CI/CS WORKSHOP

THE COMMUNITY TOGETHER

End to End Workflow Monitoring and Execution

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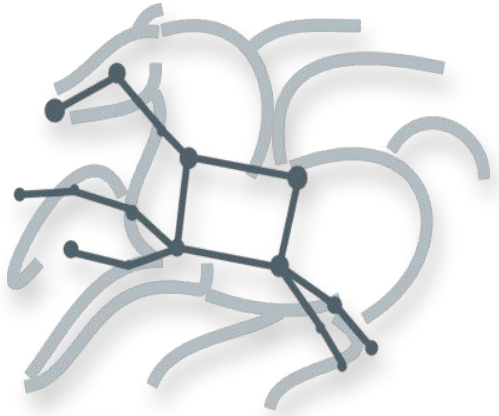
The Pegasus Workflow Management System

- Bridges the scientific domain and execution environment by **mapping high level workflow descriptions onto distributed resources**
- Enables scientists to:
  - **Automate** their work, as portable workflows
  - **Recover** from failures at runtime
  - **Debug** failures in their computations
- Built on top of HTCondor, a proven DHTC workhorse



Pegasus

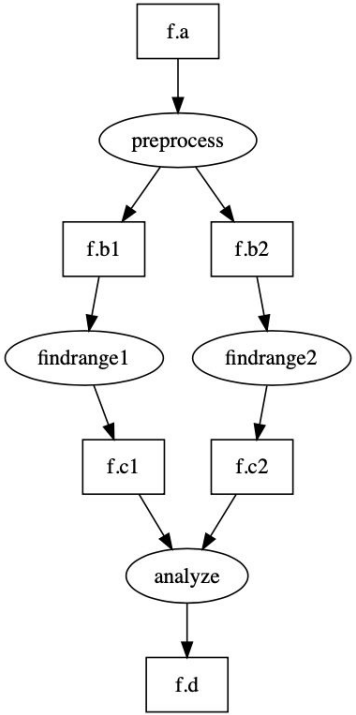
HTCondor
High Throughput Computing

Outline

- ~~Introducing the Pegasus WMS~~
- **Concepts**
- Features
- Production Use

Workflows as DAGs

- Workflows are multi-step computational tasks organized as directed acyclic graphs (DAG)
- Define abstract workflow using one of our Python, Java, or R APIs
  - Abstract in the sense that users need not map jobs to resources or create file transfer jobs for input and output files
  - Pegasus will plan the abstract workflow into an executable workflow
- Example..



Defining Workflow Inputs

```
fa = File("f.a").add_metadata(creator="ryan")
rc = ReplicaCatalog().add_replica("local", fa, Path(".").resolve() / "f.a")

preprocess = Transformation(
                "preprocess",
                site="condorpool",
                pfn="/usr/bin/pegasus-keg",
            )

findrange = Transformation(
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analyze = Transformation(
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tc = TransformationCatalog().add_transformations(preprocess, findrange, analyze)
```

