

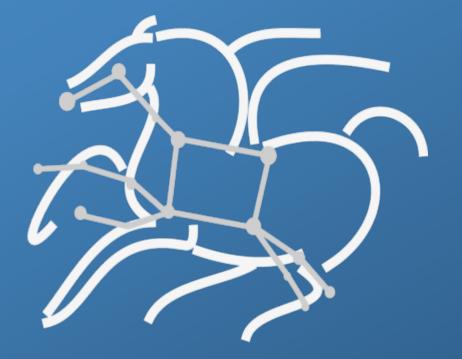
Enhancing Scientific Computations with Scientific Workflows

Pegasus Workflow Management System

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ichool of Engineering Information Sciences Institute



http://pegasus.isi.edu

OUTLINE

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Intr	nd	CTION
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Scientific Workflows Pegasus Overview Successful Stories

Pegasus Overview

Basic Concepts Features System Architecture

Break

5min - 10min Break

Features

Data Staging Information Catalogs Fault-Tolerance

Demo

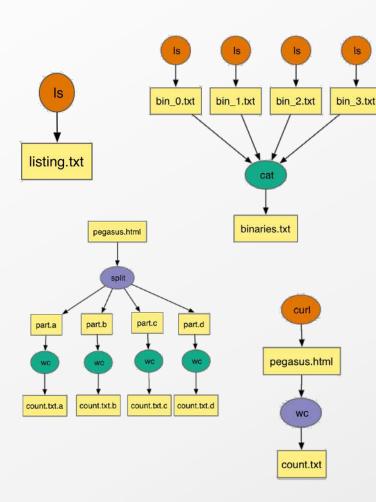


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Compute Pipelines Building Blocks



Compute Pipelines

- Allows scientists to connect different codes together and execute their analysis
- Pipelines can be very simple (independent or parallel) jobs or complex represented as DAG's
- Helps users to automate scale up

However, it is still up-to user to figure out

Data Management

• How do you ship in the small/large amounts data required by your pipeline and protocols to use?

How best to leverage different infrastructure setups

• OSG has no shared filesystem while XSEDE and your local campus cluster has one!

Debug and Monitor Computations

- Correlate data across lots of log files
- Need to know what host a job ran on and how it was invoked

Restructure Workflows for Improved Performance

• Short running tasks? Data placement

http://pegasus.isi.edu

Why Pegasus?

Automates complex, multi-stage processing pipelines

Enables parallel, distributed computations

Automatically executes data transfers

Reusable, aids reproducibility

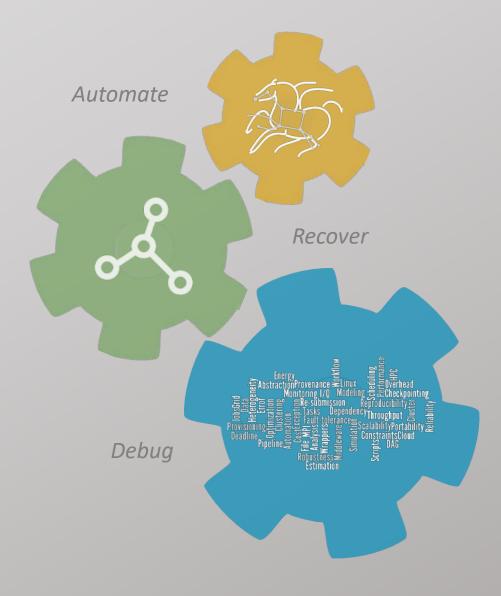
Records how data was produced (provenance)

Handles failures with to provide reliability

Keeps track of data and files



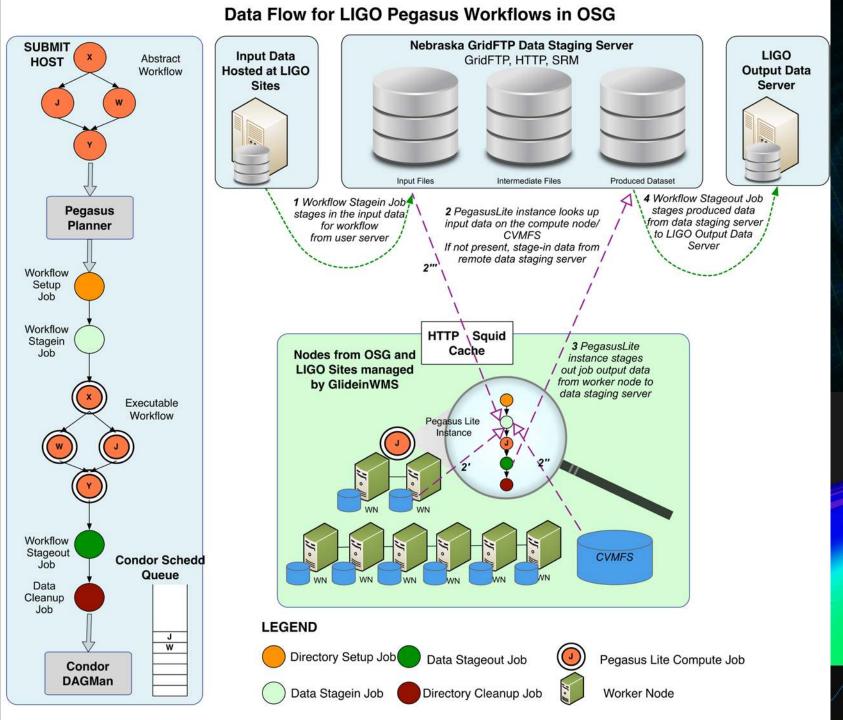
NSF funded project since 2001, with close collaboration with HTCondor team





Some of the successful stories...

