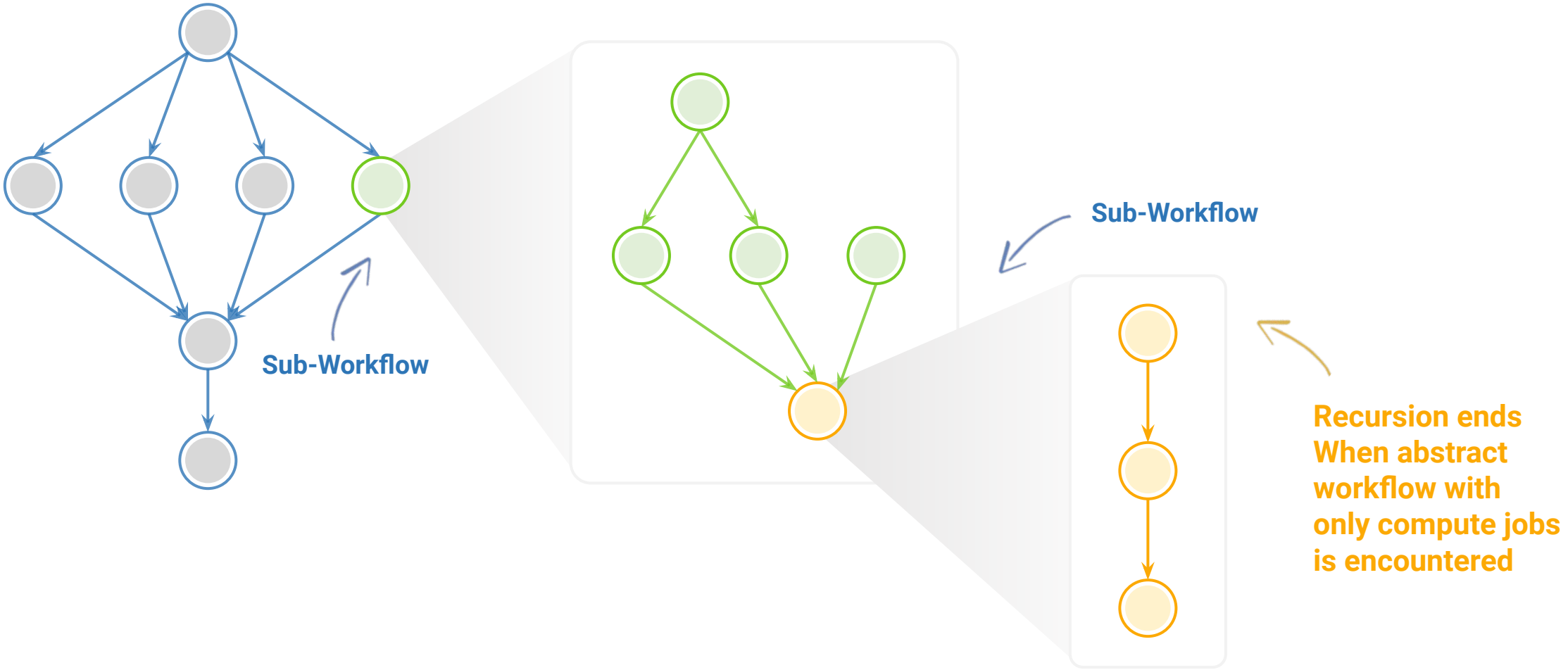
Allows sub-graphs of a Pegasus workflow to be submitted as monolithic jobs to remote resources