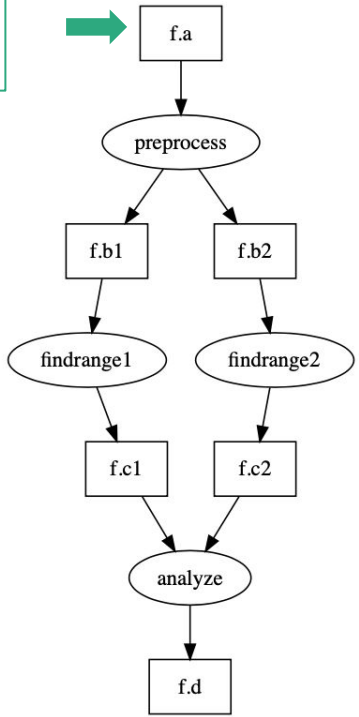

Defining Workflow Executables

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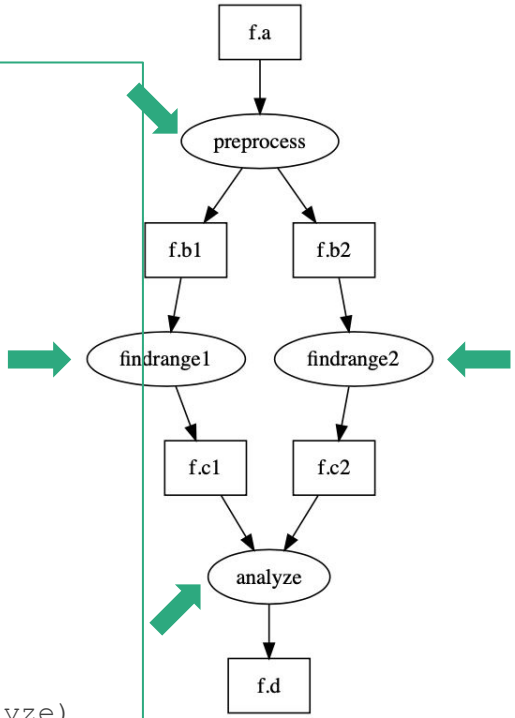

Defining the Workflow

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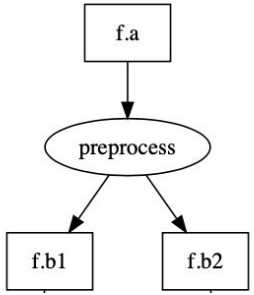

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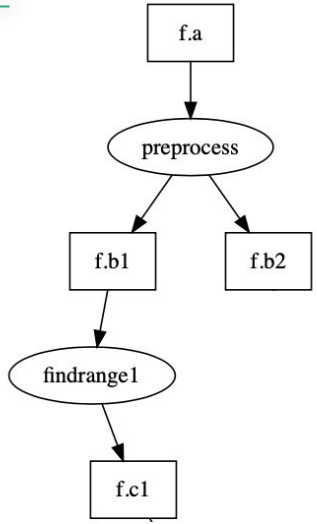

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job_findrange_2 = Job(findrange)\
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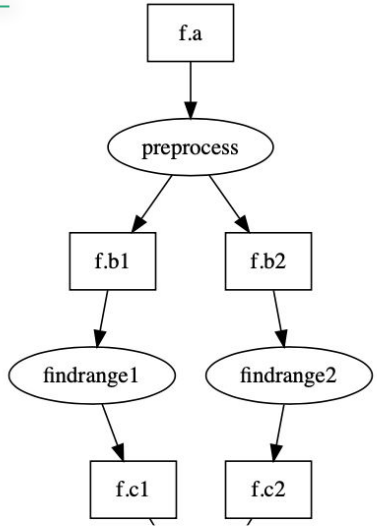

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fd = File("f.d")
job_analyze = Job(analyze)\
                .add_args("-a", "analyze", "-T", "3", "-i", fc1, fc2, "-o", fd)\
                .add_inputs(fc1, fc2)\
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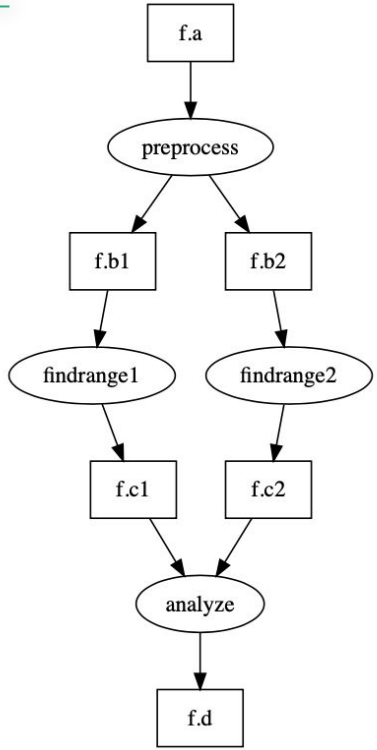
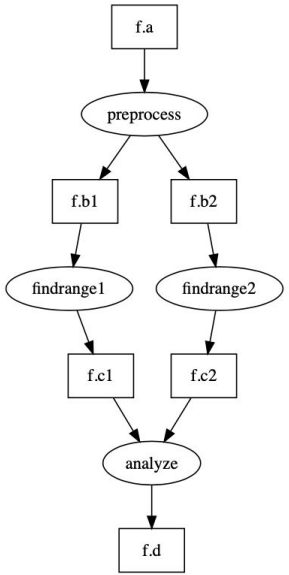