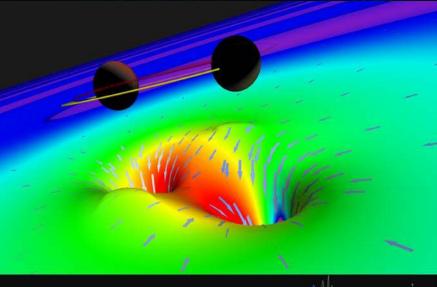




Advanced LIGO – Laser Interferometer Gravitational Wave Observatory

60,000 compute tasks Input Data: 5000 files (10GB total) Output Data: 60,000 files (60GB total)

> executed on LIGO Data Grid, Open Science Grid and XSEDE



Advanced LIGO PyCBC Workflow

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

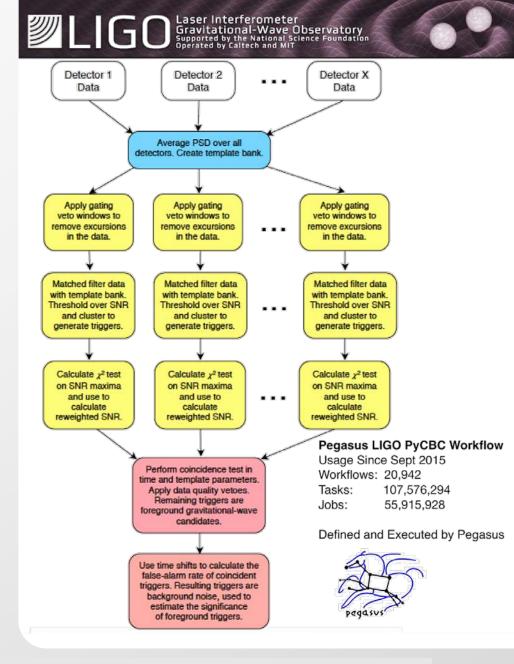
Contains **100's of thousands of jobs** and accesses on order of **terabytes of data**

Uses data from multiple detectors

For the detection, the pipeline was executed on Syracuse and Albert Einstein Institute Hannover

A single run of the binary black hole + binary neutron star search through the O1 data (about 3 calendar months of data with 50% duty cycle) requires a **workflow** with **194,364 jobs**

Generating the final O1 results with all the review required for the first discovery took about **20 million core hours**





PyCBC Papers: An improved pipeline to search for gravitational waves from compact binary coalescence. Samantha Usman, Duncan Brown et al. The PyCBC search for gravitational waves from compact binary coalescence, Samantha Usman et al (https://arxiv.org/abs/1508.02357)

PyCBC Detection GW150914: First results from the search for binary black hole coalescence with Advanced LIGO. *B. P. Abbott et al.*

Southern California Earthquake Center's CyberShake

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

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

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

GPU jobs: 439,000 node-hours

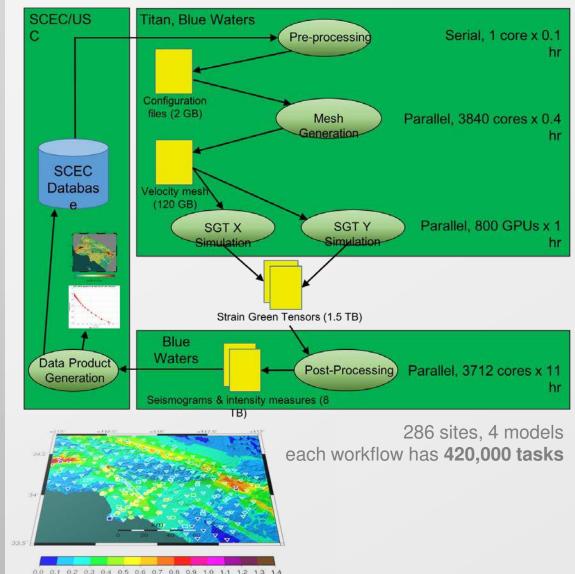
AWP-ODC finite-difference code

5 billion points per volume, 23000 timesteps 200 GPUs for 1 hour

Titan:

421,000 CPU node-hours, 110,000 GPU node-hours Blue Waters:

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



3s SA (q)



Impact on DOE Science

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

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

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

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

https://pegasus.isi.edu

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ome News Diamonds that deliver

Diamonds that deliver

Water is seen as small red and

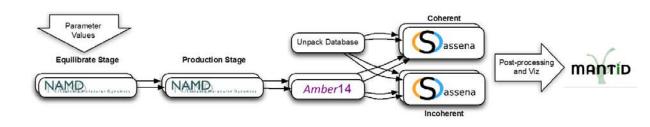
white molecules on large

nanodiamond spheres. The colored tRNA can be seen on

the nanodiamond surface. (Image Credit: Michael

Mattheson, OLCF, ORNL)

Neutrons, simulation analysis of tRNA-nanodiamond combo could transform drug delivery design principles Related Topics: Advanced Materials Neutron Science Q



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



Soybean Workflow

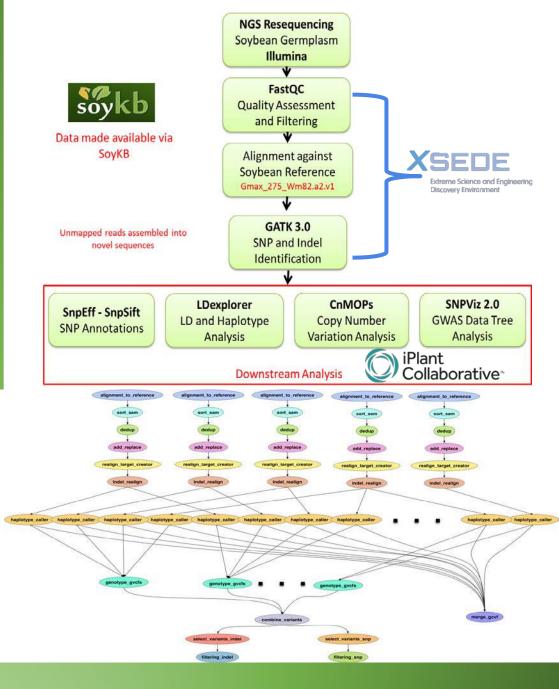
TACC Wrangler as Execution Environment

Flash Based Shared Storage

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

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







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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

