Building Community Resources For Scientific Workflow Research

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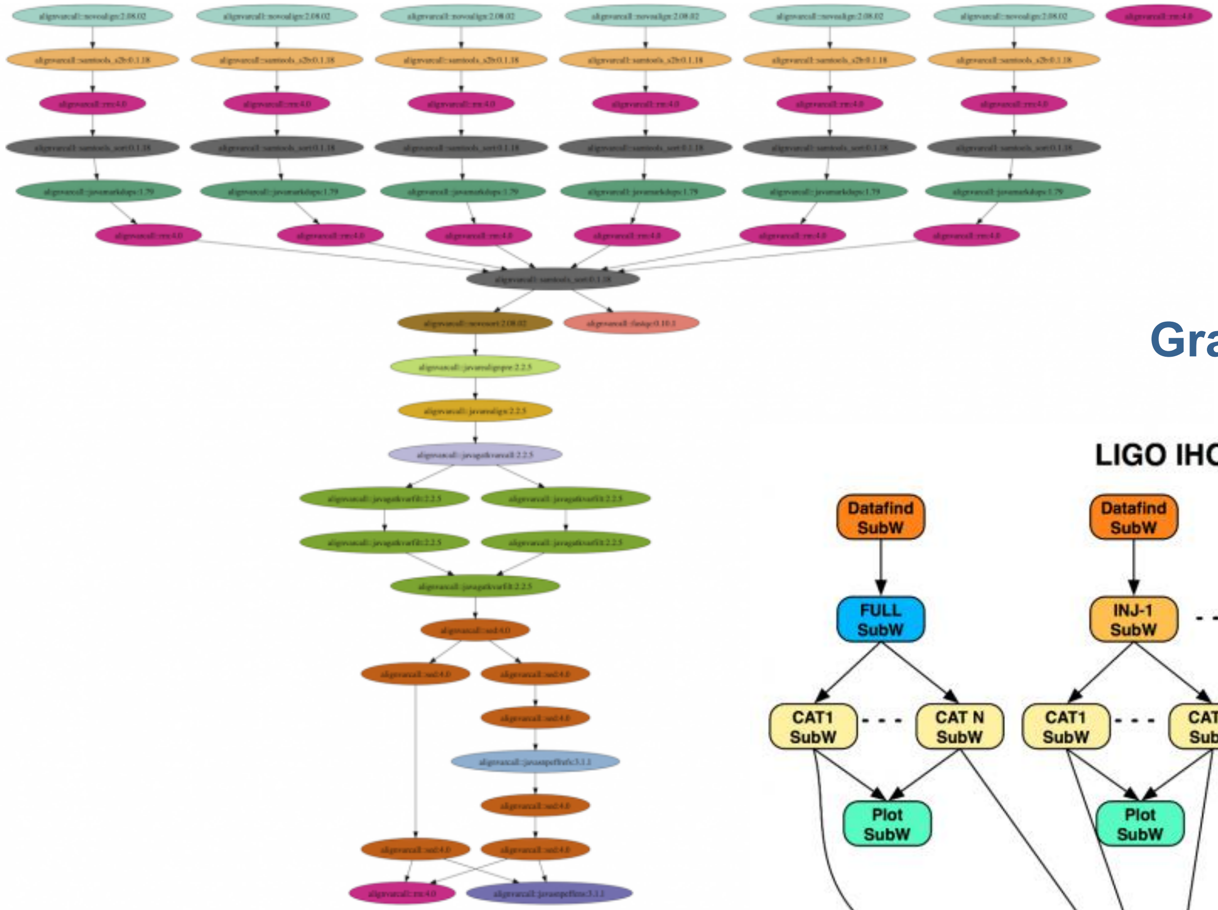
Community Resources for Enabling Scientific Workflow Research

