Pegasus – Enhancing LIGO DAGMan Experience

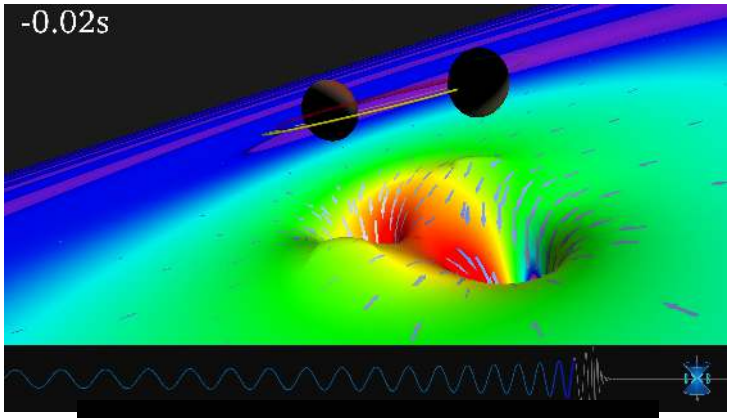
Karan Vahi

Science Automation Technologies Group

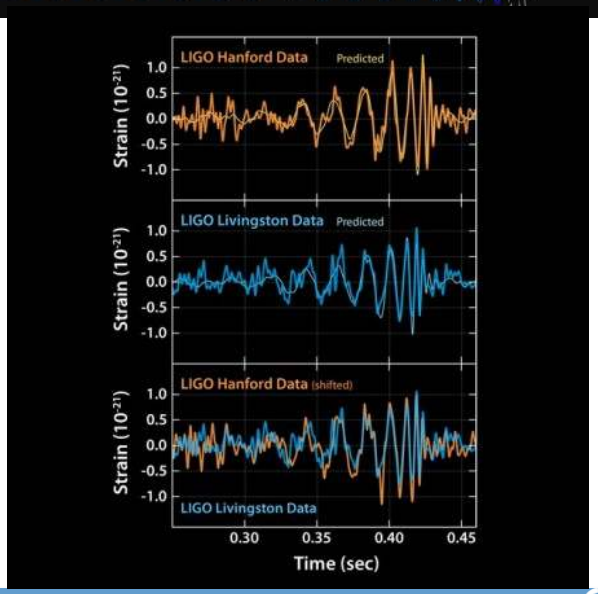
USC Information Sciences Institute

LIGO Gravitational Wave Detection

- **LIGO recently announced first ever detection of gravitational waves.**
  - Created as a result of coalescence of a pair of dense, massive black holes.
  - Confirms major prediction of Einstein Theory of Relativity



- **Detection Event**
  - Detected by both of the operational Advanced LIGO detectors (4km long L shaped interferometers)
  - Event occurred at September 14, 2015 at 5:51 a.m. Eastern Daylight Time



Detection Paper: Observation of Gravitational Waves from a Binary Black Hole Merger B. P. Abbott et al. (LIGO Scientific Collaboration and Virgo Collaboration) Phys. Rev. Lett. 116, 061102 – Published 11 February 2016