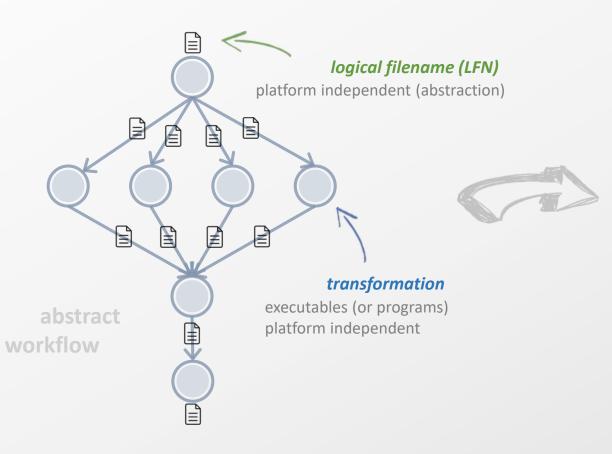


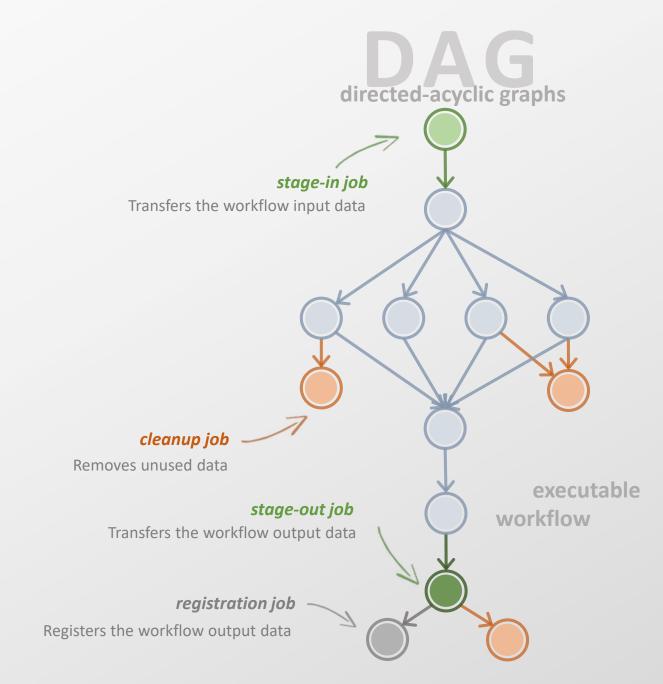


Portable Description

egasus

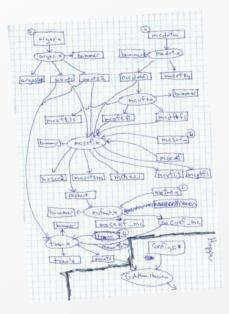
Users do not worry about low level execution details



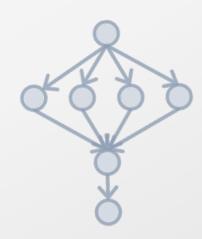


https://pegasus.isi.edu

Pegasus also provides tools to generate the abstract workflow



#!/usr/bin/env python	n python
<pre>from Pegasus.DAX3 import * import sys</pre>	C pyrion
import os	
# Create a abstract dag dax = ADAG(" <mark>hello_world</mark> ")	لَقِي Java
# Add the hello job	E
<pre>hello = Job(namespace="hello_world",</pre>	
<pre>b = File("f.b")</pre>	
hello.uses(a, link=Link.INPUT) hello.uses(b, link=Link.OUTPUT)	
dax.addJob(hello)	
<pre># Add the world job (depends on the hello job) world = Job(namespace="hello_world",</pre>	
c = File("f.c")	perl 🙀
world.uses(b, link=Link.INPUT)	heitki
world.uses(c, link=Link.OUTPUT) dax.addJob(world)	
# Add control-flow dependencies	
dax.addDependency(Dependency(parent=hello, child=world))	Jupyter
# Write the DAX to stdout	
dax.writeXML(sys.stdout)	
25	



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

<uses name="f.b" link="output"/>
<uses name="f.a" link="input"/>
</job>

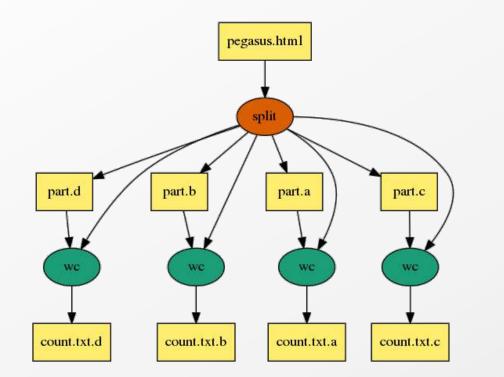
<uses name="f.b" link="input"/>
<uses name="f.c" link="output"/>
</job>







An example Split Workflow



Visualization Tools:

Pegasus

pegasus-graphviz pegasus-plots

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

n python"

#!/usr/bin/env python

import os, pwd, sys, time
from Pegasus.DAX3 import *

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

webpage = File("pegasus.html")

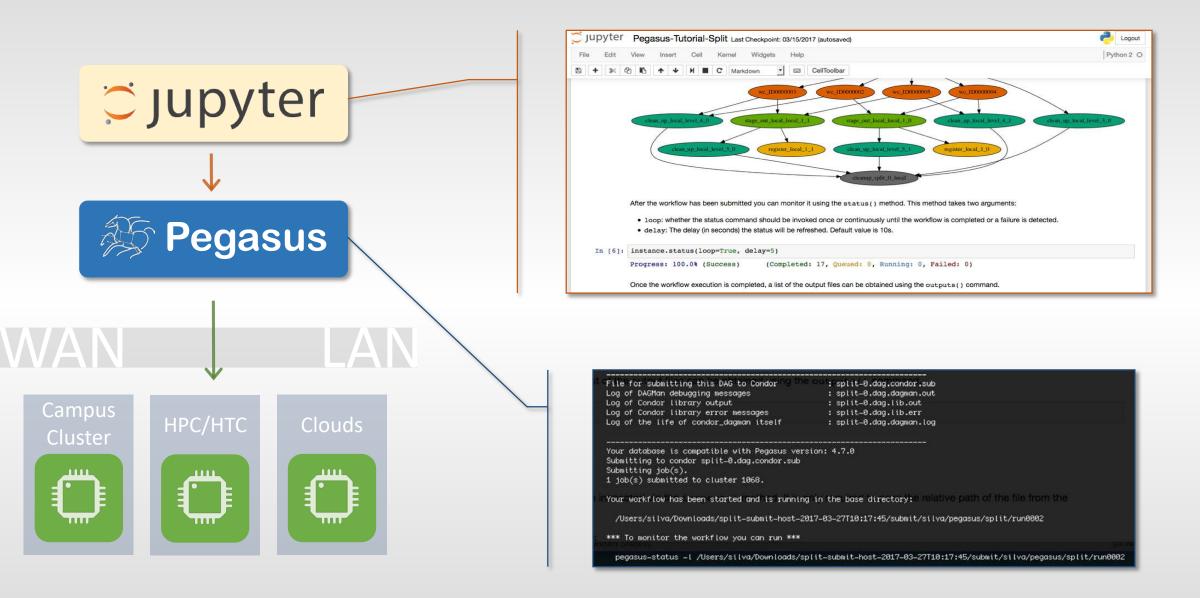
the split job that splits the webpage into smaller chunks split = Job("split") split.addArguments("-1","100","-a","1",webpage,"part.") split.uses(webpage, link=Link.INPUT) # associate the label with the job. all jobs with same label # are run with PMC when doing job clustering split.addProfile(Profile("pegasus","label","p1")) dax.addJob(split)

