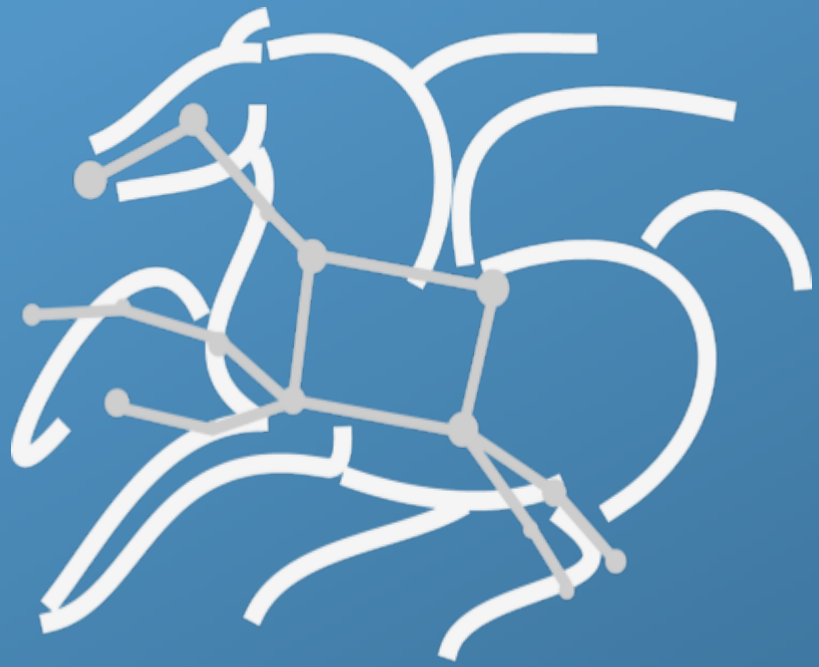
Compute Pipelines using Pegasus Workflows: An Introduction



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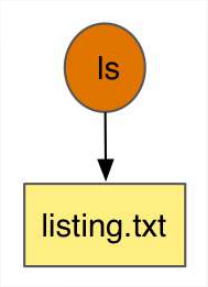
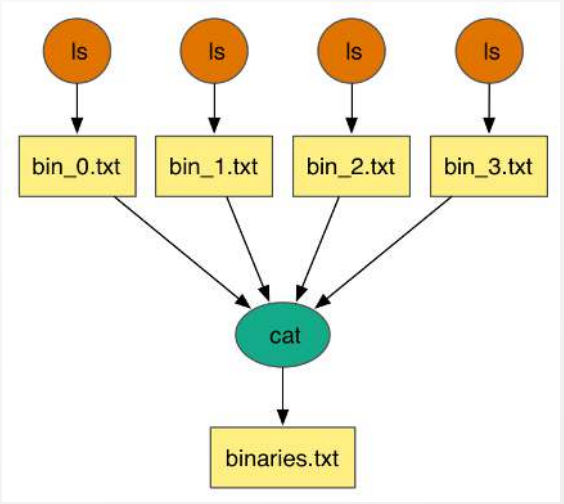
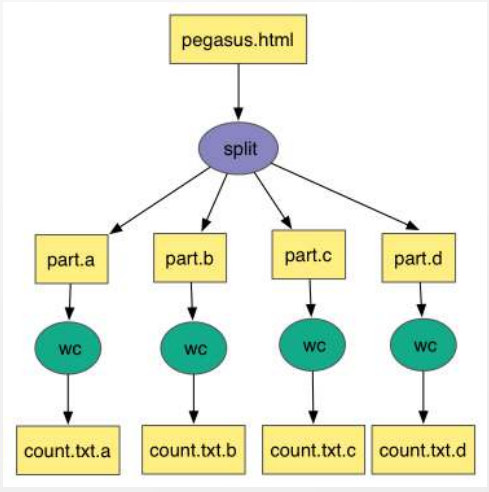
Information Sciences Institute

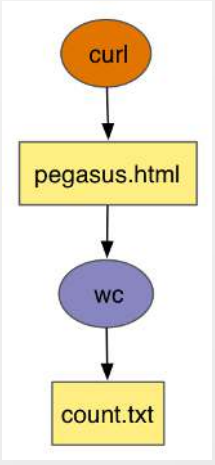
https://pegasus.isi.edu

Compute Pipelines – Building Blocks









Challenges scientists face while developing pipelines

Portability
How can you run a pipeline on Amazon EC2 one day, and a PBS cluster the next?

Data Management
How do you ship in the small/large amounts data required by your pipeline?
Different protocols: Can I use SRM? How about GridFTP? HTTP and Squid proxies?
Can I use Cloud based storage like S3 on EC2?

Debug and Monitor Computations.
Users need automated tools to go through the log files
Need to correlate data across lots of log files
Need to know what host a job ran on and how it was invoked

Restructure Pipelines for Improved Performance
Short running tasks?
Data placement?

Why Pegasus?

Automates complex, multi-stage processing pipelines

Enables parallel, distributed computations

Portable: Describe once; execute multiple times

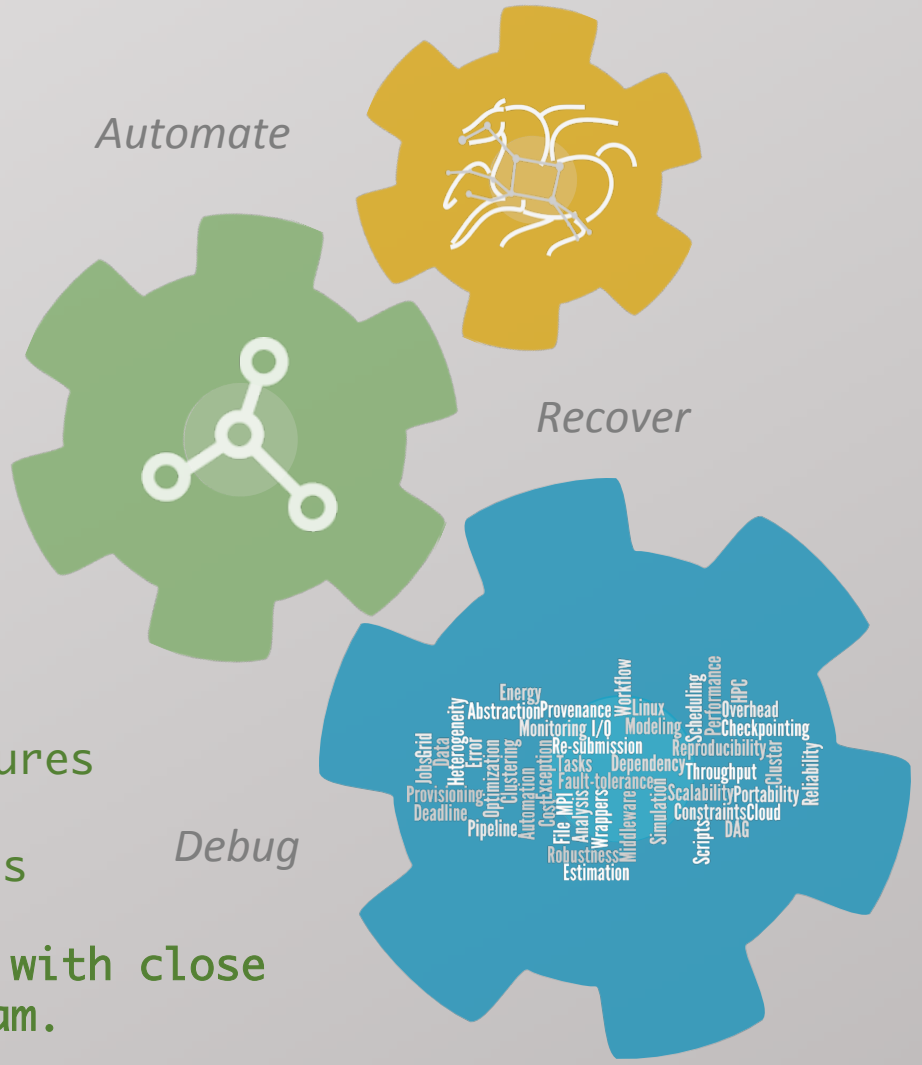
Automatically executes data transfers

Reusable, aids reproducibility

Records how data was produced (provenance)