Workflow Planning

- Workflow planning process
  - Data reuse module will optionally prune jobs for which output files already exist
  - Task clustering optimizations may be performed for small independent jobs
  - Mapping jobs onto physical compute resources
  - Add auxiliary jobs for data staging, cleanup, file registration, etc.
- Generated executable workflow submitted to through HTCondor to be run



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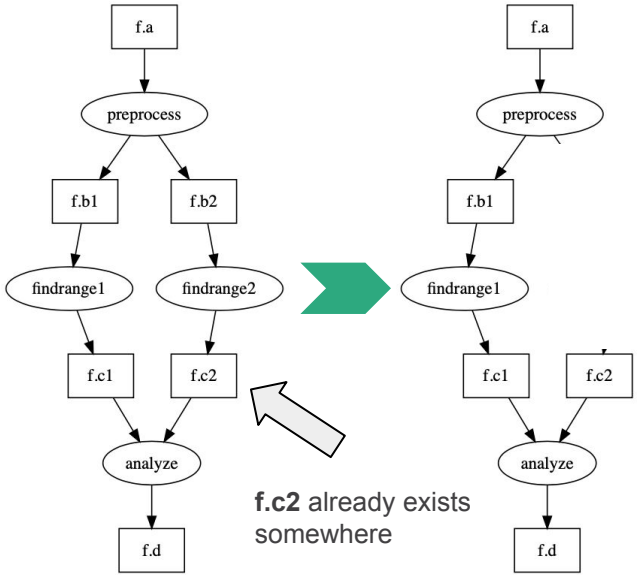

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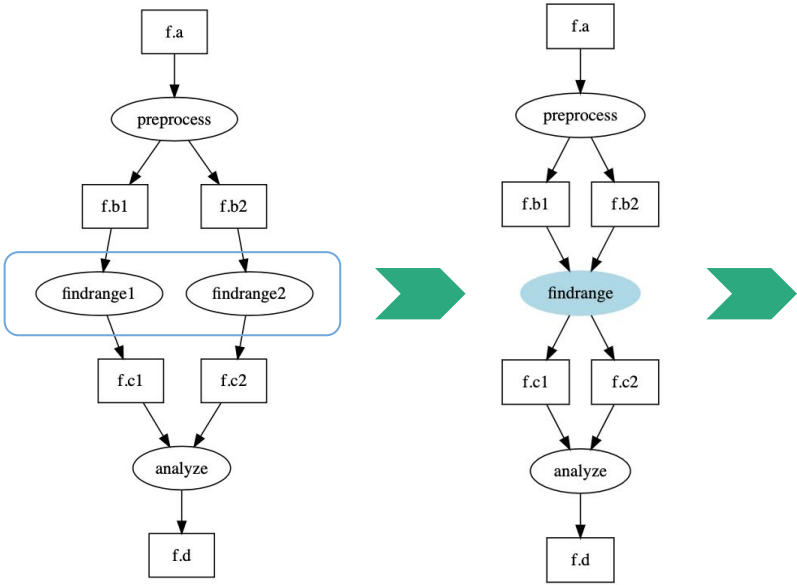

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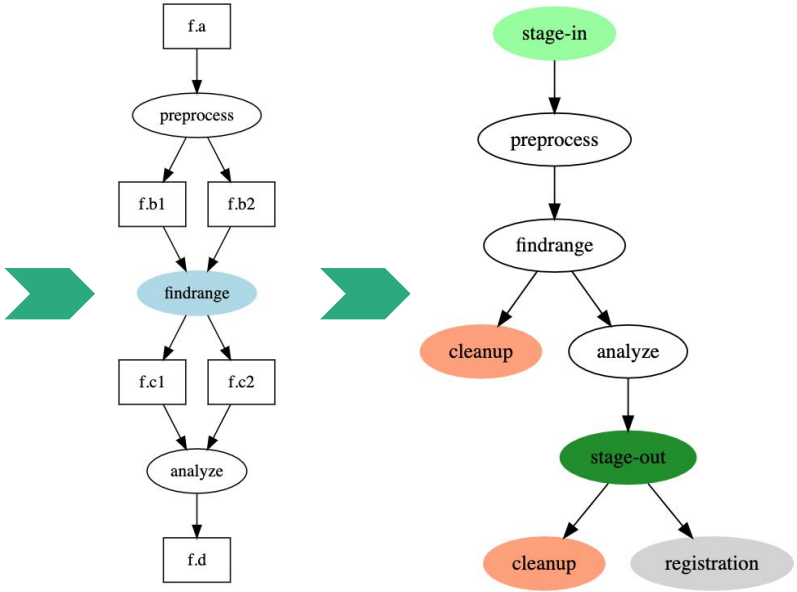