we do a parmeter sweep on the first 4 chunks created for c in "abcd": part = File("part.%s" % c) split.uses(part, link=Link.OUTPUT, transfer=False, register=False) count = File("count.txt.%s" % c) wc = Job("wc") wc.addProfile(Profile("pegasus","label","p1")) wc.addArguments("-1",part) wc.setStdout(count) wc.uses(part, link=Link.INPUT) wc.uses(count, link=Link.OUTPUT, transfer=True, register=True) dax.addJob(wc)

#adding dependency
dax.depends(wc, split)

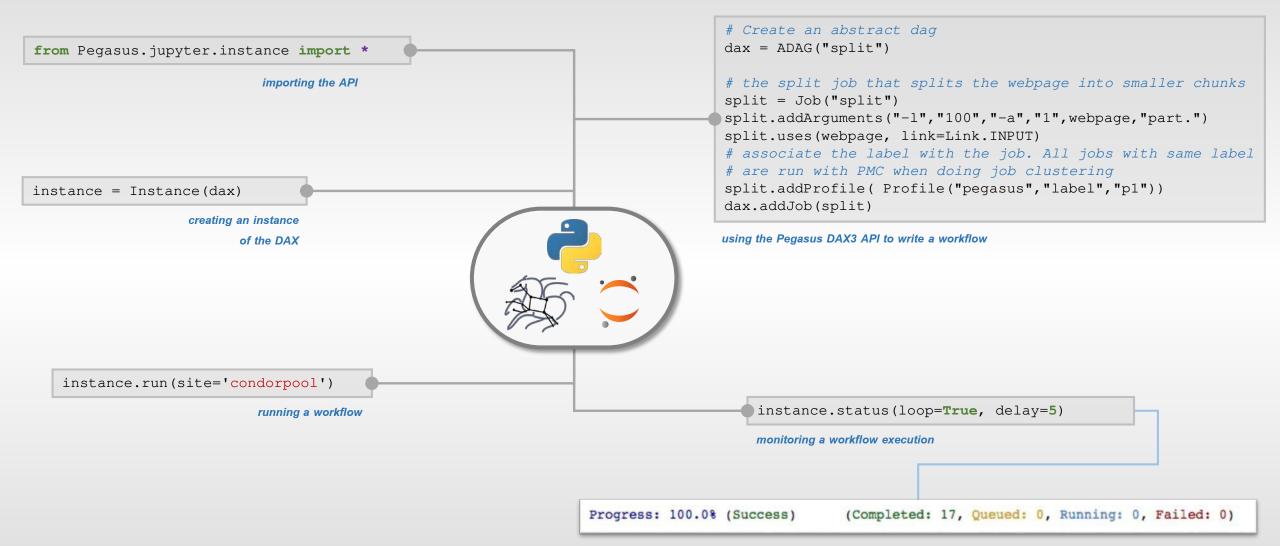
f = open("split.dax", "w")
dax.writeXML(f)
f.close()

Running Pegasus workflows with Jupyter



Pegasus

Pegasus-Jupyter Python API





Pegasus Container Support Support for Docker Singularity – Widely supported on OSG



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

Users can refer to a container they want to use. However, they let Pegasus stage their executable to the node.

Useful if you want to use a site recommended/standard container image.

Users are using generic image with executable staging.

Future Plans

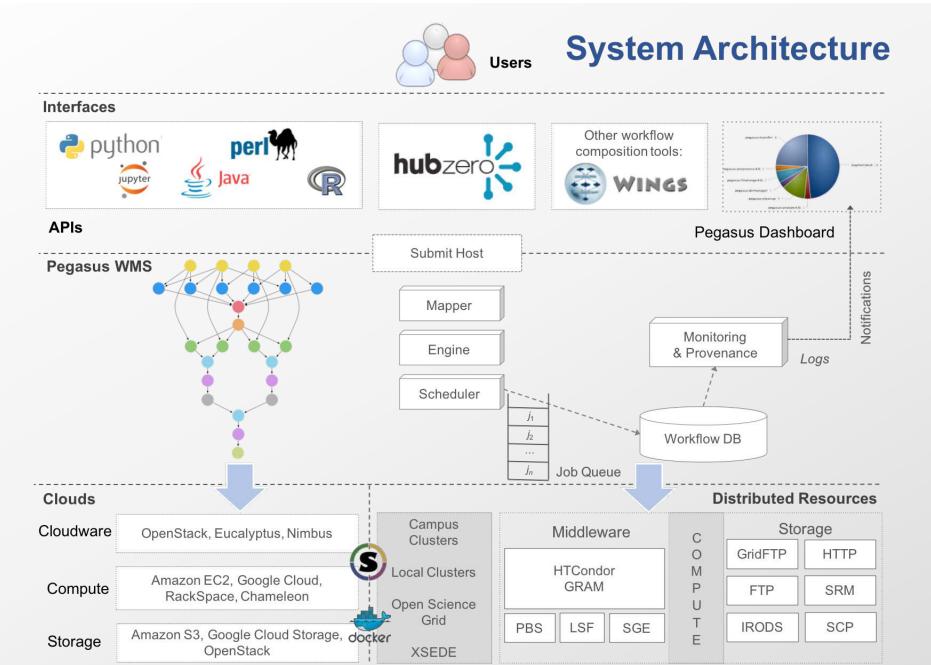
Users can specify an image buildfile for their jobs.

Pegasus will build the Docker image as separate jobs in the executable workflow, export them at tar file and ship them around (planned for 4.8.X)



Data Management for Containers

- Users can refer to container images as
 - Docker or Singularity Hub URL's
 - Docker Image exported as a TAR file and available at a server , just like any other input dataset.
- We want to avoid hitting Docker/Singularity Hub repeatedly for large workflows
 - Extend pegasus-transfer to pull image from Docker Hub and then export it as tar file, that can be shipped around in the workflow.
- Ensure pegasus worker package gets installed at runtime inside the user container.