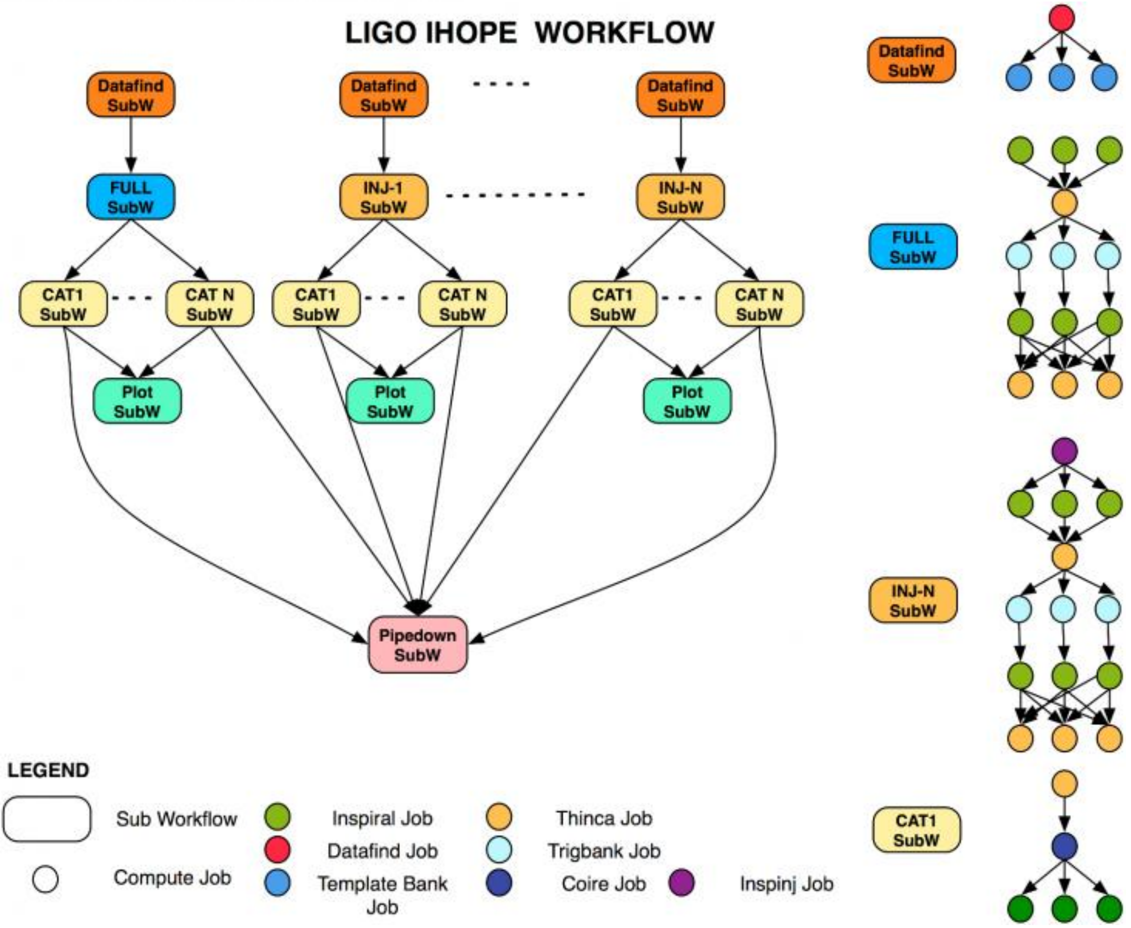
- Execution traces
- Synthetic workflow generator
- Workflow execution simulator