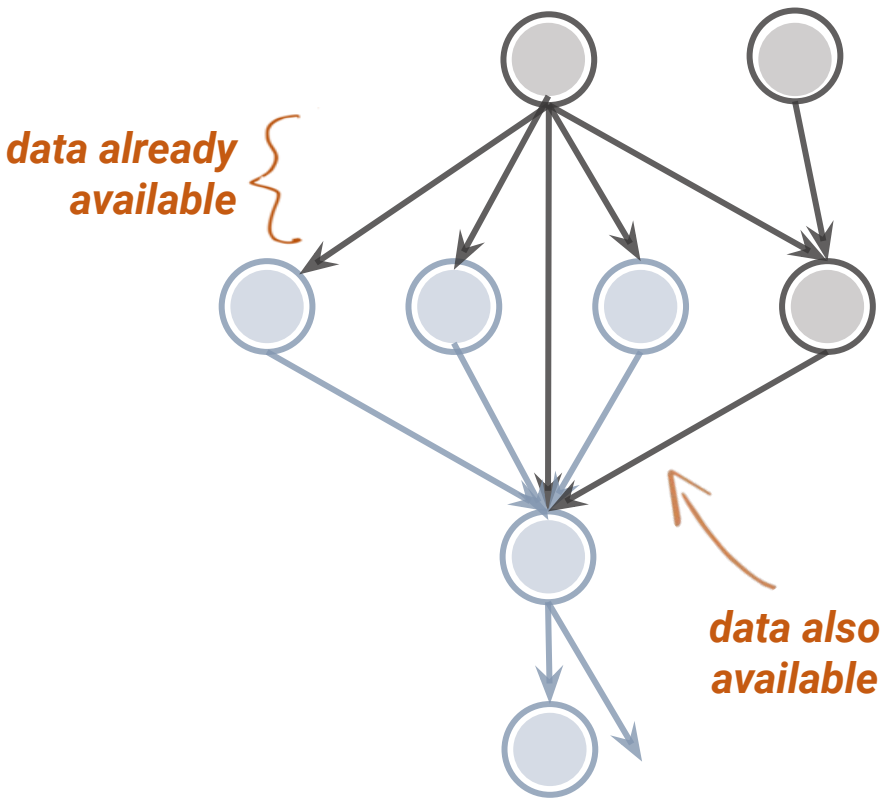
Performance.
Why not improve it?



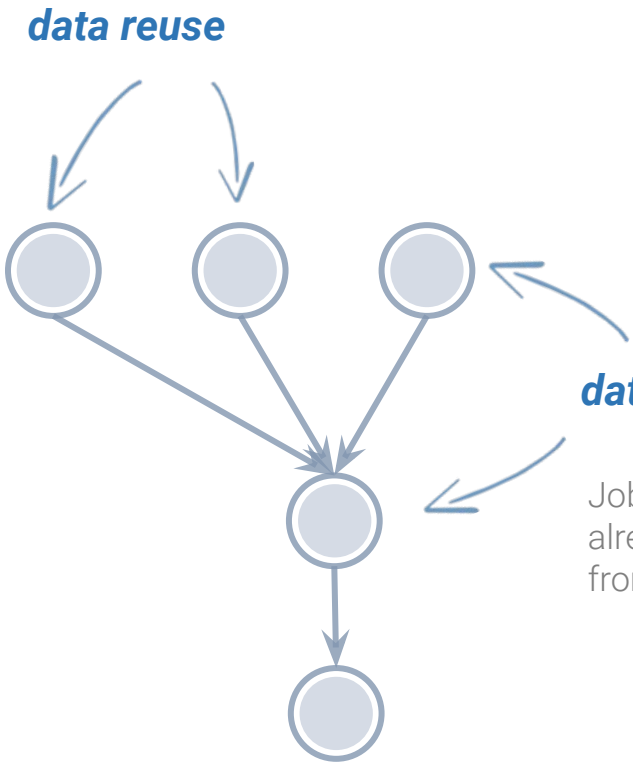
Pegasus also handles large-scale workflows



Data Reuse prune jobs if output data already exists



workflow reduction



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

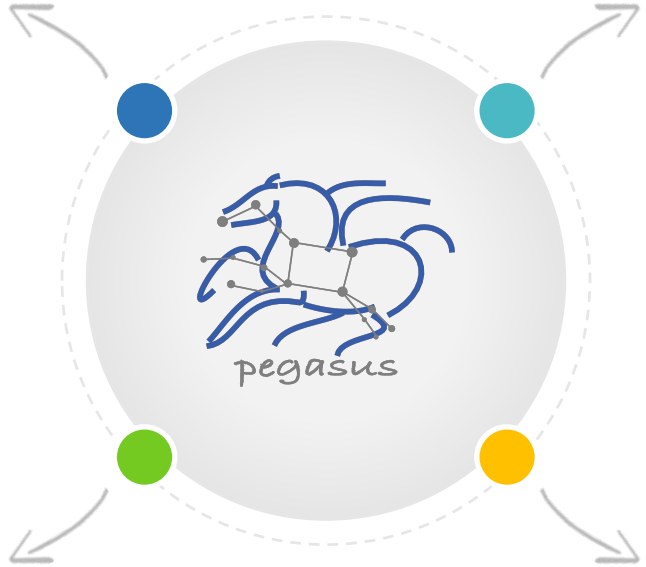
And if a job fails?