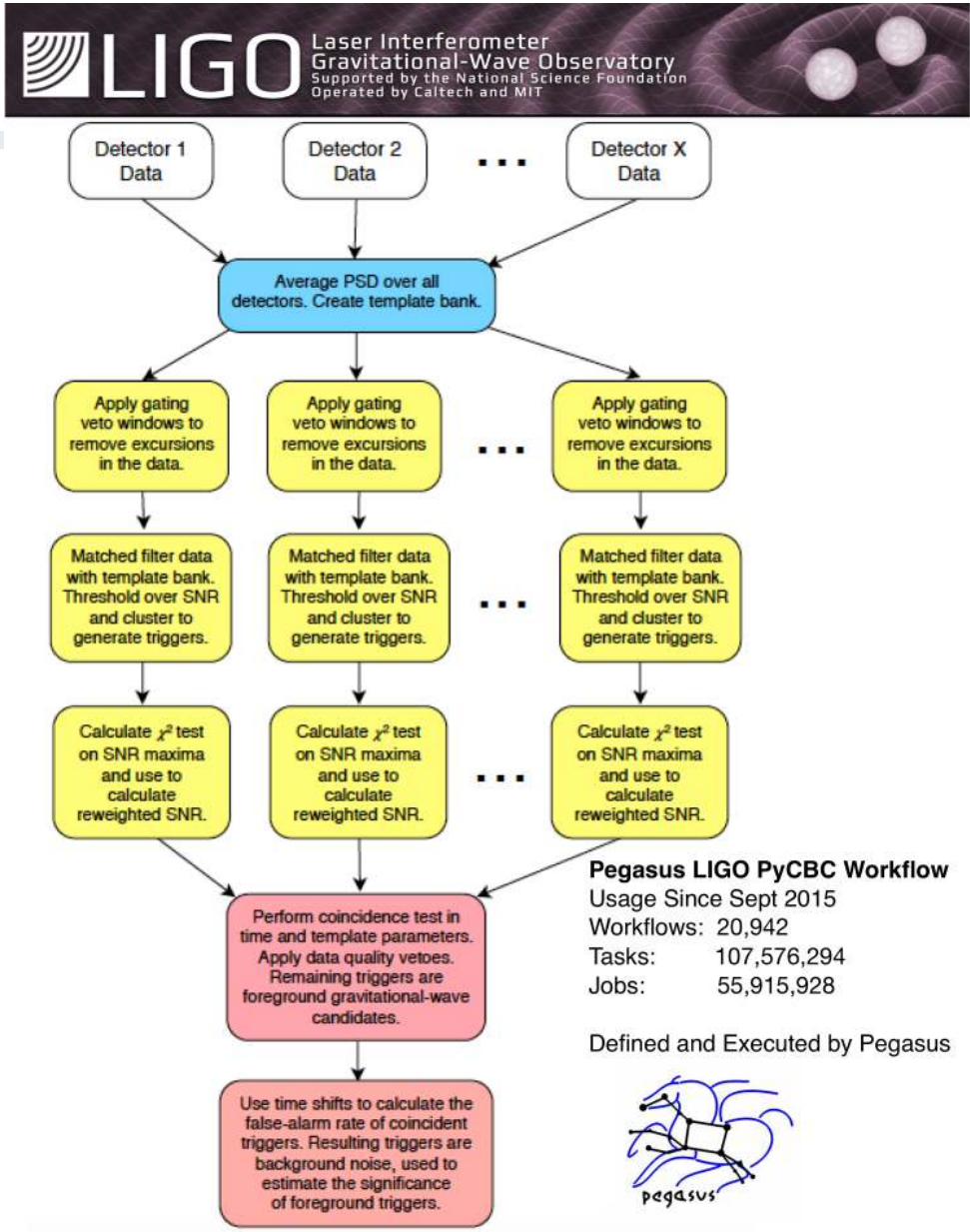
Image Credits: *0.2 Second before the black holes collide: SXS/LIGO*
Signals of Gravitational Waves Detected: Caltech/MIT/LIGO Lab

LIGO Detection – Behind the Scenes

- **A variety of complex analysis pipelines were executed.**
- **Some were low latency that initially alerted people to look at a specific piece of data containing the signal.**
- **However, to verify that signal is a valid candidate,**
  - a large amount of data needs to be analyzed.
  - Statistical significance of the detection should be at 5-sigma level
- **Pipelines are mainly executed on LSC Data Grid**
  - Consists of approximately 11 large clusters at various LIGO institutions and affiliates
  - Each cluster has Grid middleware and HTCondor installed.
  - GridFTP used for data transfers.
- **Pipelines are modeled as scientific workflows**

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.
- **Exclusively managed by Pegasus WMS and an earlier version was used for the blind injection test in 2011**
- For the detection, the pipeline was executed on Syracuse and Albert Einstein Institute Hannover

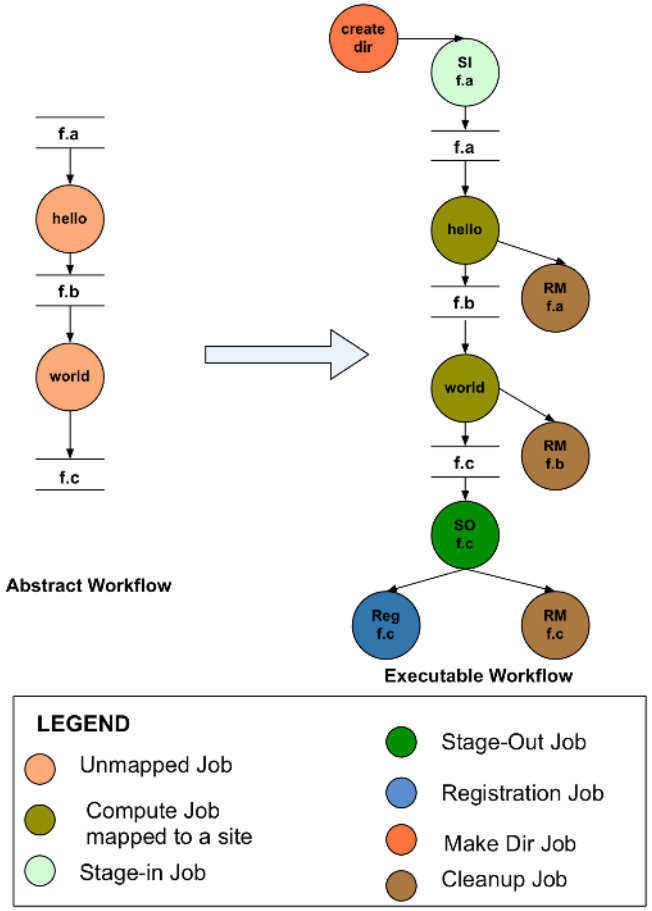


PyCBC Paper: An improved pipeline to search for gravitational waves from compact binary coalescence. *Samantha Usman, Duncan Brown et al.*