Provides to tools to handle and debug failures

Keeps track of data and files



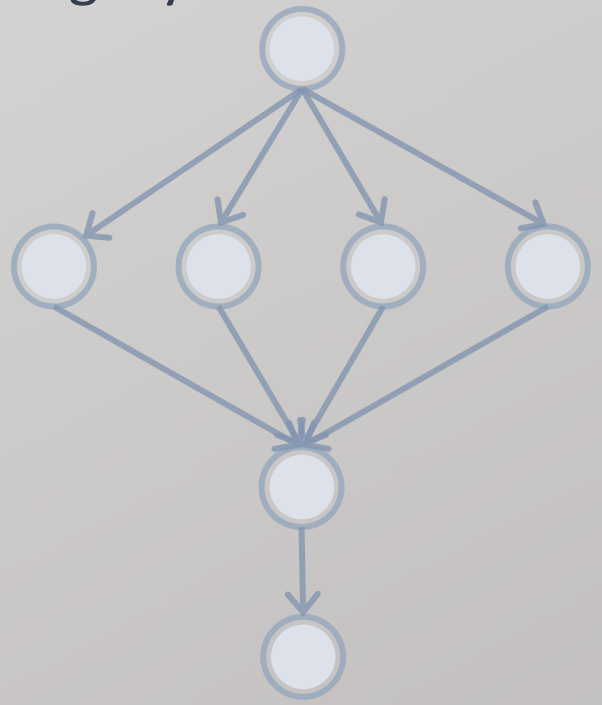
HTCondor
High Throughput Computing

NSF funded project since 2001, with close Collaboration with HTCondor team.

Key Pegasus Concepts

Pegasus WMS == Pegasus planner (mapper) + DAGMan workflow engine + HTCondor scheduler/broker + Pegasus Monitoring layer

- Pegasus maps workflows to infrastructure
- DAGMan manages dependencies and reliability
- HTCondor is used as a broker to interface with different schedulers
- Monitoring layer parses condor logs and puts them in a relational database



Workflows are DAGs (or hierarchical DAGs)

- Nodes: jobs, edges: dependencies
- No while loops, no conditional branches

Planning occurs ahead of execution

- (Except hierarchical workflows)

Planning converts an abstract workflow into an executable workflow

- Planner is like a workflow compiler. Compiles user workflows to target execution environment.