Outline

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- ~~Concepts~~
- **Features**
- Production Use

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
  - Submit host used as staging site
- 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
  - Internal file transfer tool “pegasus-transfer” handles all file transfers
- Shared File System (HPC sites, XSEDE, campus clusters, …)
  - I/O directly against the shared file system

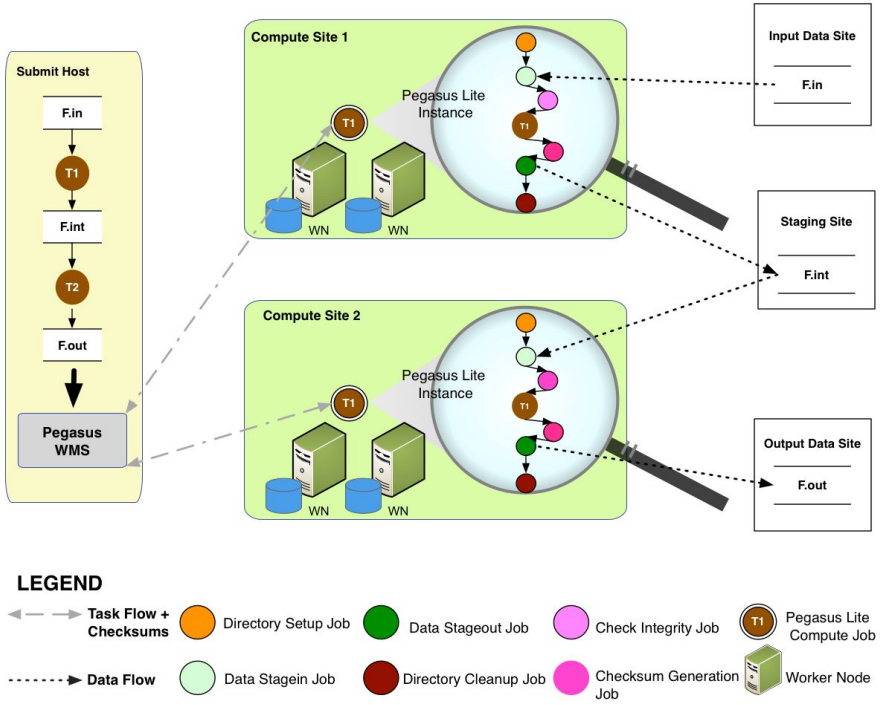
pegasus-transfer internal file transfer utility

- Directory creation, file removal
- Two stage transfers between incompatible protocols
  - E.g., GridFTP to S3 is executed as: GridFTP to local file, local file to S3
- Parallel transfers
- Automatic retries
- Credential management

```
HTTP
SCP
GridFTP
Globus Online
iRods
Amazon S3
Google Storage
SRM
FDT
Stashcp
Rucio
cp
ln -s
```

Automatic Integrity Checking

- Pegasus automatically performs integrity checksums on input files right before jobs begin
  - Checksums can be specified for inputs coming from external sources
  - All intermediate and output files have checksums which are generated and tracked within the system
- Checksum validation failure results in job failure