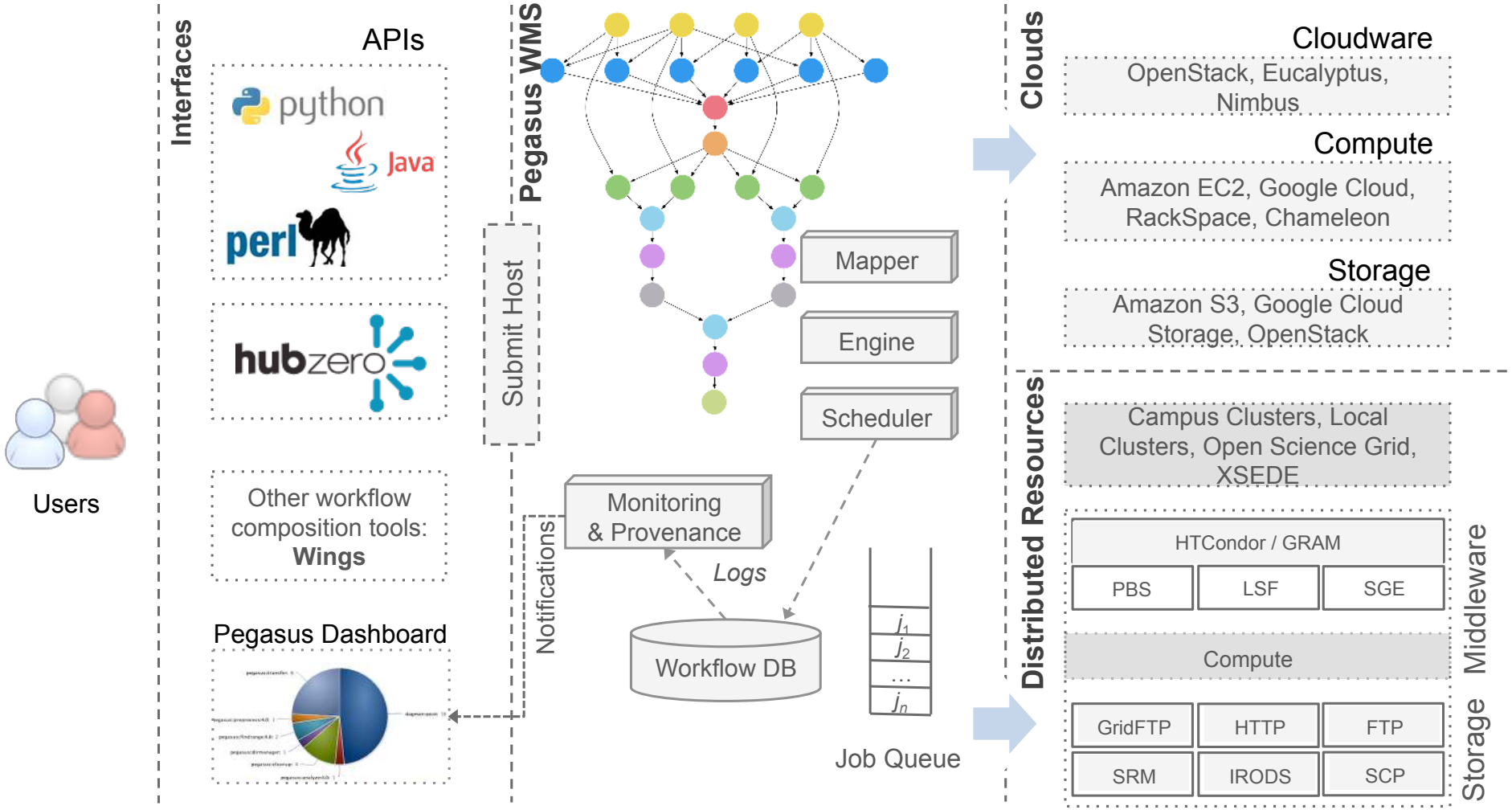
PyCBC Detection GW150914: First results from the search for binary black hole coalescence with Advanced LIGO. *B. P. Abbott et al.*

Pegasus Workflow Management System

- **NSF funded project since 2001**
  - Developed as a collaboration between USC Information Sciences Institute and the HTCondor Team at UW Madison
- **Builds on top of HTCondor DAGMan.**
- **Abstract Workflows - Pegasus input workflow description**
  - Workflow "high-level language"
  - Only identifies the computation, devoid of resource descriptions, devoid of data locations
  - File Aware – For each task you specify the input and output files
- **Pegasus is a workflow "compiler" (plan/map)**
  - Target is DAGMan DAGs and Condor submit files
  - Transforms the workflow for performance and reliability
  - Automatically locates physical locations for both workflow components and data
  - Collects runtime provenance