Taking a closer look into a Pegasus workflow…

abstract workflow

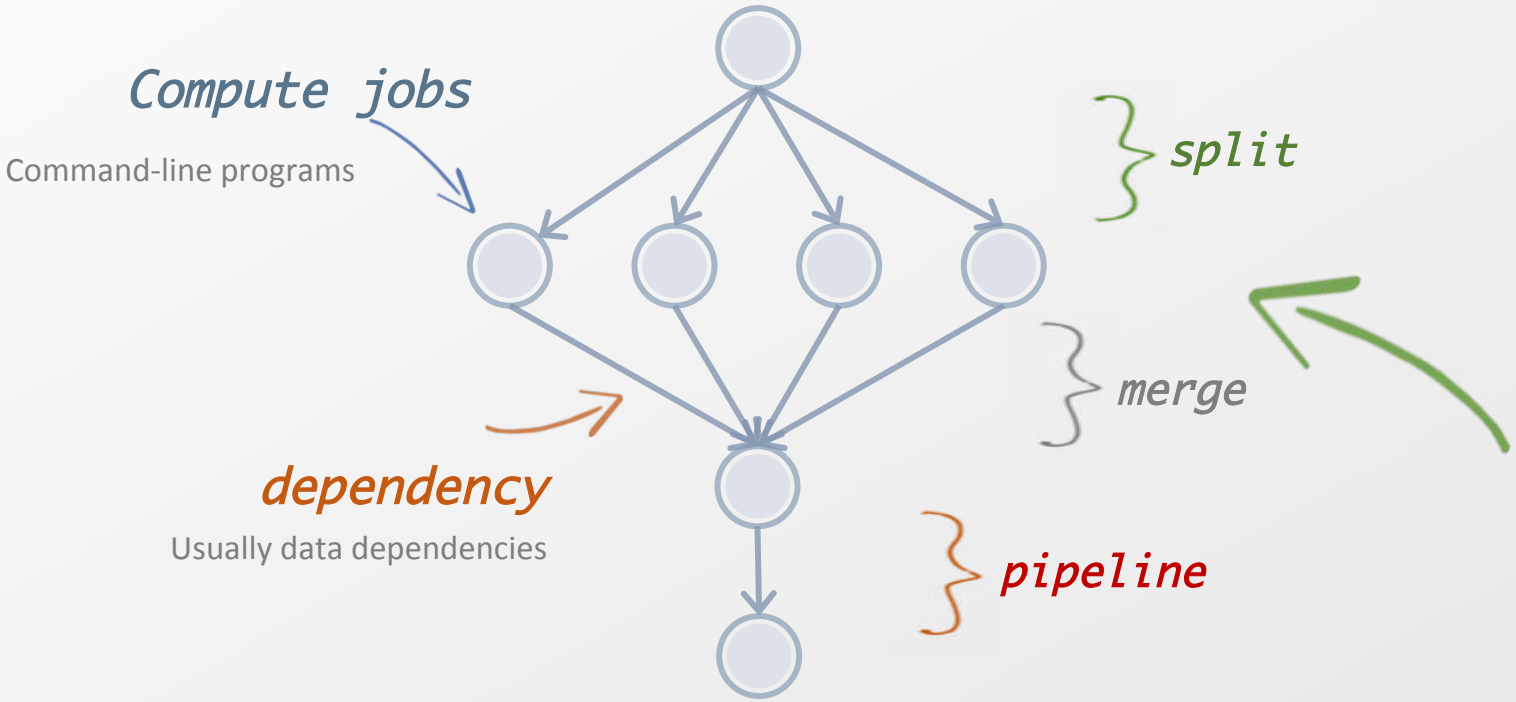
executable workflow

optimizations

storage constraints

DAG

directed-acyclic graphs



DAX

DAG in XML

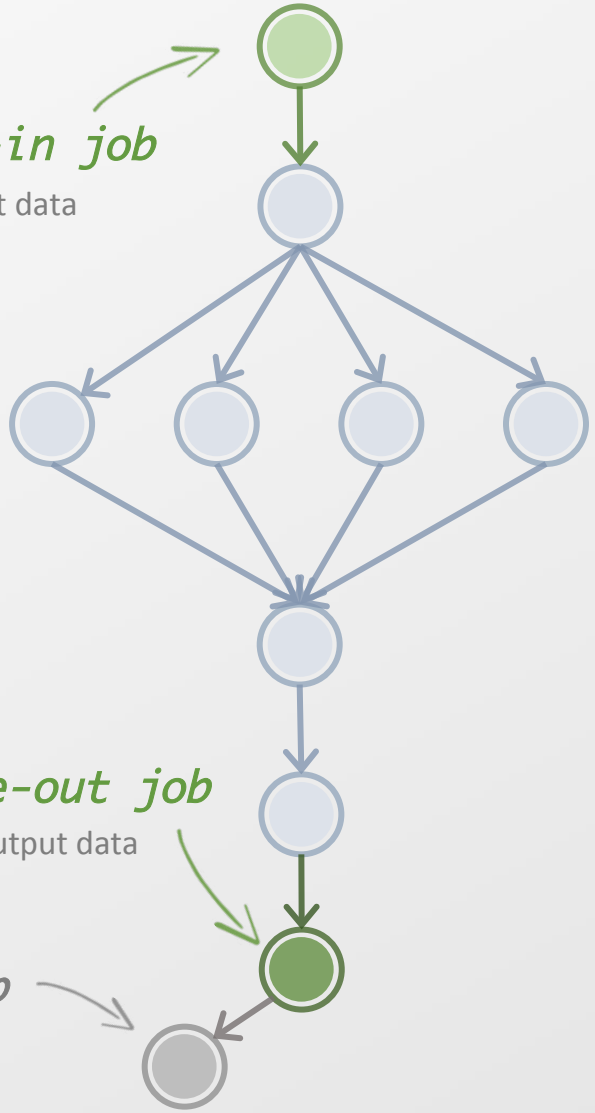
Pegasus input workflow description

Looks very similar to how users describe their pipelines

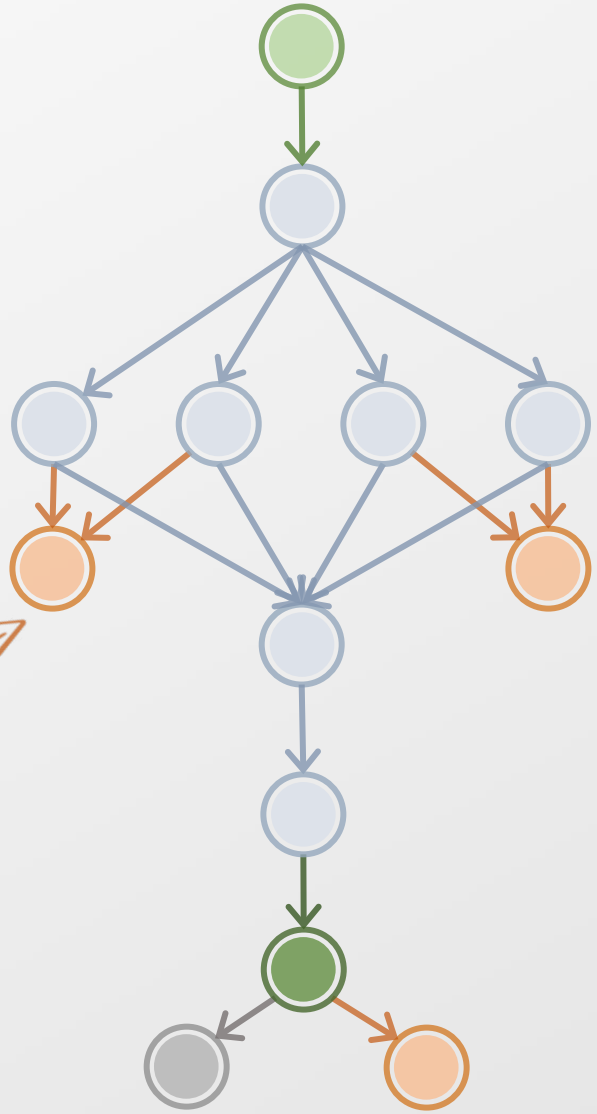
Only identifies computation steps, devoid of resource descriptions and data locations

File aware For each node you specify the input and output files by use of logical identifiers

From the abstraction to execution!



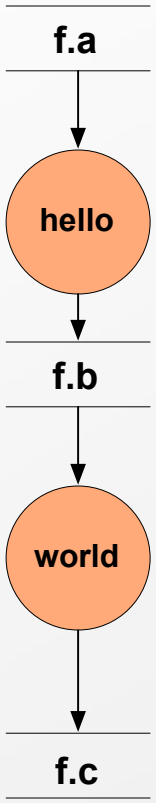
Optimizing storage usage…



cleanup job

Removes unused data

Pegasus also provides tools to generate the abstract workflow



Java

perl

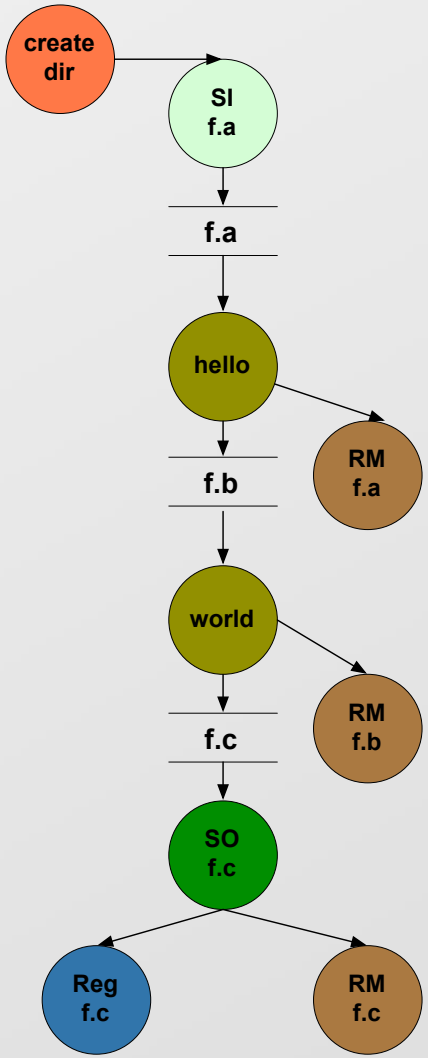
python

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

from Pegasus.DAX3 import *
import sys
import os

# Create a abstract dag
dax = ADAG("hello_world")

# Add the hello job
hello = Job(namespace="hello_world",
            name="hello", version="1.0")
b = File("f.b")
hello.uses(a, link=Link.INPUT)
hello.uses(b, link=Link.OUTPUT)
dax.addJob(hello)

# Add the world job (depends on the hello job)
world = Job(namespace="hello_world",
            name="world", version="1.0")
c = File("f.c")
world.uses(b, link=Link.INPUT)
world.uses(c, link=Link.OUTPUT)
dax.addJob(world)

# Add control-flow dependencies
dax.addDependency(Dependency(parent=hello,
                             child=world))

# Write the DAX to stdout
dax.writeXML(sys.stdout)
```

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

<!-- generator: python -->
<adag xmlns="http://pegasus.isi.edu/schema/DAX"
            version="3.4" name="hello_world">

    <!-- describe the jobs making
        up the hello world pipeline -->
    <job id="ID0000001" namespace="hello_world"
                    name="hello" version="1.0">

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

    <job id="ID0000002" namespace="hello_world"
                    name="world" version="1.0">

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

    <!-- describe the edges in the DAG -->
    <child ref="ID0000002">
        <parent ref="ID0000001"/>
    </child>
</adag>
```

DAG in XML

Plan



So, what information does Pegasus need?

Transformation Catalog

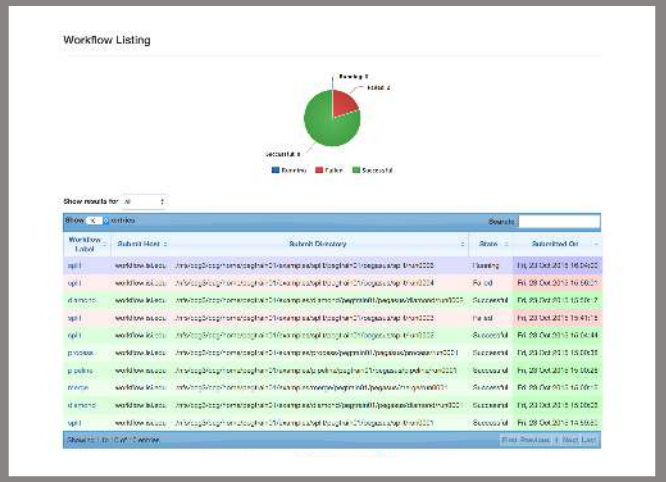
describes all of the executables (called “transformations”) used by the workflow

Site Catalog

describes the sites where the workflow jobs are to be executed

Replica Catalog

describes all of the input data stored on external servers



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

>_ But, if you prefer the 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%)
```

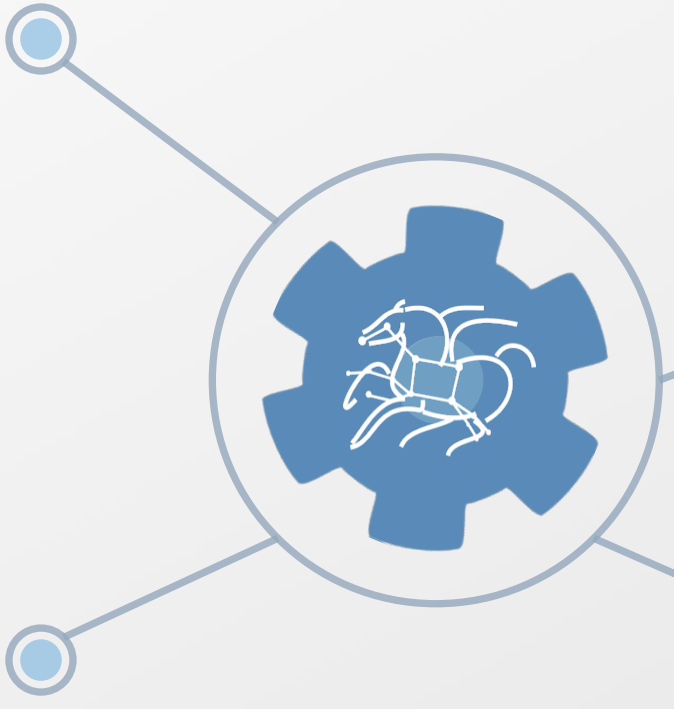
```
$ pegasus-statistics -s all pegasus/examples/split/run0001
------------------------------------------------------------------------------
Type           Succeeded Failed Incomplete Total Retries Total+Retries
Tasks              5       0        0        5     0         5
Jobs              17       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 :
```

…Pegasus provides a set of concise and powerful tools

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

pegasus-kickstart

() login02.osgconnect.net — Konsole

File Edit View Bookmarks Settings Help