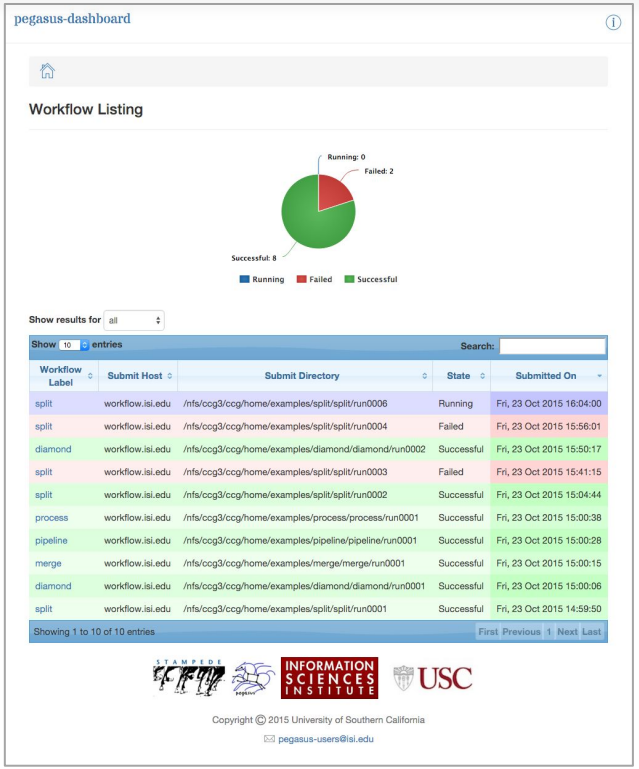


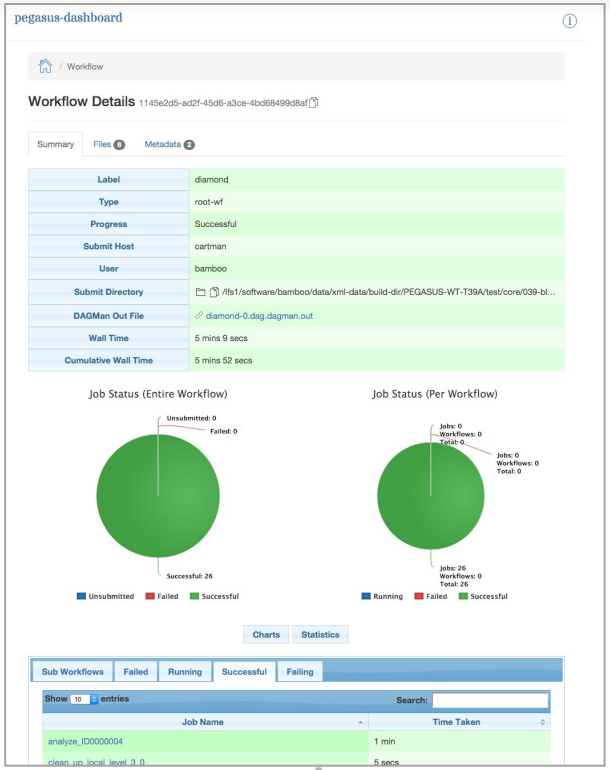
Monitoring and Debugging Tools CLI

- pegasus-status
  - View current status of running workflow
  - View summary of jobs and sub workflows
- pegasus-analyzer
  - View errors from any failed jobs
- pegasus-statistics
  - View summary of workflow statistics
  - Succeeded jobs, failed jobs, retries, workflow walltime, etc.

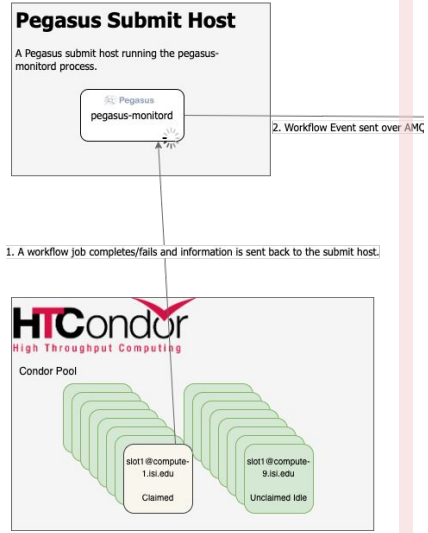
```
$ pegasus-status -l /Workflow/dags/directory
STAT  IN_STATE  JOB
Run       07:01  level-3-0
Run       06:25   |-sleep_ID000005
Run       06:20   \_subdax_level-2_ID000004
Run       05:44      |-sleep_ID000003
Run       05:39      \_subdax_level-1_ID000002
Run       05:03         \_sleep_ID000001
Summary: 6 Condor jobs total (R:6)

UNRDY READY   PRE  IN_Q  POST  DONE  FAIL %DONE STATE   DAGNAME
    0     0     0     1     0     1     0  50.0 Running level-2_ID
    0     0     0     2     0     1     0  33.3 Running level-2_ID
    0     0     0     3     0     1     0  25.0 Running *level-3-0
    0     0     0     6     0     3     0  33.3         TOTALS (9
 Summary: 3 DAGs total (Running:3)
```