Some workflows are structurally complex

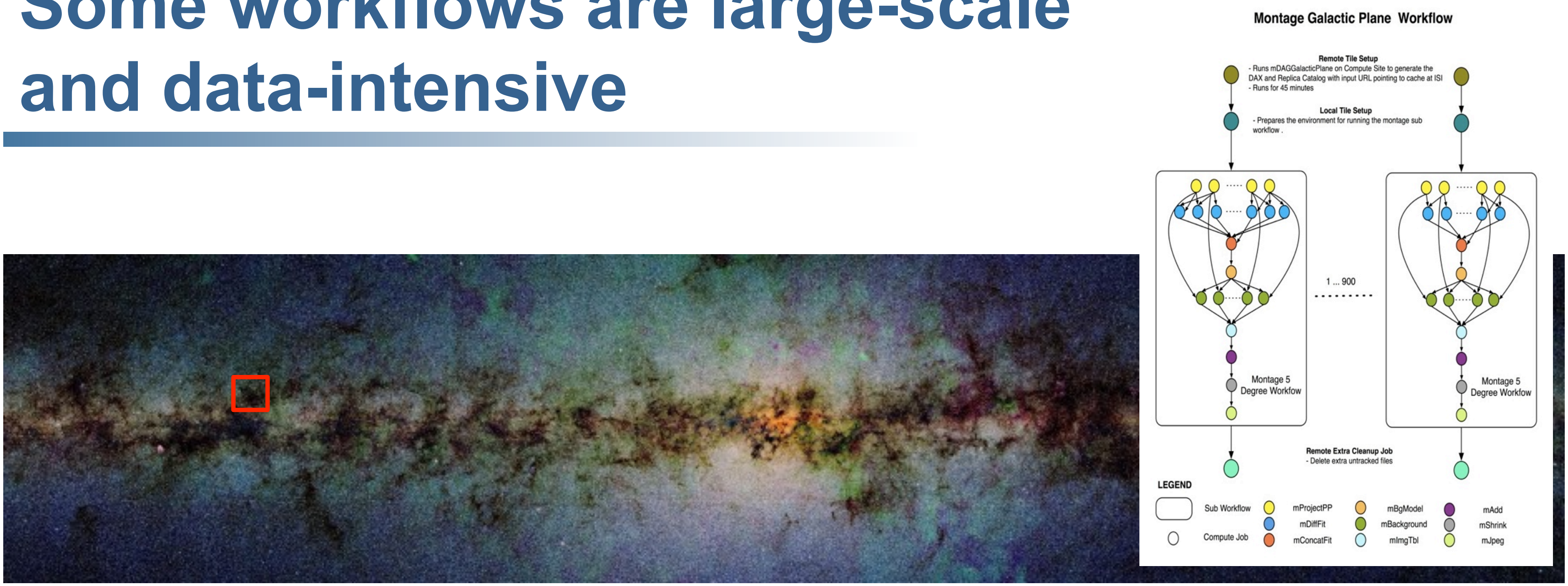


Genomics Workflow

Gravitational-wave physics



Some workflows are large-scale and data-intensive



John Good (Caltech)

- **Montage Galactic Plane Workflow**
  - **18 million input images (~2.5 TB)**
  - **900 output images (2.5 GB each, 2.4 TB total)**
  - **10.5 million tasks (34,000 CPU hours)**

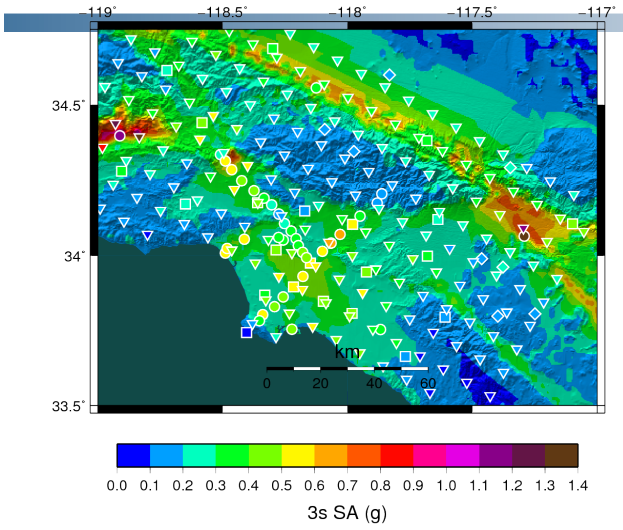
× 17

- **Need to support hierarchical workflows and scale, workflow ensembles**

Southern California Earthquake Center, T. Jordan, USC

CyberShake PSHA Workflow

- **Description**
  - 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)



1,144 geographic locations

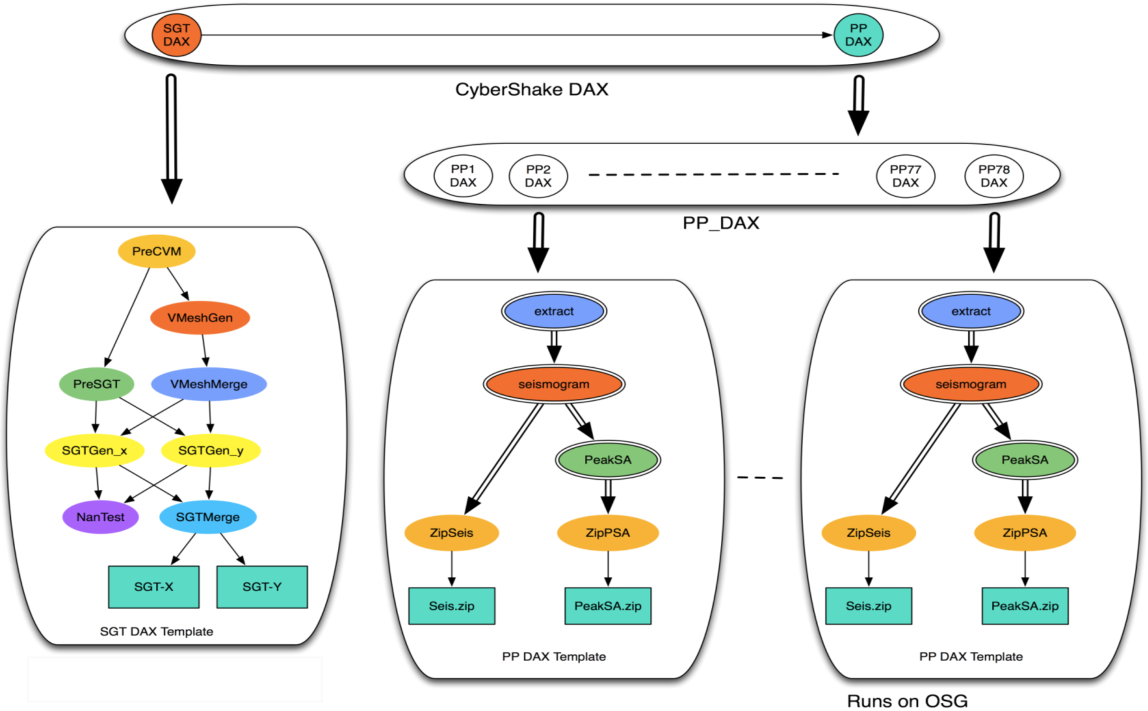
Uses Pegasus with execution on TACC’s Stampede