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

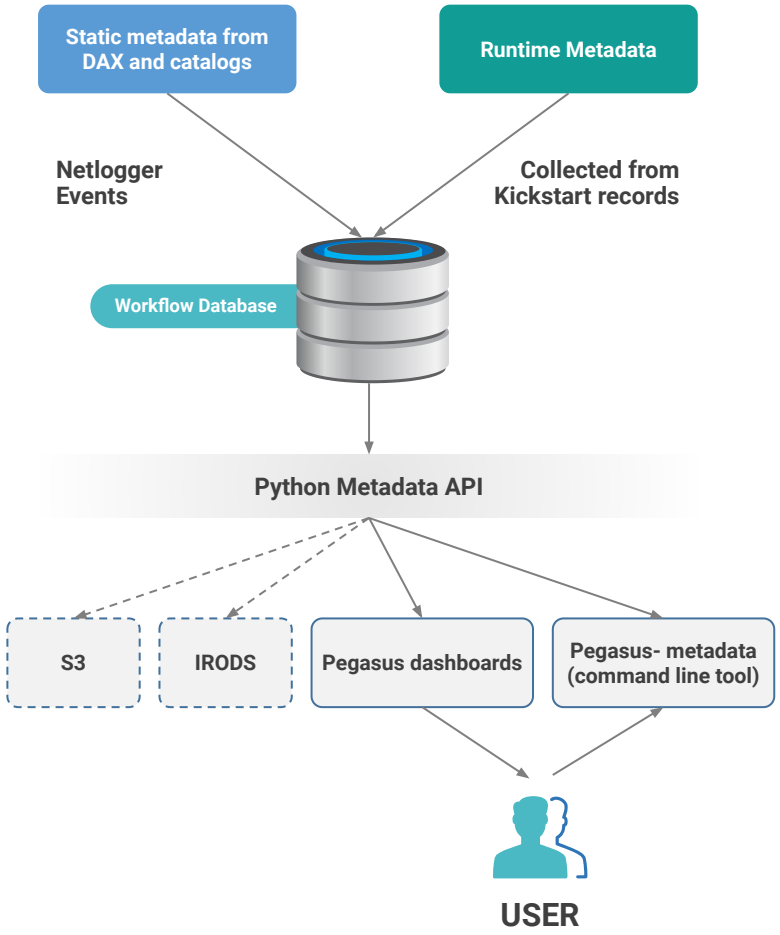
Static: application parameters
Runtime: performance metrics

Workflow, Job, File

```
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
```

Select Data Based on Metadata

Register Data With Metadata



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.