Monitoring and Debugging Tools dashboard





Monitoring and Debugging Tools AMQP endpoint



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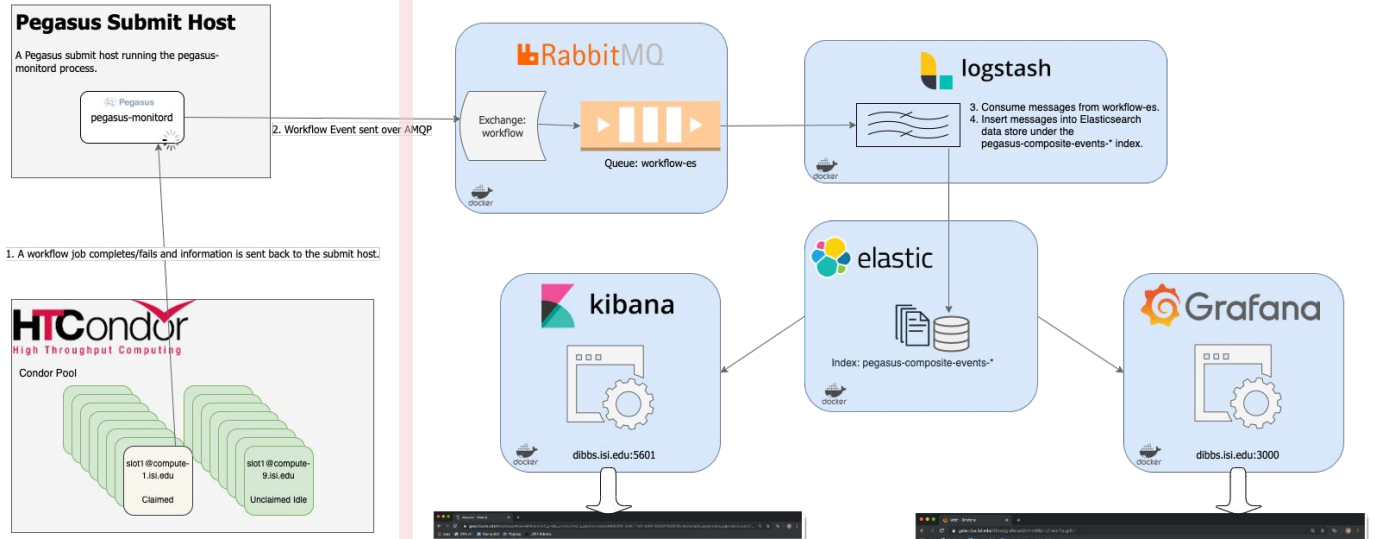
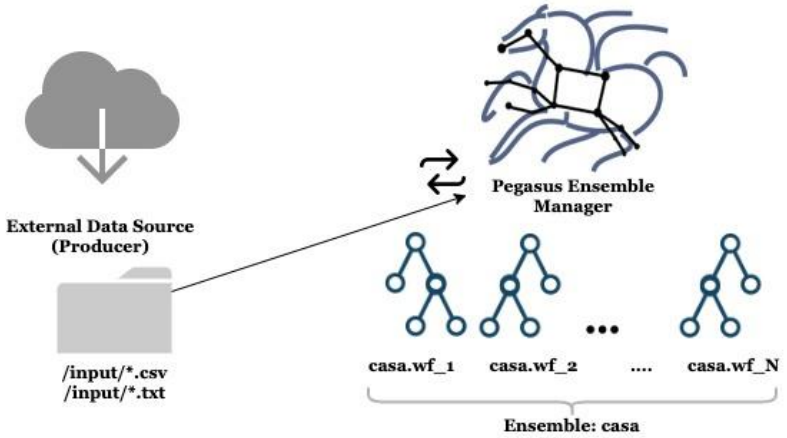


5. Workflow events can be conveniently viewed through the Kibana web interface

5. Interactive visualizations can be viewed through the Grafana web interface.

Ensemble Manager workflow management & dynamic triggering

- Service for managing collections of workflows called ensembles
- Allows for throttling of concurrent planning and running workflows
- Support for triggering of new workflow runs based on arrival of new input files which match one or more given patterns