```
<?xml version="1.0" encoding="UTF-8"?>
<invocation xmlns="http://pegasus.isi.edu/schema/invocation" xmlns:xsi="http://www.w3.org/2001/XMLSchema-instance" xsi:schemaLocation="http://pegasus.isi.edu/schema/invocation http://pegasus.isi.edu/schema/iv-2.3.xsd" version="2.3" start="2016-11-28T14:27:48.909-06:00" duration="11200.691" transformation="job-wrapper.sh" derivation="ID0013214" resource="condorpool" wf-label="particleshower" wf-stamp="2016-11-22T21:14:13-06:00" interface="eth0" hostaddr="131.225.208.240" hostname="fnpc4593.fnal.gov" pid="1725084" uid="12740" user="osg" gid="9652" group="osg" umask="0022">
  <mainjob start="2016-11-28T14:27:49.007-06:00" duration="11200.593" pid="1725089">
    <usage utime="10921.591" stime="30.304" maxrss="395820" minflt="128741" majflt="18" nswap="0" inblock="85776" outblock="1717424" msgsnd="0" msgrcv="0" nsignals="0" nvcsw="7676" nivcsw="185495"/>
    <status raw="0"><regular exitcode="0"/></status>
    <statcall error="0">
      <file name="/storage/local/data1/condor/execute/dir_1227464/glide_bSxwfe/execute/dir_1724937/pegasus.XRZ1p3/job-wrapper.sh">23212F62696E2F626173680A0A736574</file>
      <statinfo mode="0100755" size="1305" inode="16648869" nlink="1" blksize="4096" blocks="8" mtime="2016-11-28T12:10:53-06:00" atime="2016-11-28T14:27:48-06:00" ctime="2016-11-28T14:27:48-06:00" uid="12740" user="osg" gid="9652" group="osg"/>
    </statcall>