Pegasus

http://pegasus.isi.edu

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web interface for monitoring and debugging workflows

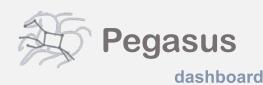
	Warkflow Wall Time						
Workflow Cumulative Job Wall Time							
Cumulative Job Waltime as seen from Sobmit Side						9 mins 35 secs.	
Workflow Cumulative Badput Time						9 mine 23 secs	
Cumulative Job Badput Walitime as seen from Submit Side						9 mins 20 secs	
		Workflow Ret	ries			1	
Taska Jobs Eub Workfowa	5 16 0	0	0	s 16 0	2	5 18 0	
Increase and and			20		8	0	
Entire Workflow Type	Succeeded	Failed	Incomplete	Total	Retries	Total + Retries	
Tasks	\$	0	0	5	o	6	
Jobs	10	0	0	10	2	18	
Sub Workflows	0	0	0	0	0	0	

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



Real-time Monitoring Reporting Debugging Troubleshooting RESTful API



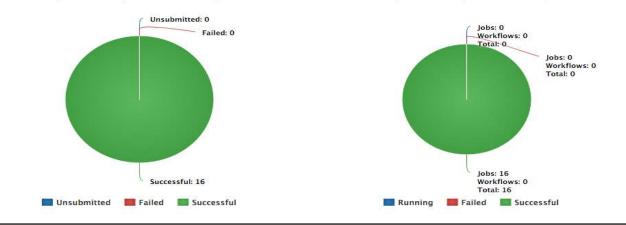


web interface for monitoring and debugging workflows

Real-time <u>monitoring</u> of workflow executions. It shows the <u>status</u> of the workflows and jobs, job <u>characteristics</u>, <u>statistics</u> and <u>performance</u> metrics. <u>Provenance</u> data is stored into a relational database. Workflow Details 5bb4de1d-e986-42b8-9160-ab9488494ecf

Label	split
Туре	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	
Wall Time	12 mins 23 secs
Cumulative Wall Time	9 mins 34 secs

Job Status (Entire Workflow)



Job Status (Per Workflow)



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...

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

Туре	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





Automate, recover, and debug scientific computations.

Get Started

Pegasus Online Office Hours

https://pegasus.isi.edu/blog/online-pegasus-office-hours/

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

HipChat



Pegasus Website
 http://pegasus.isi.edu

Users Mailing List pegasus-users@isi.edu

• Support pegasus-support@isi.edu

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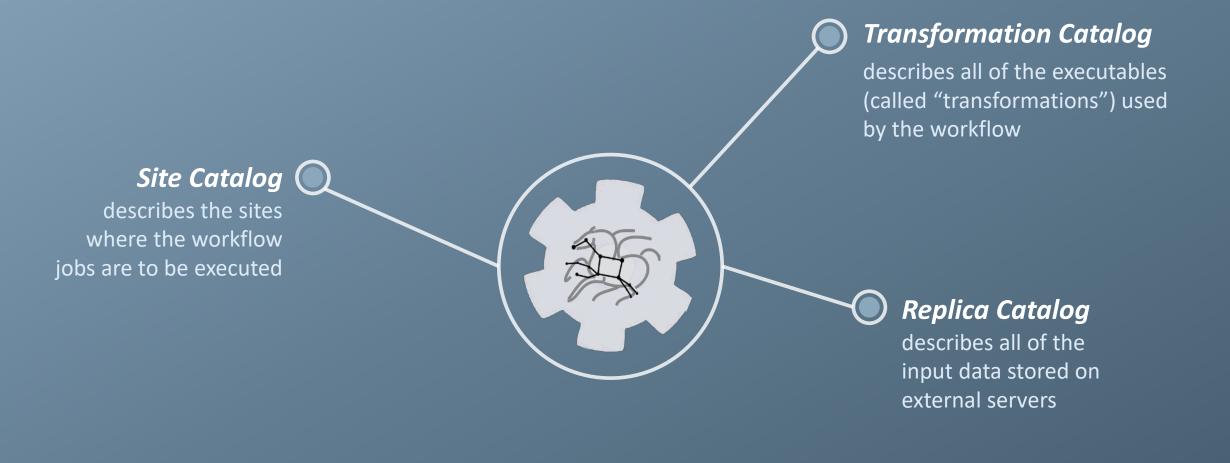
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Understanding Pegasus features...



So, what information does Pegasus need?





How does Pegasus decide where to execute?

site catalog

transformation catalog

replica catalog

site description - describes the compute resources

scratch

tells where temporary data is stored

storage

tells where output data is stored

profiles

key-pair values associated per job level

Pegasus

<!-- The local site contains information about the submit host -->
<!-- The arch and os keywords are used to match binaries in the -->
<!-- transformation catalog -->
<site handle="local" arch="x86 64" os="LINUX">

<!-- These are the paths on the submit host were Pegasus stores data --> <!-- Scratch is where temporary files go -->

<directory type="shared-scratch" path="/home/tutorial/run">
 <file-server operation="all" url="file:///home/tutorial/run"/>
</directory>