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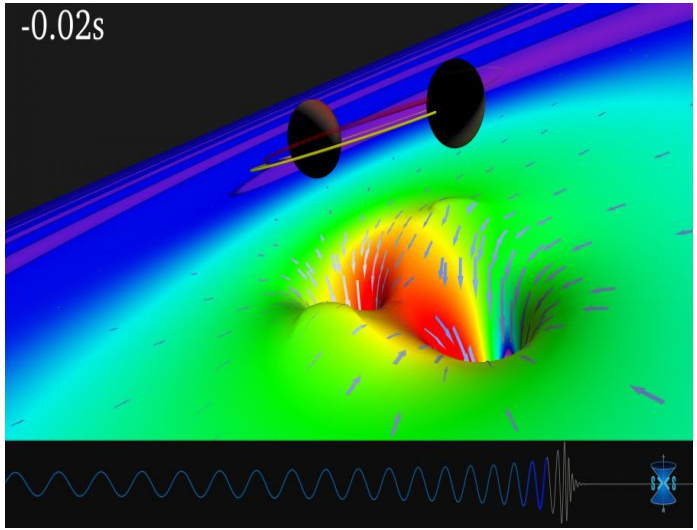
- ~~Features~~
- **Production Use**

LIGO PyCBC Workflows for Gravitational Wave Science

- Laser Interferometer Gravitational Wave Observatory
  - Facility for gravitational wave research
  - Methods:
    - PyCBC software package
    - Pegasus WMS workflows
    - Compute using OSG, XSEDE, etc.

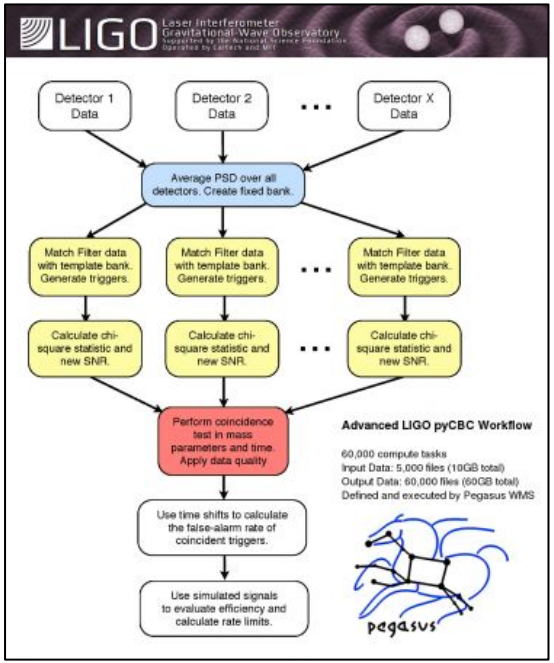
What do these workflows look like..



0.2 Second before the black holes collide.
Image credit: SXS/LIGO

LIGO PyCBC Workflows for Gravitational Wave Science

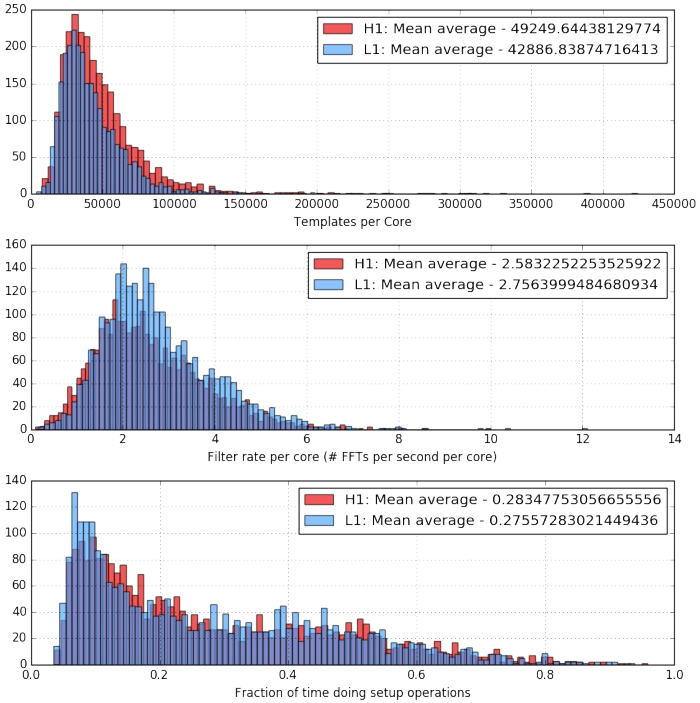
- Advanced PyCBC Workflows
  - 40,000 compute tasks
  - 1,100 input files
  - 63 output files
  - 725 GB processed data
  - Compute: LIGO Data Grid, OSG, EGI, XSEDE