    <argument-vector>
      <arg nr="1">100</arg>
      <arg nr="2">0</arg>
      <arg nr="3">gamma</arg>
      <arg nr="4">62</arg>
      <arg nr="5">VERITAS</arg>
      <arg nr="6">corsika.tar.gz</arg>
      <arg nr="7">corsika75000Linux_QGSII_urqmd</arg>
      <arg nr="8">13213</arg>
    </argument-vector>
  </mainjob>
  <jobids condor="547839.0"/>
  <cwd>/storage/local/data1/condor/execute/dir_1227464/glide_bSxwfe/execute/dir_1724937/pegasus.XRZ1p3</cwd>
  <usage utime="0.013" stime="0.085" maxrss="828" minflt="2448" majflt="0" nswap="0" inblock="0" outblock="0" msgsnd="0" msgrcv="0" nsignals="0" nvcsw="1" nivcsw="12"/>
  <machine page-size="4096">
    <stamp>2016-11-28T14:27:48.909-06:00</stamp>
    <uname system="linux" nodename="fnpc4593.fnal.gov" release="2.6.32-642.6.2.el6.x86_64" machine="x86_64">#1 SMP Tue Oct 25 15:06:33 CDT 2016</uname>
    <linux>
      <ram total="65319608" free="1071948" shared="0" buffer="148224"/>
      <swap total="8388604" free="7741364"/>
      <boot idle="45893257.760">2016-11-09T16:40:54.260-06:00</boot>
      <cpu count="32" speed="2000" vendor="AuthenticAMD">AMD Opteron(tm) Processor 6128</cpu>
      <load min1="26.35" min5="27.70" min15="24.33"/>
      <procs total="881" running="23" sleeping="854" waiting="3" zombie="1" vmsize="65009304" rss="14780272"/>
      <task total="1273" running="24" sleeping="1243" waiting="5" zombie="1"/>
    </linux>
```