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

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

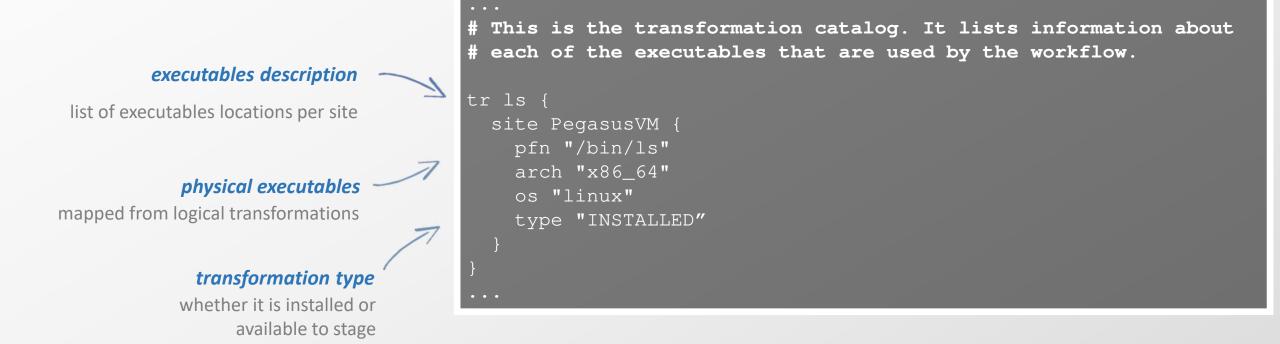
</site>

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

transformation catalog

replica catalog

site catalog



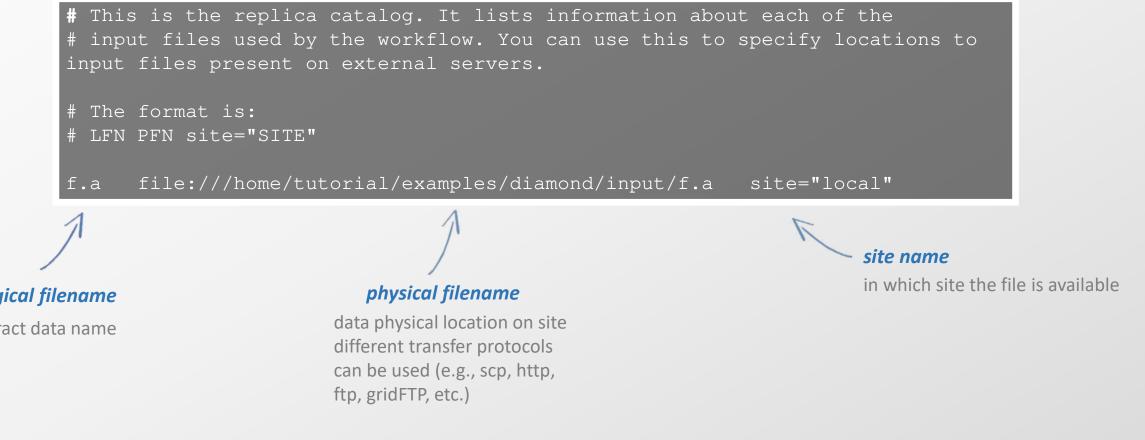


What if data is not local to the submit host?

site catalog

transformation catalog

replica catalog



logical filename abstract data name

aasus

http://pegasus.isi.edu

Replica catalog multiple sources

site catalog

transformation catalog

replica catalog

pegasus.conf

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

rc.data

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

- # The format is:
- # LFN PFN site="SITE"
- f.a file:///cvmfs/oasis.opensciencegrid.org/diamond/input/f.a site="cvmfs"
- f.a file:///local-storage/diamond/input/f.a site="prestaged"
- f.a gridftp://storage.mysite/edu/examples/diamond/input/f.a site="storage"



Data Staging Configurations

HTCondor I/O (HTCondor pools, OSG, ...)

Worker nodes do not share a file system

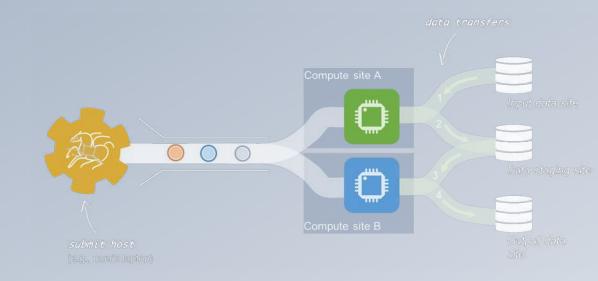
Data is pulled from / pushed to the submit host via HTCondor file transfers Staging site is the submit host

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

Worker nodes do not share a file system

Data is pulled / pushed from a staging site, possibly not co-located with the computation

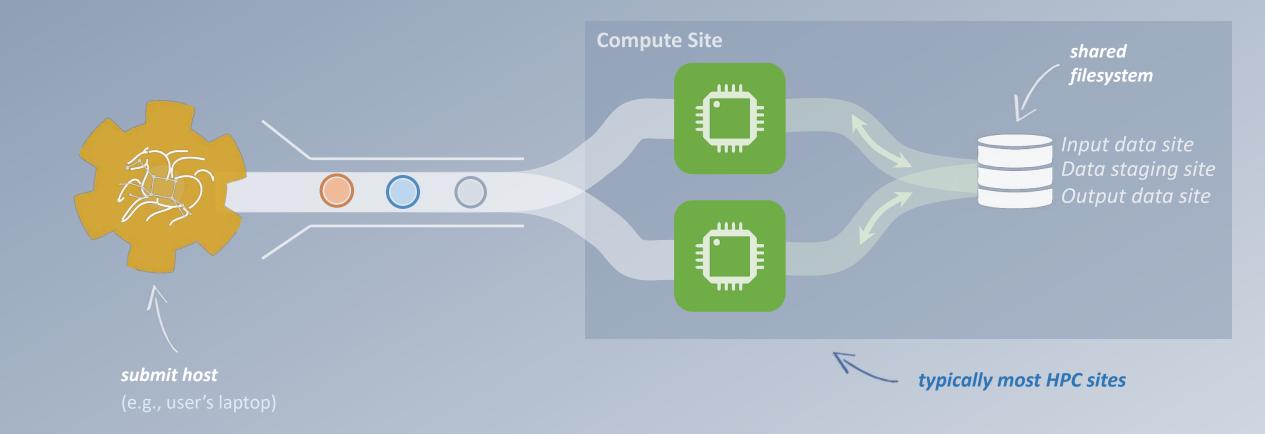
Shared File System (HPC sites, XSEDE, Campus clusters, ...) I/O is directly against the shared file system





High Performance Computing

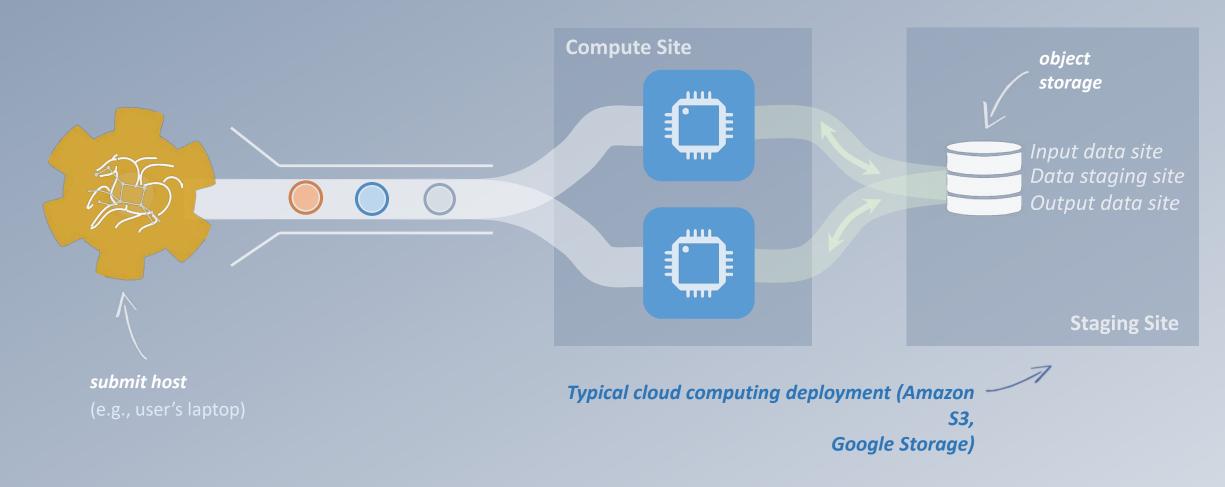
There are several possible configurations...