Pegasus Deployment



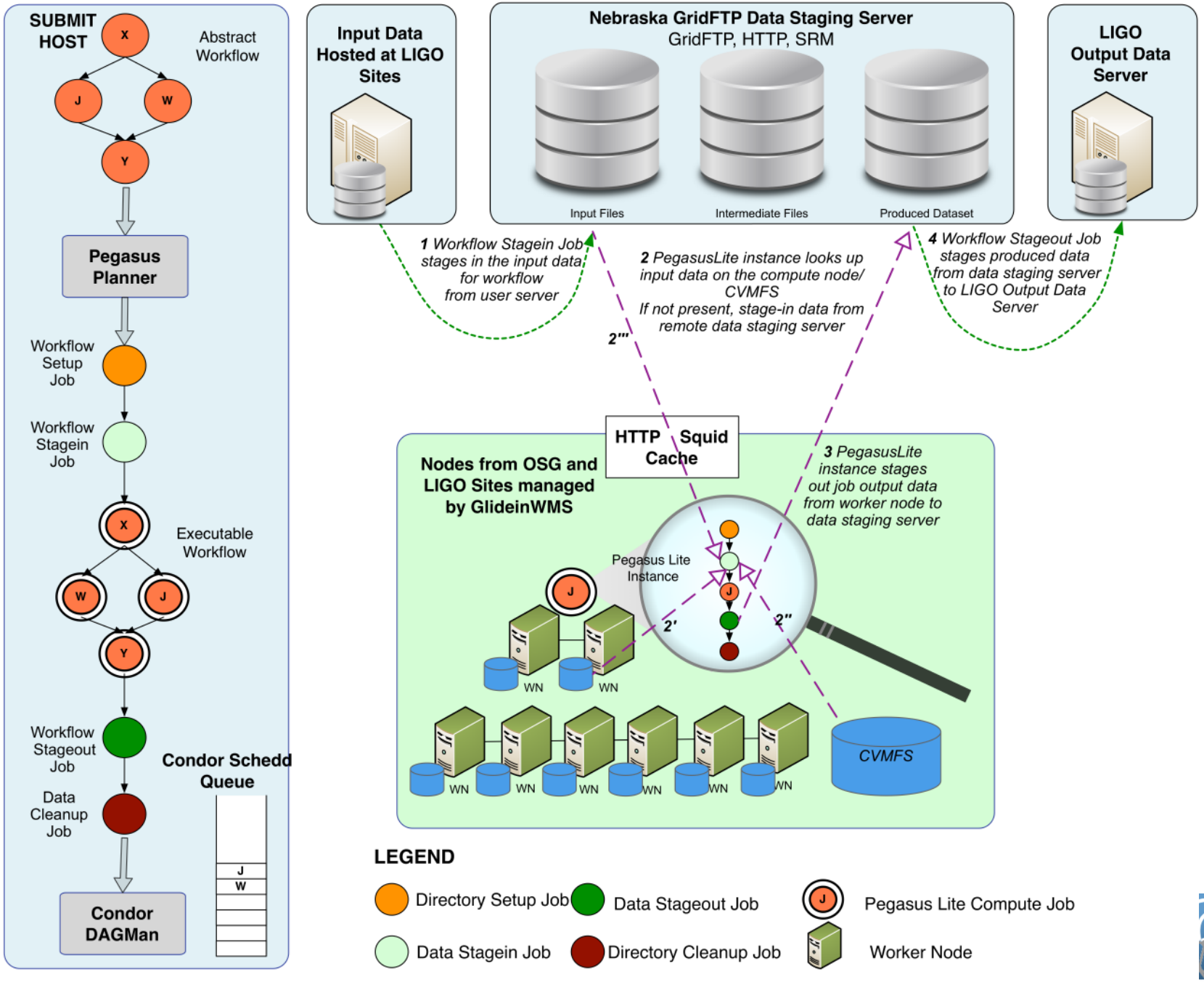
Benefits to LIGO provided by Pegasus- Expanded Computing Horizons

- **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.