5,5 Top

() login02.osgconnect.net

Data Staging Configurations

- Condor I/O (HTCondor pools, OSG, …)
  - Worker nodes do not share a file system
  - Data is pulled from / pushed to the submit host via HTCondor file transfers
  - Staging site is the submit host
- Non-shared File System (clouds, OSG, …)
  - Worker nodes do not share a file system
  - Data is pulled / pushed from a staging site, possibly not co-located with the computation
- Shared File System (HPC sites, XSEDE, Campus clusters, …)
  - I/O is directly against the shared file system

pegasus-transfer

- Pegasus' internal data transfer tool
- Supports many 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
- Checkpoint and restart transfers
- Credential management
  - Uses the appropriate credential for each site and each protocol (even 3rd party transfers)

Protocols

- HTTP
- SCP
- GridFTP
- iRods
- Amazon S3
- Google Storage
- SRM
- FDT
- stashcp
- cp
- ln -s

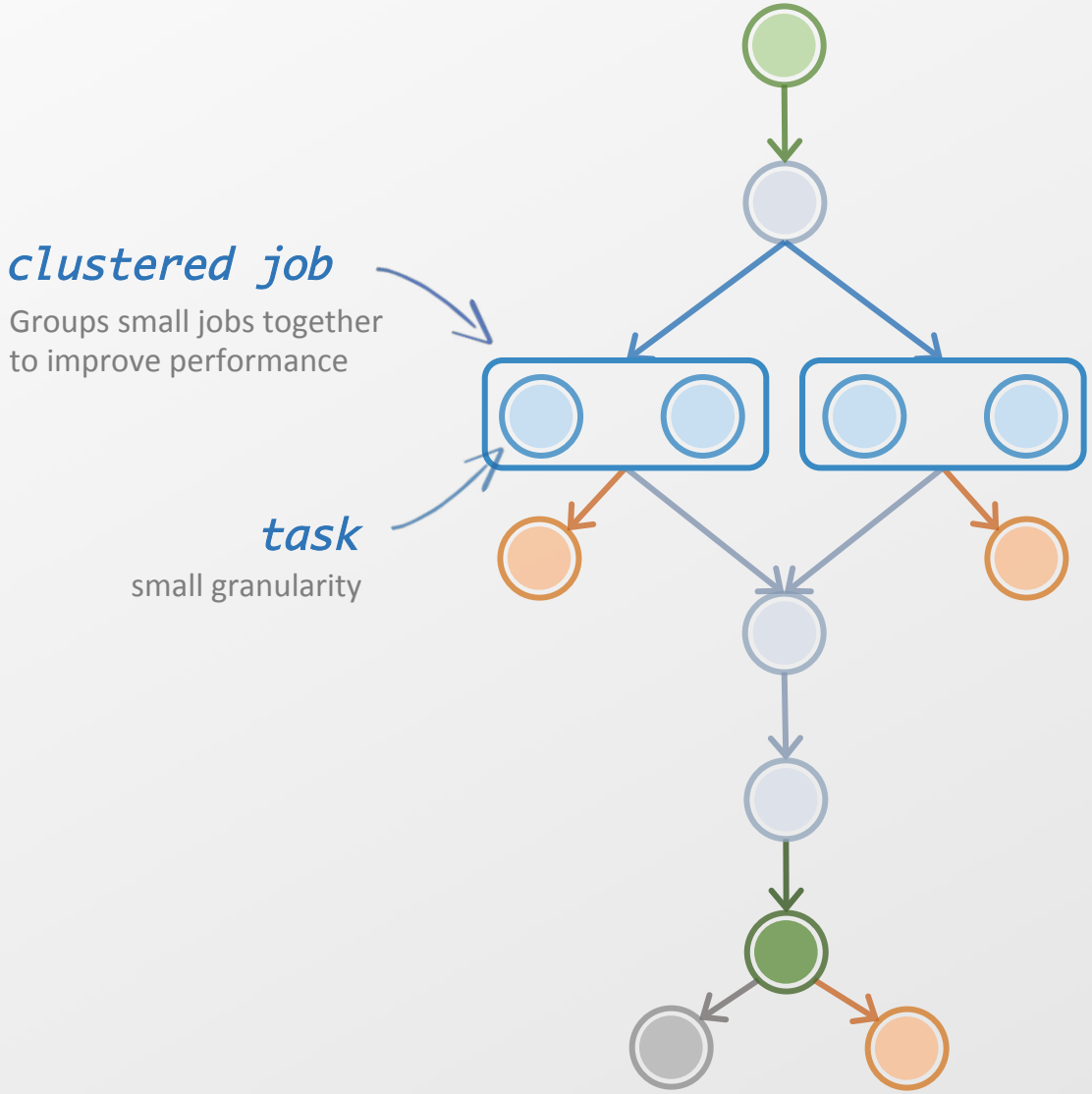
A few more features…

Performance, why not improve it?

workflow restructuring

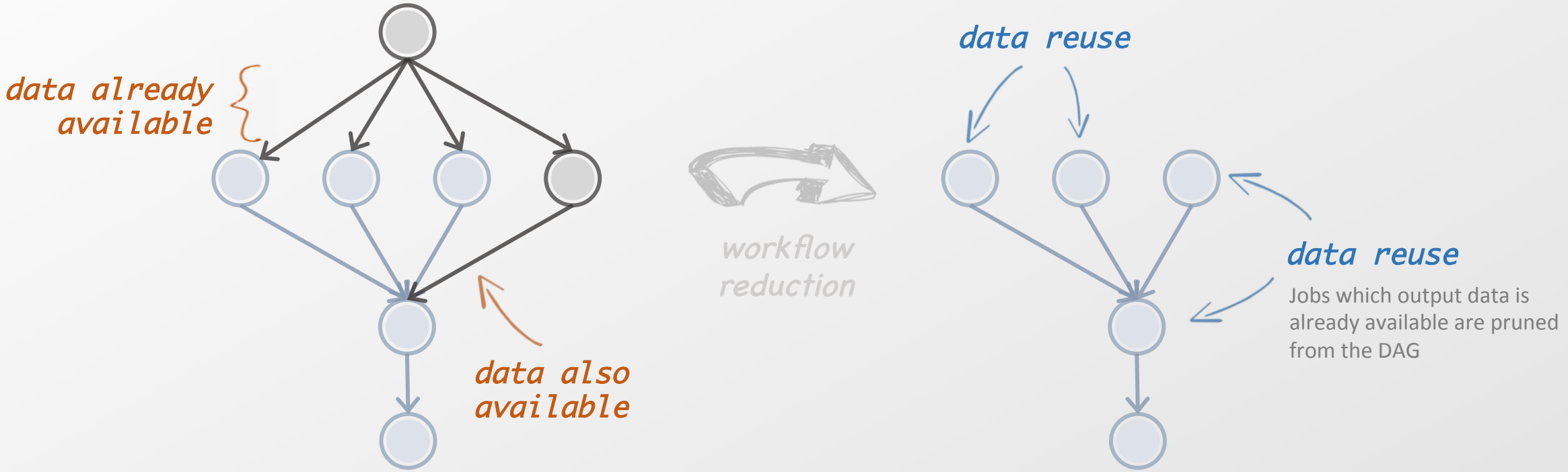
workflow reduction

hierarchical workflows



http://pegasus.isi.edu

What about data reuse?



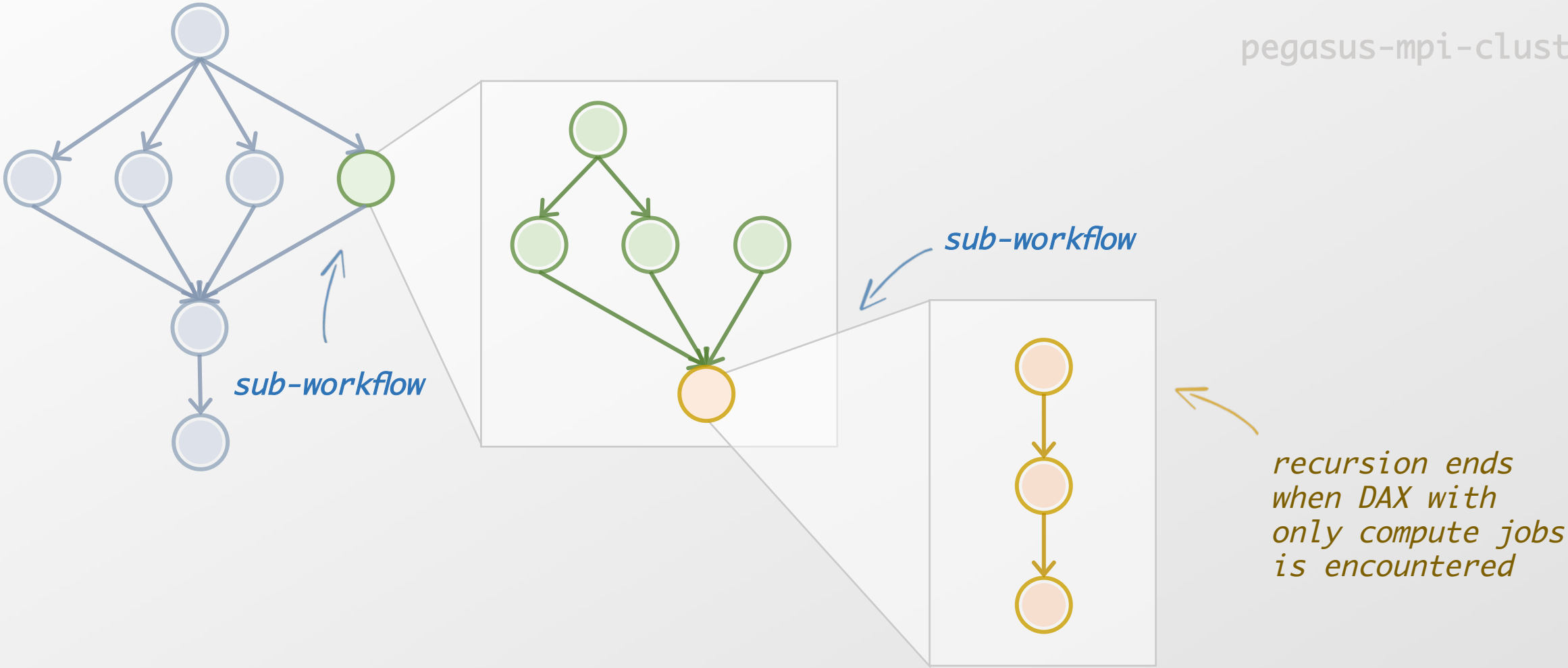
Pegasus also handles **large-scale workflows**

workflow restructuring

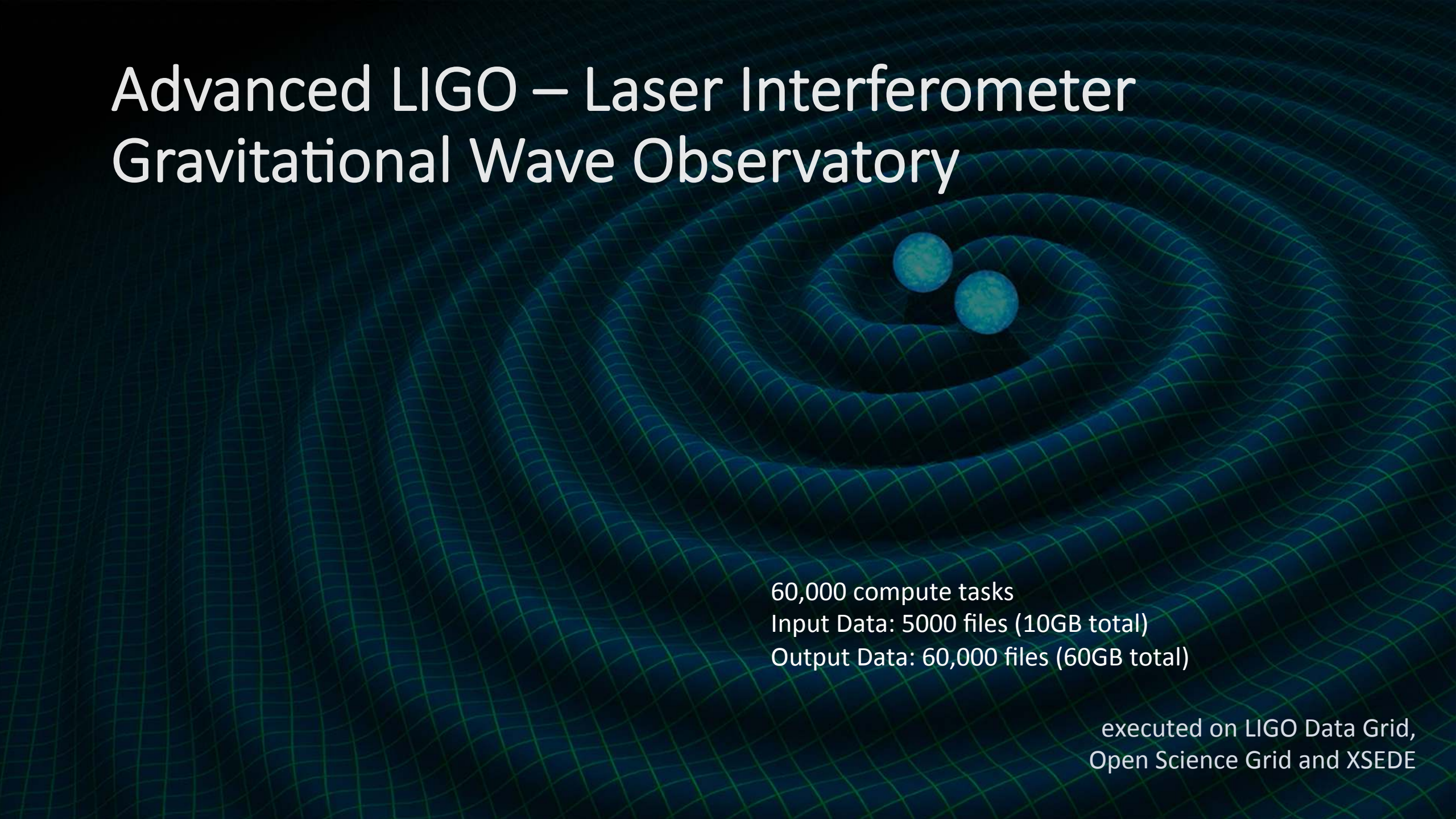
workflow reduction

hierarchical workflows

pegasus-mpi-cluster