Cloud Computing

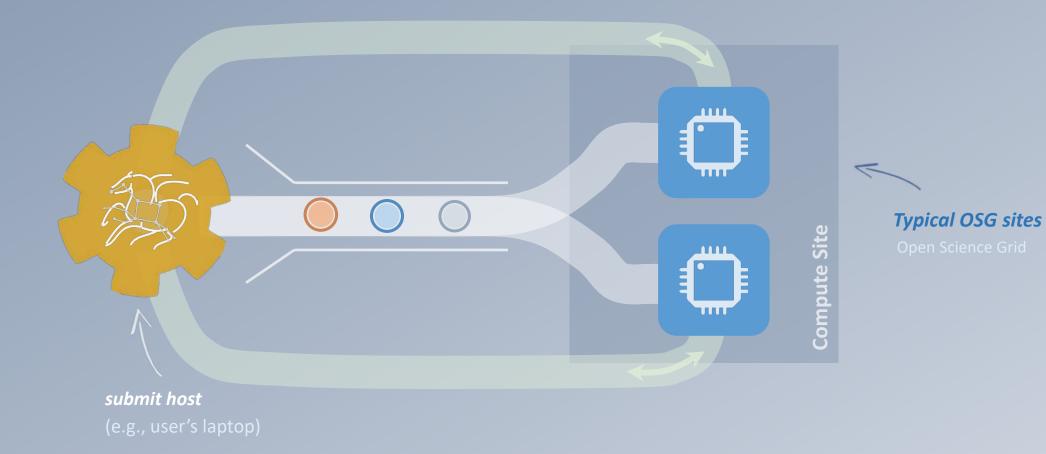
high-scalable object storages





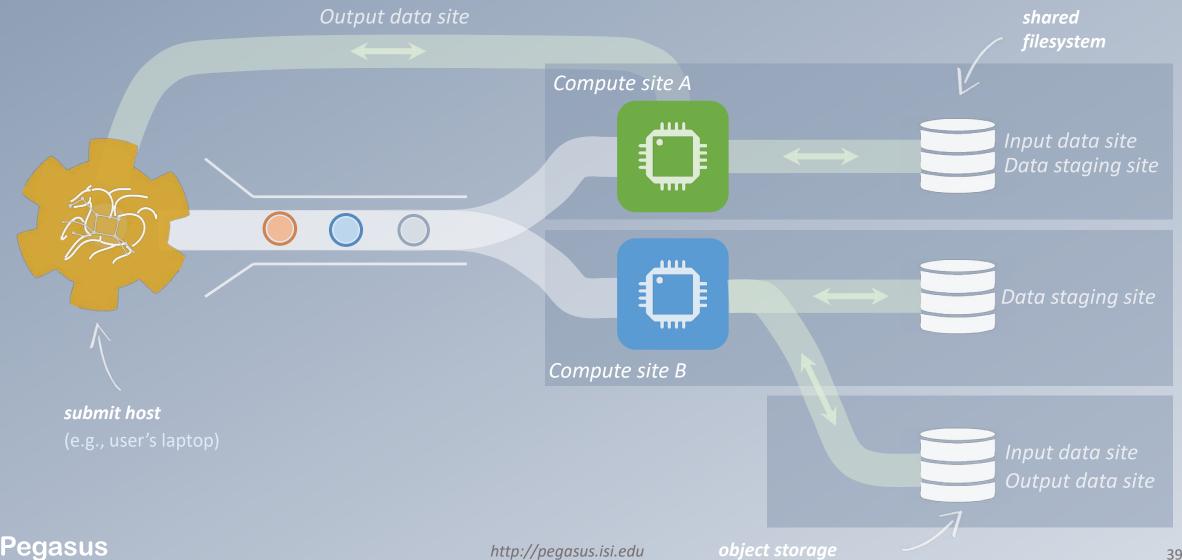
Grid Computing

local data management





And yes... you can mix everything!



Running workflows on AWS

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

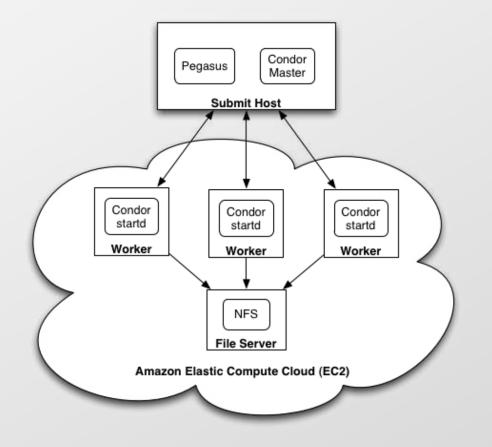
The simplest way is to use a submit machine outside the cloud, and to provision several worker nodes and a file server node in the cloud

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

Guidelines for Tutorial VM:

https://pegasus.isi.edu/documentation/vm amazon.php







pegasus-transfer

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

Directory creation, file removal

If protocol supports, used for cleanup

Two stage transfers

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

Parallel transfers

Automatic retries

Credential management

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

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



And if a job fails?