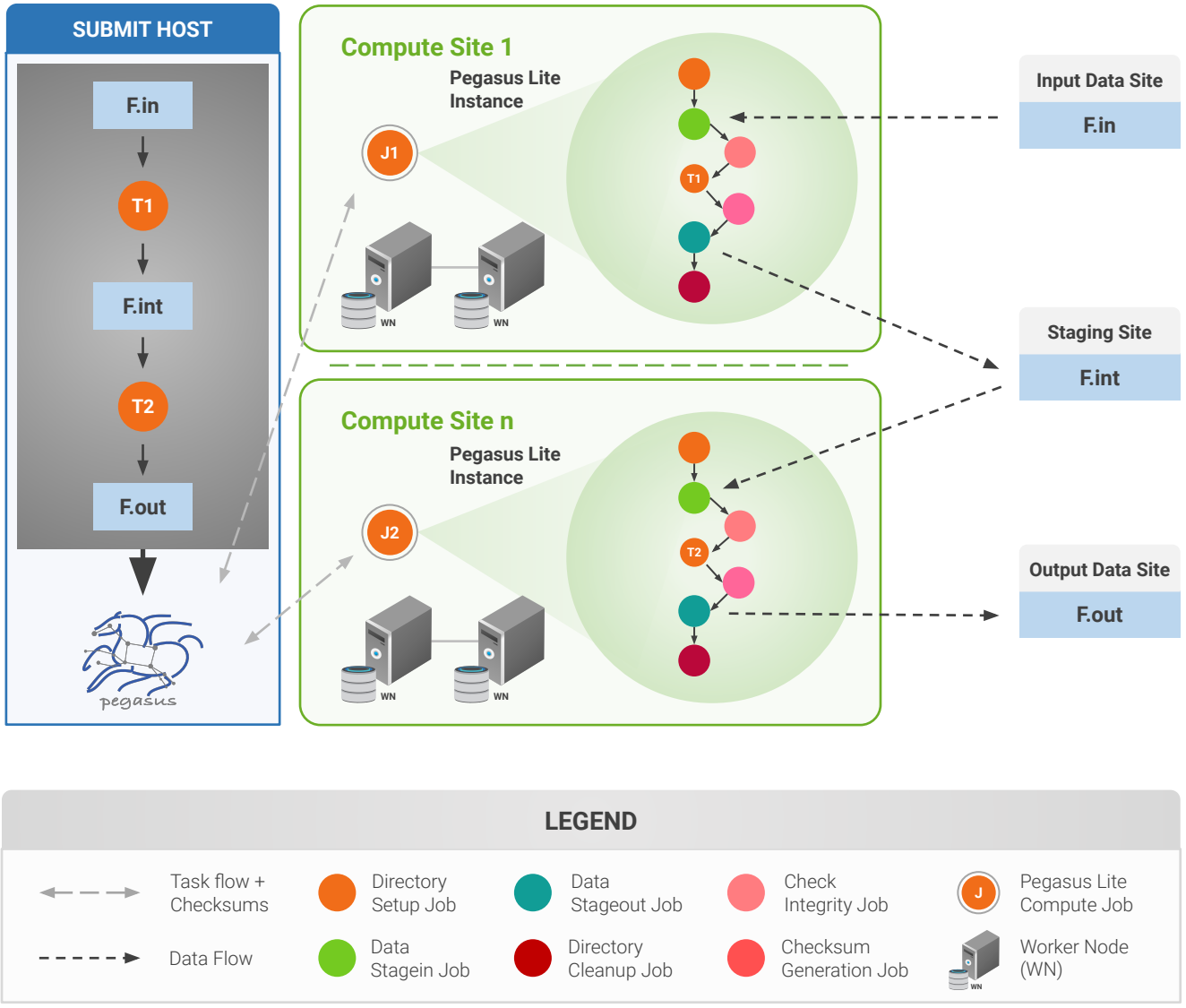
User Perception: "Am I not already protected? I have heard about TCP checksums, encrypted transfers, checksum validation, RAID and erasure coding – is that not enough?"

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



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

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

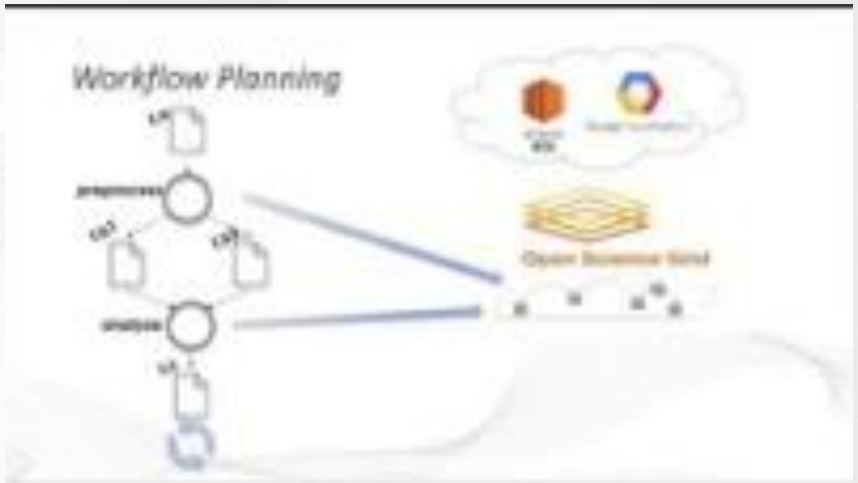
Slack
Ask for an invite by trying to join pegasus-users.slack.com in the Slack app

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