Advanced LIGO – Laser Interferometer Gravitational Wave Observatory

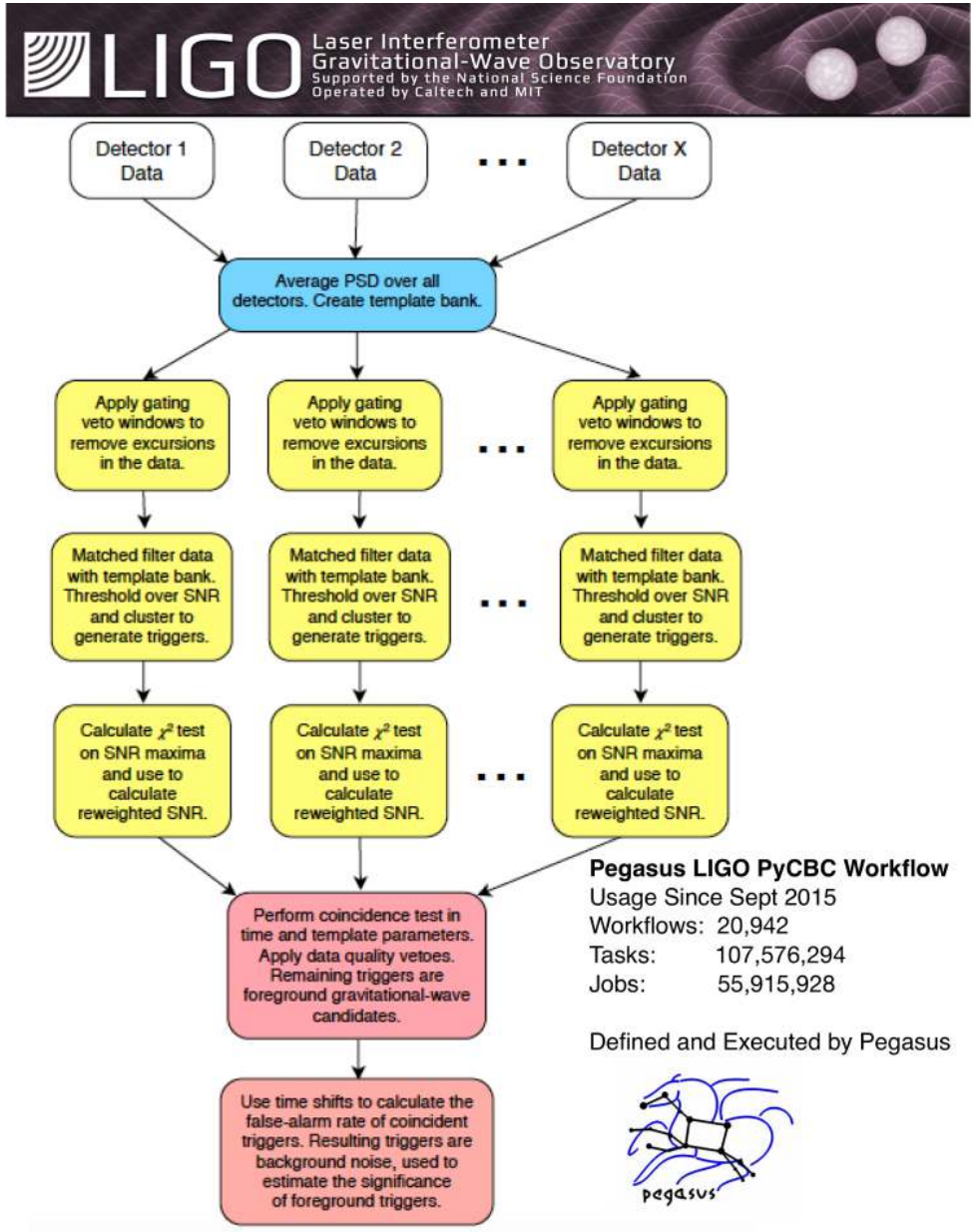


60,000 compute tasks
Input Data: 5000 files (10GB total)
Output Data: 60,000 files (60GB total)

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.*

Benefits to LIGO provided by Pegasus- Expanded Computing Horizons

- No longer limited to a single execution resource
  - Non Pegasus LIGO pipelines can often only run on LIGO clusters
  - Input is replicated out of band , in a rigid directory layout.
  - Rely on the shared filesystem to access data.

- Pegasus made it possible to leverage Non LDG Computing Resources

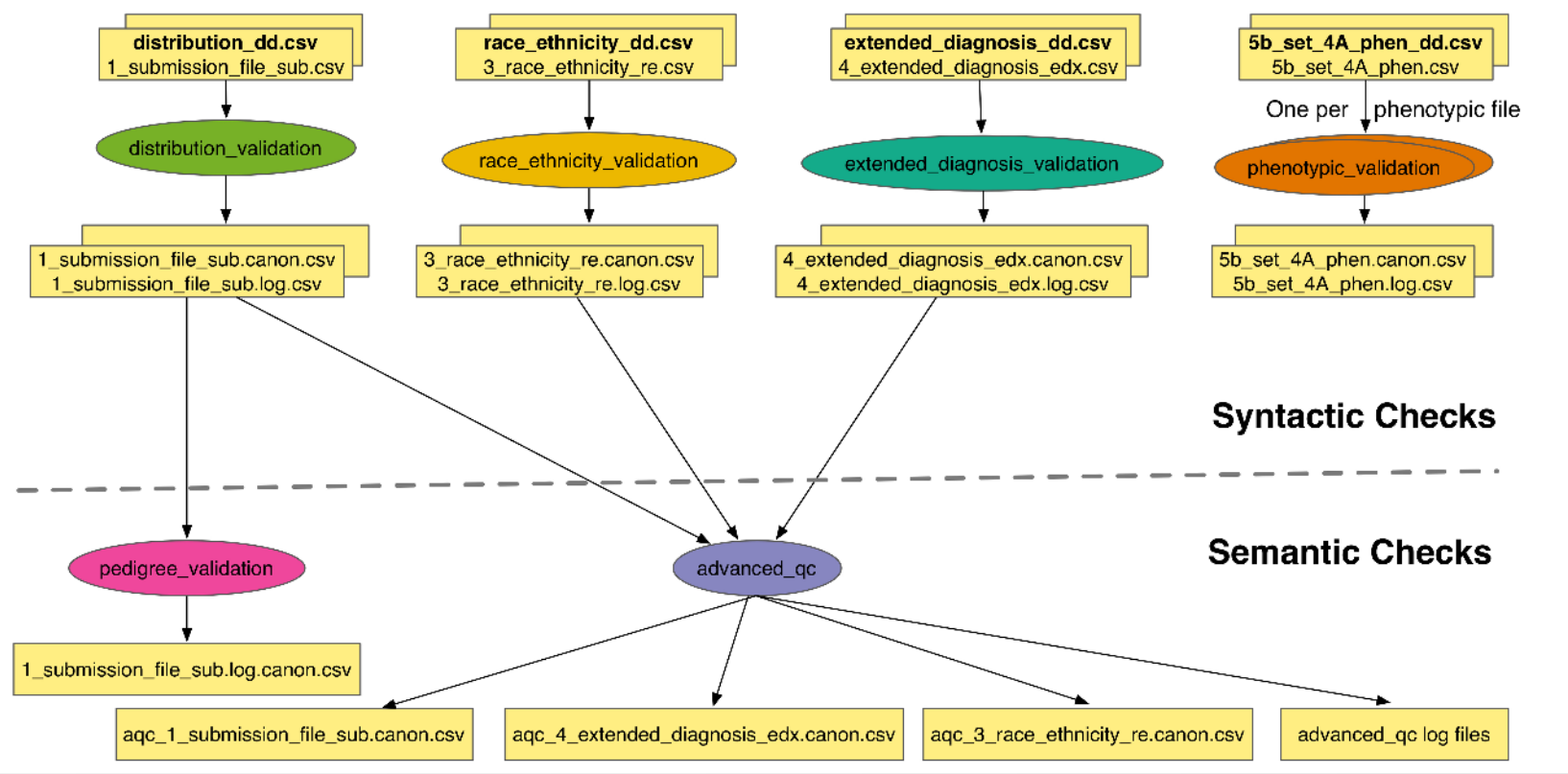
  - Open Science Grid
    - Dynamic – Best Effort Resource with no shared filesystem available

  - Large NSF Supercomputing Clusters XSEDE
    - No HTCondor
    - Geared for Large MPI jobs, not thousands of single node jobs
    - LIGO tried to setup XSEDE cluster as a LDG site but mismatch in setup.
    - Pegasus enabled LIGO to use XSEDE without changes at LIGO or at XSEDE

  - VIRGO Resources in Europe
    - Clusters with no shared filesystem and different storage management infrastructure than LDG
    - No HTCondor

Automated Quality Control Workflows for NIMH-NRGR

The NIMH Repository and Genomics Resource (NIMH-RGR) is large NIH funded center that facilitates psychiatric genetic research by providing a collection of over 150,000 well characterized, high quality patient and control bio-samples.