Job Failure Detection 🤘

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

Job Retry

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

Checkpoint Files

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

Rescue DAGs

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

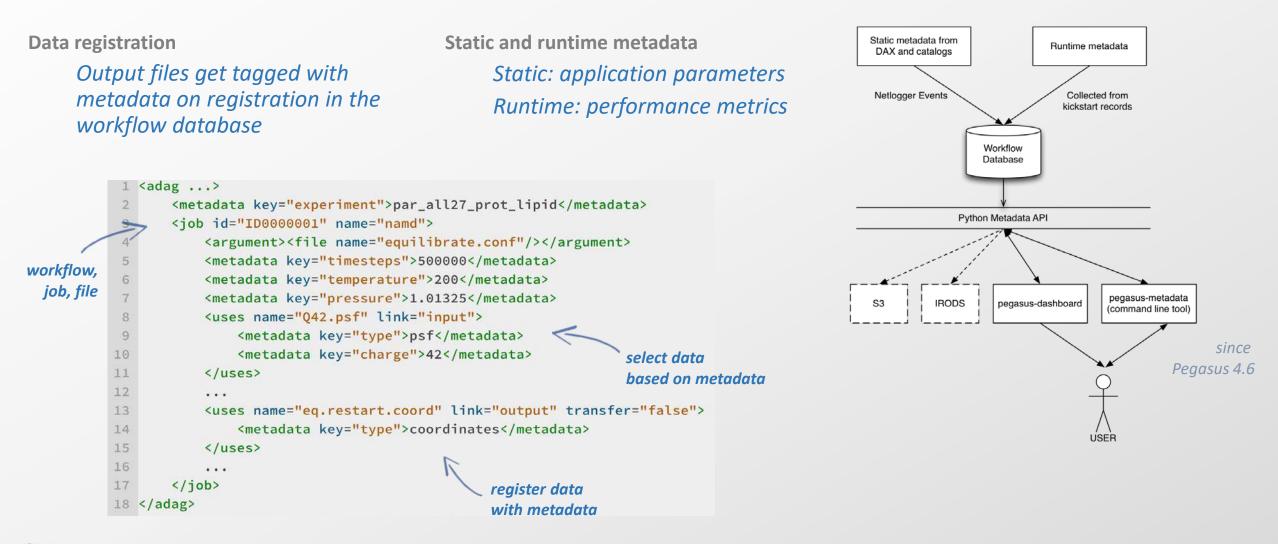


A few more features...



Metadata

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





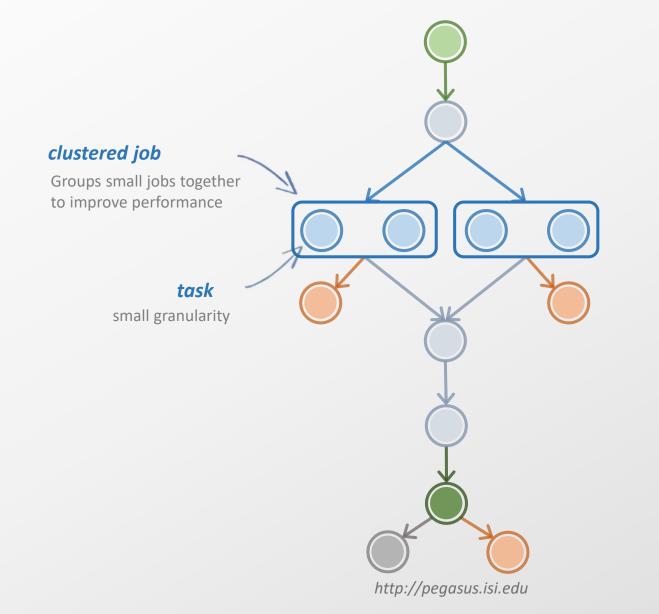
Performance, why not improve it?

workflow restructuring

workflow reduction

hierarchical workflows

pegasus-mpi-cluster





What about data reuse?

workflow restructuring

workflow reduction

hierarchical workflows

data already available data also available data also available



workflow restructuring Pegasus also handles large-scale workflows workflow reduction hierarchical workflows pegasus-mpi-cluster sub-workflow sub-workflow recursion ends when DAX with only compute jobs is encountered



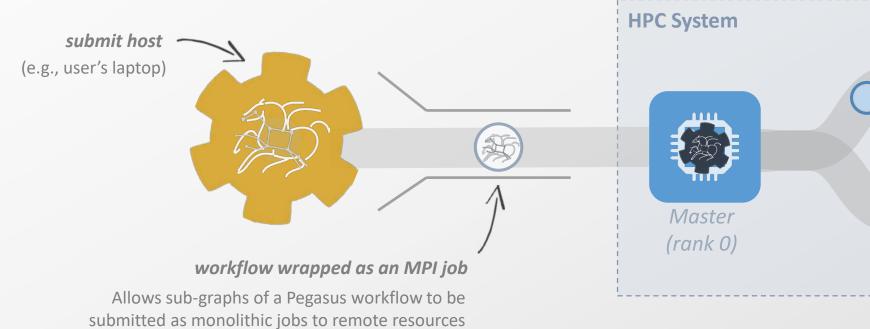
Running **fine-grained** workflows on HPC systems...

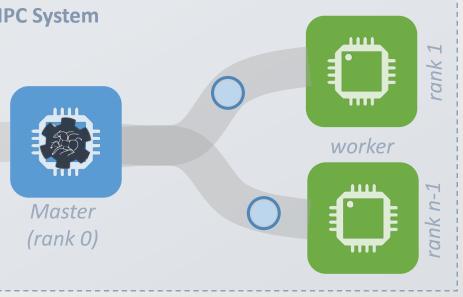
workflow restructuring

workflow reduction

hierarchical workflows

pegasus-mpi-cluster









Automate, recover, and debug scientific computations.

Get Started

Pegasus Online Office Hours

https://pegasus.isi.edu/blog/online-pegasus-office-hours/

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

HipChat



Pegasus Website
 http://pegasus.isi.edu

Users Mailing List pegasus-users@isi.edu

• Support pegasus-support@isi.edu



Automate, recover, and debug scientific computations.

Summer Office Hours

When ? Every Monday and Wednesday from 10am to 12pm

For how long ? From June 20th to August 8th 2018 !!!

But Where? ORNL Building 5100 (Joint Institute for Computational Sciences), Room 227

Can I get in touch ? Yes! Email me at georgpap@isi.edu

https://pegasus.isi.edu/2018/06/13/summer-pegasus-office-hours-ornl/

Demo...





Automate, recover, and debug scientific computations.

Hands On Tutorial

Thursday, June 21st Joint Institute For Computational Sciences JICS Lecture Hall (Room 128) From 1pm – 3pm

Survey: https://goo.gl/forms/uohZ0PklOcPodG942