- **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

- **Pegasus enables users to run workflows across different computing environments!**

Data Flow for LIGO Pegasus Workflows in OSG



LIGO on XSEDE

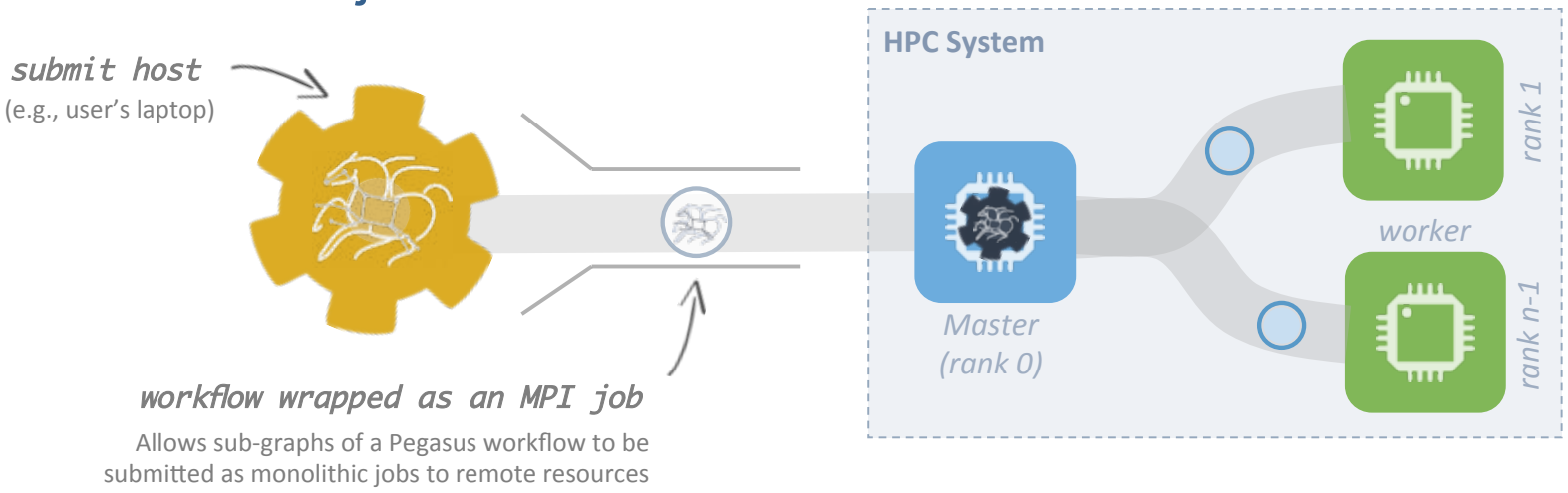
- **Problem: Many scientific workflows are fine-grained**
  - Thousands of tasks
  - Short duration
  - Serial
- **Collectively, these tasks require distributed resources to finish in a reasonable time, but individually they are relatively small**
  - Touch many GB or TB of data
  - Consume thousands of CPU hours
- **Many large-scale compute resources are optimized for a few, large, parallel jobs, not many small, serial jobs**
  - Serial tasks face long queue times due to low priority
  - Batch schedulers have low throughput

Results in poor workflow performance

Pegasus MPI Cluster

Solution: Pegasus-MPI-Cluster

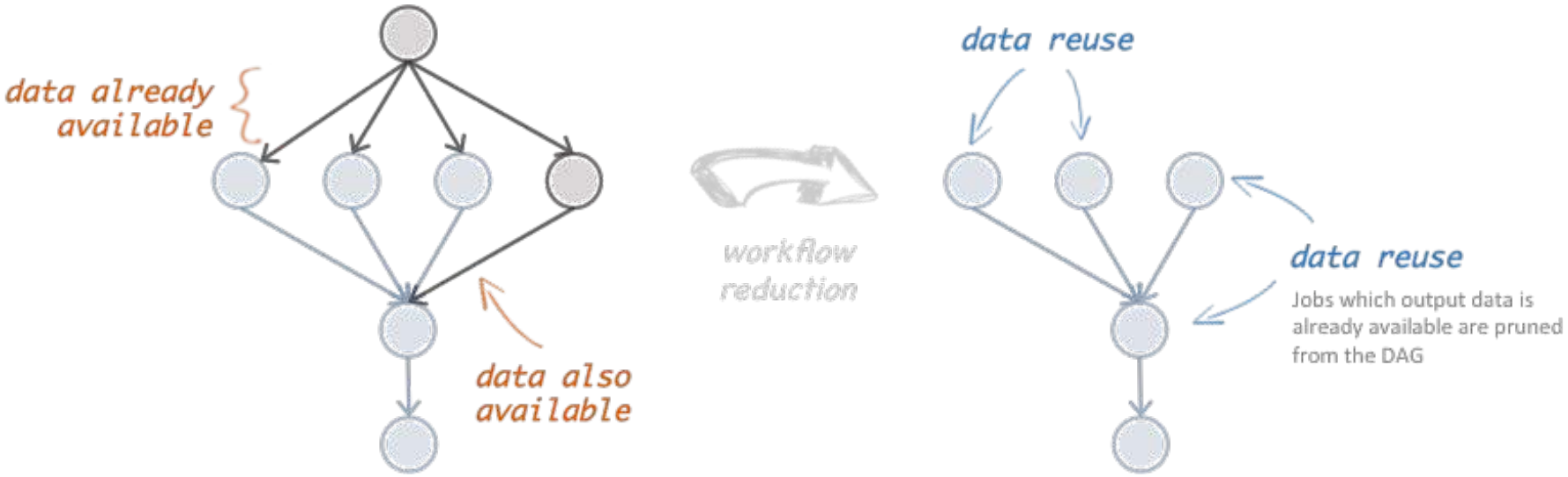
- A master/worker task scheduler for running fine-grained workflows on batch systems
- Runs as an MPI job
  - Uses MPI to implement master/worker protocol
- Allows sub-graphs of a Pegasus workflow to be submitted as monolithic jobs to remote resources