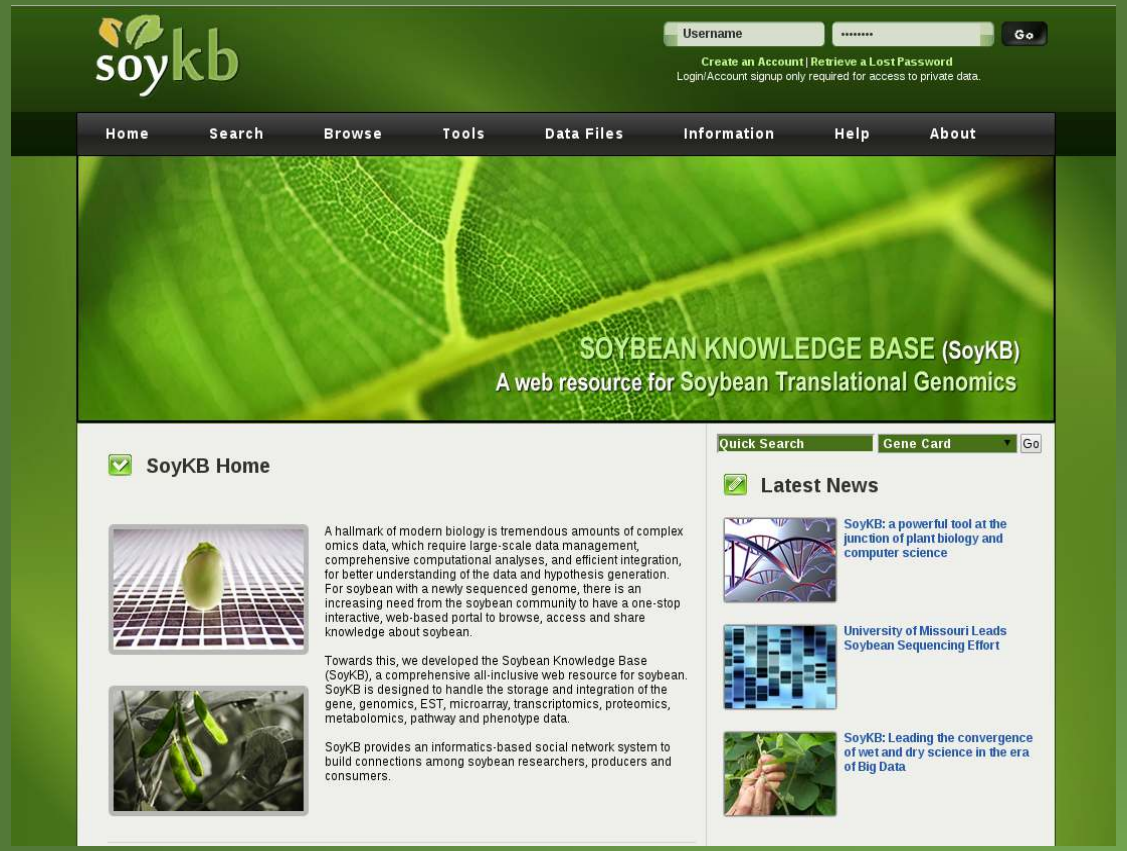


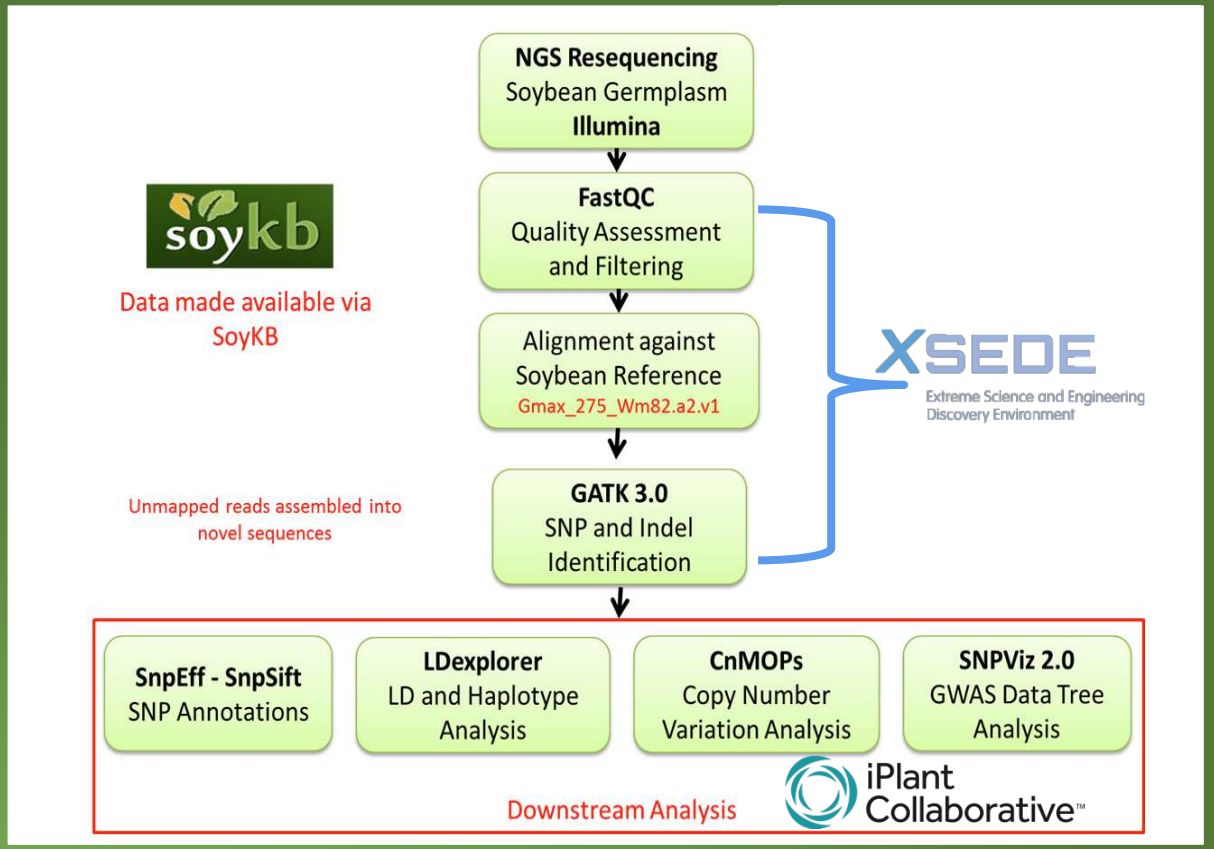
Pipeline to automate quality control checks on incoming phenotypic data to the center

Earlier curation process was manual done by analysts at the center, that was often error prone

Web based system developed on top of Pegasus WMS by the center.

https://www.nimhgenetics.org/submit_data/

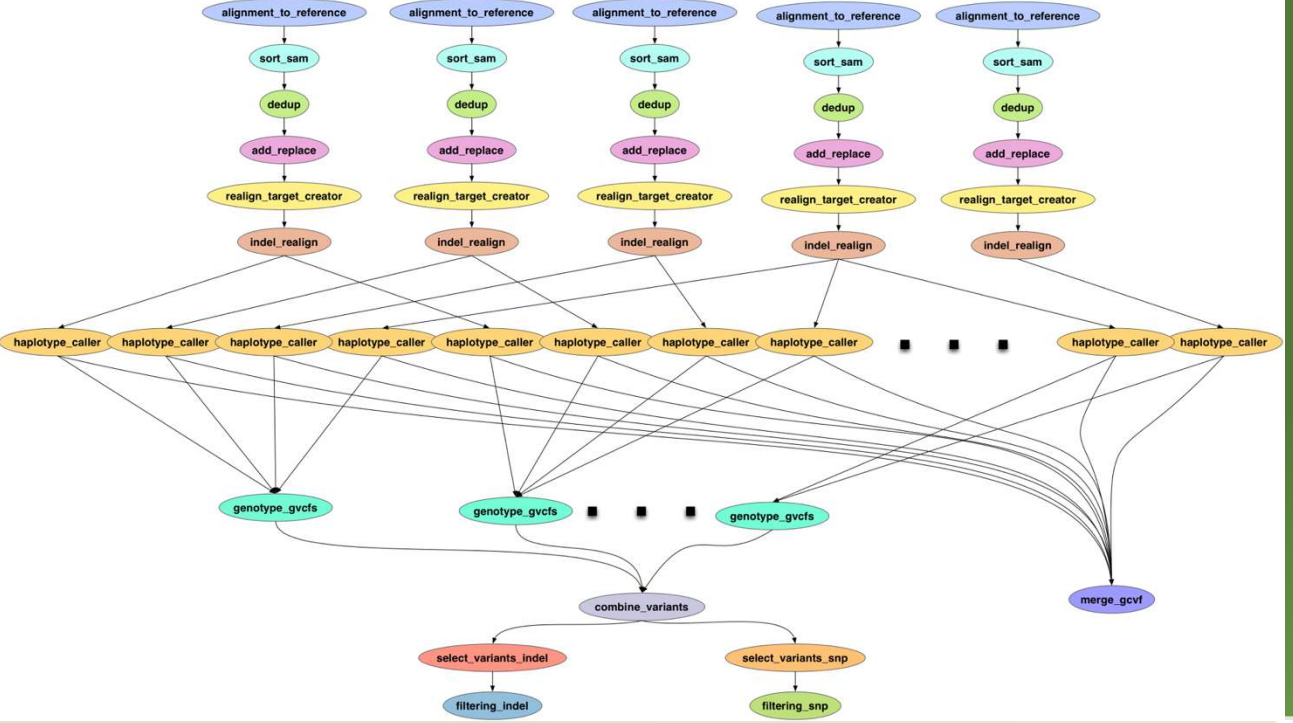




http://soykb.org

XSEDE Allocation
PI: Dong Xu
Trupti Joshi, Saad Kahn, Yang Liu, Juexin Wang, Badu Valliyodan, Jiaojiao Wang

https://github.com/pegasus-isi/Soybean-Workflow



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

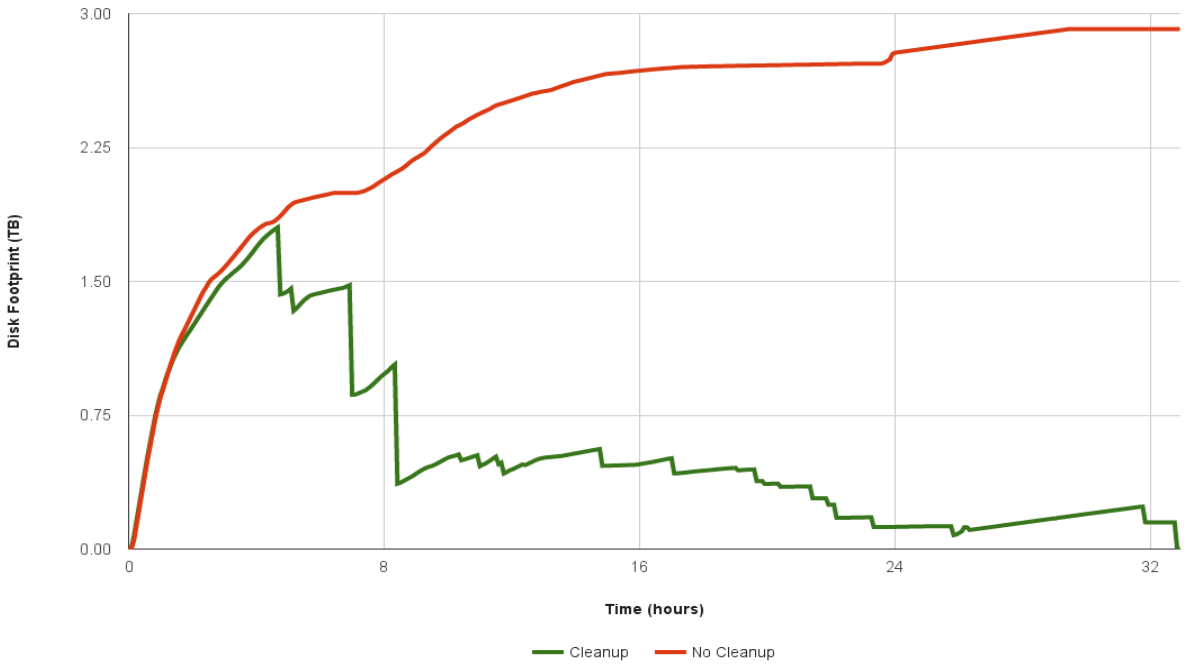
TACC Wrangler as Execution Environment

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



Pegasus est. 2001

Automate, recover, and debug scientific computations.

Get Started

Pegasus Website

http://pegasus.isi.edu

Users Mailing List

pegasus-users@isi.edu

Support

pegasus-support@isi.edu

HipChat

Pegasus est. 2001

Automate, recover, and debug scientific computations.

Thank You

Questions?

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School of Engineering
Information Sciences Institute

Meet our team


Ewa Deelman


Karan Vahi


Mats Rynge


Rajiv Mayani


Rafael Ferreira da Silva

NSF U.S. DEPARTMENT OF ENERGY NIH