Advanced LIGO pyCBC Workflow. Image Credit: Samantha Usman, Duncan Brown et al

LIGO PyCBC Workflows for Gravitational Wave Science

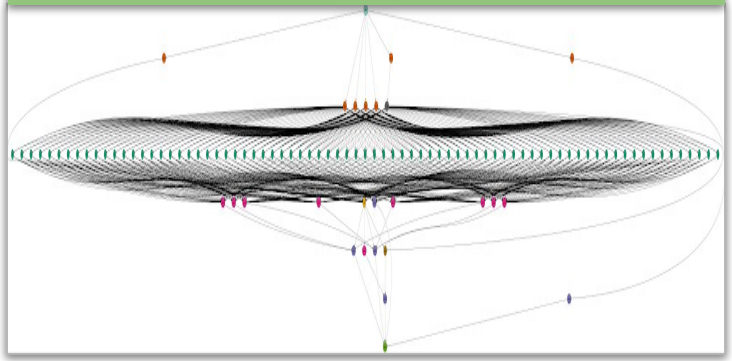
- Plots typically generated as part of post run analysis
- Using the AMQP data collection setup, these charts are able to be updated live as jobs complete, affording LIGO researchers better monitoring capabilities of the PyCBC workflow runs



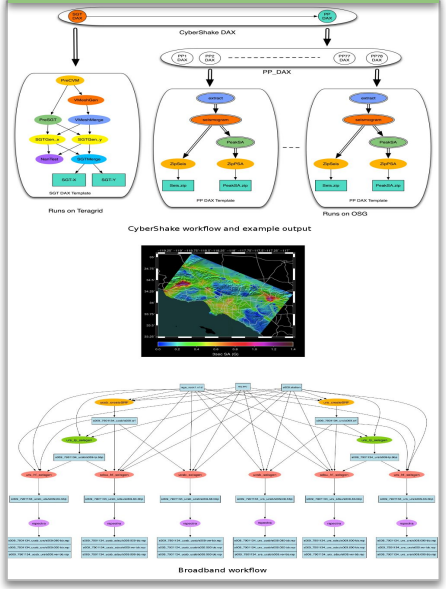
Other Production Use

In the last 12 months, Pegasus users ran **240K workflows**, **145M jobs**

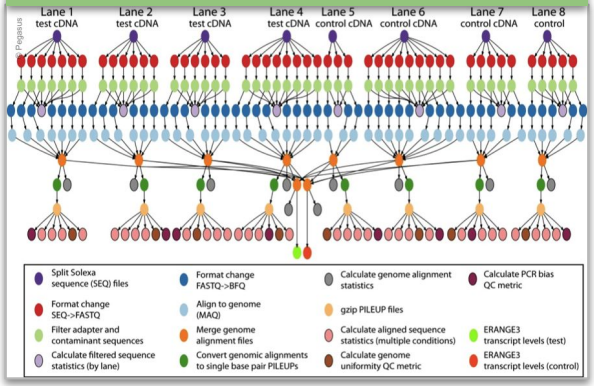
XENONnT - Dark Matter Search



SCEC CyberShake



Epigenomics (USC)



Pegasus est. 2001

Automate, recover, and debug scientific computations

Pegasus5.0 coming soon! Beta1 is out.

Get Started

Pegasus Online Office Hours

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

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

Pegasus Website

https://pegasus.isi.edu/

Users Mailing List

pegasus-users@isi.edu

Pegasus Website

pegasus-support@isi.edu

Pegasus office hours

USC Viterbi
Information Sciences Institute

Questions?

Thank you!

tanaka@isi.edu