Benefits to LIGO provided by Pegasus- Smart Data Management

- **Automated Discovery of Data**
  - Symlink against locally available inputs
  - Fallback to remote file servers if data not available locally
  - Support for retrieving data using various protocols
- **Automated Cleanup of Data**
  - Data that is no longer required is automatically cleaned up.
  - **Reduces peak storage requirements.**
- **Data Reuse**
  - If output data is already computed or exists, Pegasus automatically prunes the pipeline accordingly
  - **Reduces amount of computing resources used!**
- **Job Checkpoint Files**
  - Long running jobs write out checkpoint files that are managed by Pegasus
  - **Can run long running jobs on sites where limits on runtime of a single job.**

Reusing Data Products

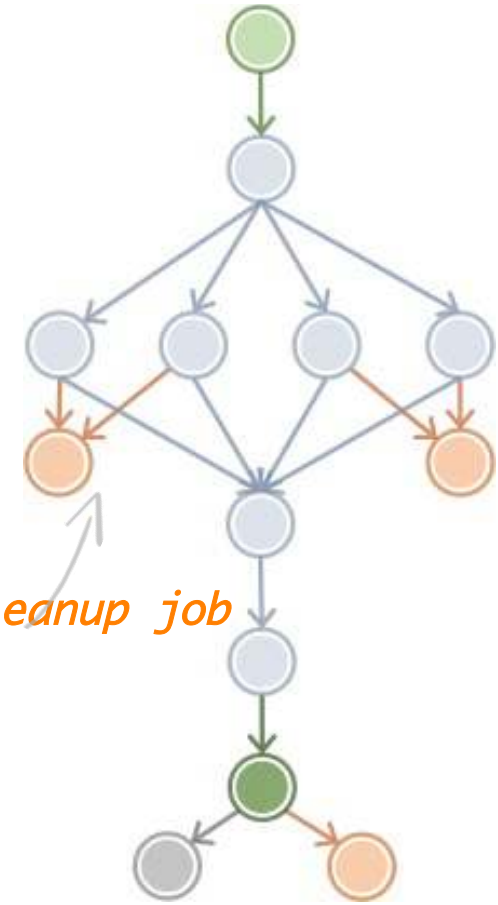


Solution: Workflow Reduction

- Don’t execute jobs at runtime for which data products already exist.
- Similar to make style semantics for compiling code

File cleanup

- **Solution**
  - **Do cleanup after workflows finish**
    - Does not work as the scratch may get filled much before during execution
  - **Interleave cleanup automatically during workflow execution.**
    - Requires an analysis of the workflow to determine, when a file is no longer required
  - **Cluster the cleanup jobs by level for large workflows**
    - Too many cleanup jobs adversaly affect the walltime of the workflow.



Benefits to LIGO provided by Pegasus- Performance Improvements

- **Task Clustering**
  - LIGO workflows are mix of long running and short running tasks.
  - Pegasus clusters short running tasks into larger chunks to overcome scheduling overheads.
  - LIGO used Pegasus MPI Cluster framework for running large workflows on XSEDE.
    - Sub graphs of Pegasus Workflows submitted to remote resources as single MPI job.
- **Separation of Directories**
  - Non Pegasus LIGO pipelines rely on the shared filesystem of clusters
  - Use of Pegasus allowed workflow submit directories to be moved to local filesystems

Benefits to LIGO provided by Pegasus- Monitoring and Debugging

- **Failure Recovery**
  - Automatic retry of failed jobs as a workflow is running
  - Workflows can be restarted from they left off
- **Debug and Monitor Workflows**
  - 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
- **Pegasus Dashboard**
  - Used by LIGO users to monitor and debug workflows
- **Especially useful for LIGO users because of the size of their workflows!**

Pegasus Dashboard

Workflow Wall Time	5 days 1 hour
Workflow Cumulative Job Wall Time	2065 days 10 hours
Cumulative Job Walltime as seen from Submit Side	2066 days 23 hours
Workflow Cumulative Badput Time	58 mins 32 secs
Cumulative Job Badput Walltime as seen from Submit Side	1 hour 32 secs
Workflow Retries	5

Workflow Statistics

Job Breakdown Statistics

Workflow Statistics

Show 10 entries — Search:

Transformation	Count	Succeeded	Failed	Min	Max	Mean	Total
dagman::post	15301	14819	482	5	554	9.607	146993
inspiral-FULL_DATA-H1_ID9	7621	7620	1	901.357	20055.080	12507.034	95316108.773
inspiral-FULL_DATA-L1_ID10	6641	6640	1	1589.662	19568.902	12504.586	83042955.049
pegasus::transfer	108	108	0	0	205.304	9.664	1043.731
coinc-FULL_DATA_FULL-H1L1_ID14	20	20	0	263.256	348.672	297.379	5947.586
pegasus::dirmanager	7	7	0	0	5	2.857	20
condor::dagman	6	6	0	607	833	700.167	4201
dagman::pre	6	6	0	11	75	27.167	163
single_template-P1_0-H1_ID5	5	5	0	360.602	383.866	373.194	1865.968
single_template_plot-P1_0-H1_ID6	5	5	0	4.013	8.382	5.008	25.041

Showing 1 to 10 of 314 entries — First Previous 1 2 3 4 5 … 32 Next Last

Job Statistics

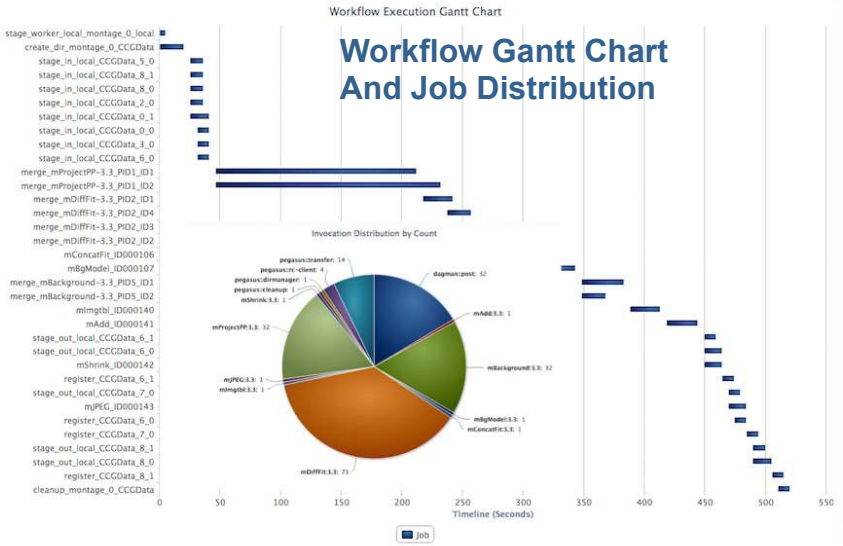
Charts

Job Distribution

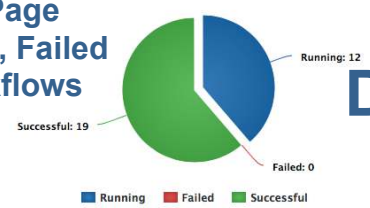
Time Chart

Gantt Chart

Workflow Gantt Chart And Job Distribution



Workflow Listing Page Shows Successful, Failed and Running Workflows



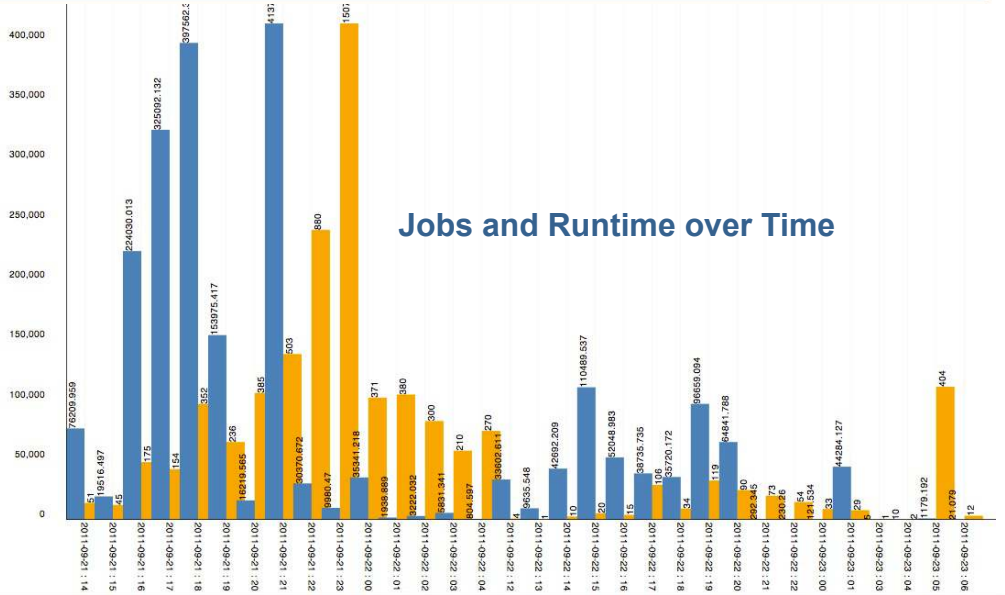
how results for all

Show 10 entries — Search: injections

Workflow Label	Submit Host	Submit Directory	State	Submitted On
analysis2-C01-injections	sugar-dev2.phy.syr.edu	/usr1/amber.lenon/pycbc-tmp.4a07mk2LXe/work	Successful	Sat, 06 Feb 2016 13:27:15
analysis8-C01-injections	sugar-dev2.phy.syr.edu	/usr1/amber.lenon/pycbc-tmp.cqBQirspEl/work	Successful	Mon, 08 Feb 2016 15:25:05
analysis7-C01-injections	sugar-dev2.phy.syr.edu	/usr1/amber.lenon/pycbc-tmp.tpHketeH7X/work	Successful	Mon, 08 Feb 2016 11:45:22
analysis3-C01-injections	sugar-dev2.phy.syr.edu	/usr1/amber.lenon/pycbc-tmp.LU6iToRyVA/work	Running	Tue, 23 Feb 2016 16:27:30
analysis4-C01-injections	sugar-dev2.phy.syr.edu	/usr1/amber.lenon/pycbc-tmp.gArV7UNU9C/work	Running	Tue, 23 Feb 2016 16:27:44
analysis5-C01-injections	sugar-dev2.phy.syr.edu	/usr1/amber.lenon/pycbc-tmp.d95VFhwkKu/work	Running	Wed, 24 Feb 2016 11:49:17
analysis6-C01-injections	sugar-dev2.phy.syr.edu	/usr1/amber.lenon/pycbc-tmp.O1anUn5hGE/work	Running	Wed, 24 Feb 2016 11:55:55
analysis9-C01-injections	sugar-dev2.phy.syr.edu	/usr1/amber.lenon/pycbc-tmp.Lf2hB7UTuG/work	Running	Wed, 24 Feb 2016 12:07:11

Showing 11 to 18 of 18 entries (filtered from 33 total entries) — First Previous 1 2 Next Last

Jobs and Runtime over Time



Pegasus LIGO Collaboration - Timeline

2001 Griphyn (Grid Physics Network) funded. Pegasus development started

2002 Pegasus LIGO demonstration at SC 2002 highlighting Virtual Data

2002 HPDC paper on Griphyn and LIGO focusing on Virtual Data

2003 Support for LDR – Globus RLS based LIGO data discovery service

2004 Development of replica selection strategies to optimize data access on LIGO Data Grid

2004 Long term collaboration with LIGO for running workflows on OSG

2005 Use of task clustering for performance improvements

2006 Development of cleanup algorithm to reduce peak storage requirements

2010 Hierarchal Workflows used by LIGO iHope workflows

2010 Developed pegasus-analyzer – a workflow debugging tool

2010-2011 Pegasus managed iHope workflows used for blind injection test

2012 Enabled LIGO iHope workflows to use VIRGO computing resources

2013 Introduced Pegasus Dashboard for LIGO users

2014 Enabled LIGO to leverage XSEDE for computations

2015 Pegasus managed pyCBC workflows used to verify gravitational wave detection

LIGO Pegasus – What's Next

- **Continued use of Pegasus to detect other interesting events**
- **Support for Metadata**
  - Automatic collection of static and runtime metadata attributes
  - Accessible via Pegasus Dashboard
  - Use for smarter data reuse – identifying what are the existing relevant data sets
- **Automatic organization of files in efficient directory structure**
  - Having thousands of files in a directory degrades filesystem performance.
  - Pegasus will automatically place them in a hierarchal data organization.
- **Increased use of Open Science Grid**
  - Seamless overflow of jobs to OSG
  - Improved Data Discovery
- **Improved error debugging and analysis via dashboard**

Pegasus

est. 2001

Automate, recover, and debug scientific computations.

Get Started

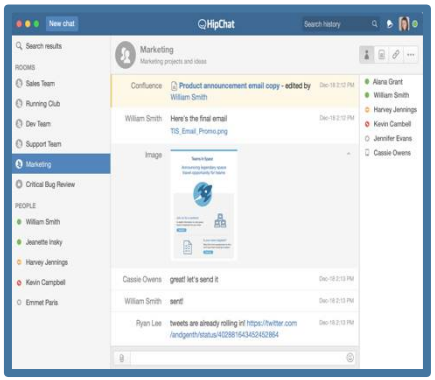
Tutorial
http://pegasus.isi.edu/documentation/

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?

Acknowledgements

LIGO – Duncan Brown, Stuart Anderson, Larne Pekowsky, Alex Nitz, Peter Couvares and many others.

Meet our team


Ewa Deelman


Karan Vahi


Gideon Juve


Mats Rynge


Rajiv Mayani


Rafael Ferreira da Silva