~ 470 million tasks total

Over 739 hours of computing

45 TB of data

12 TB being staged back for archiving



Coordination between resources is needed

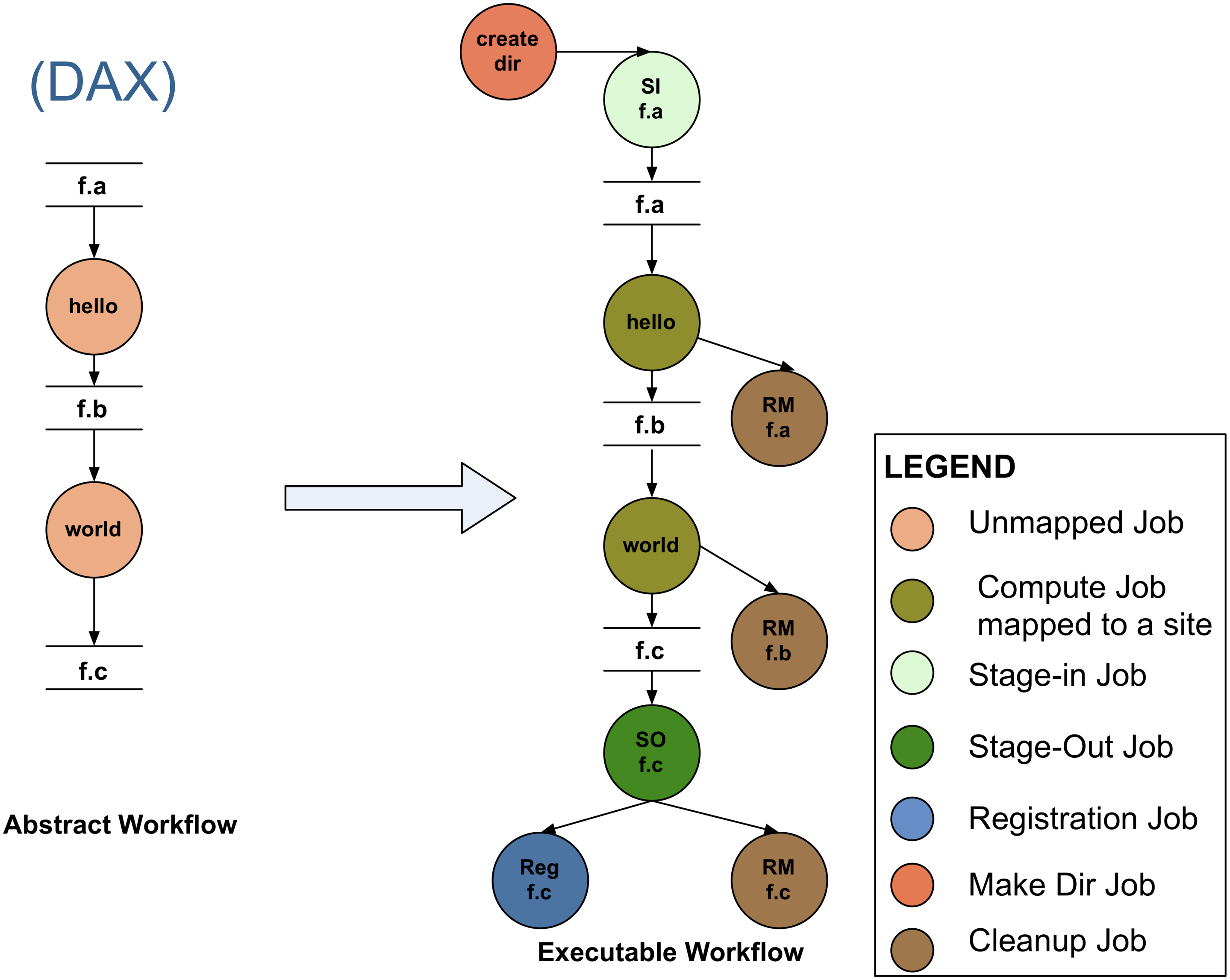
Pegasus Workflow Management System

- A workflow "compiler"
  - Input: abstract workflow description, resource-independent
  - Output: executable workflow with concrete resources
  - Transforms the workflow for performance and reliability (task clustering, data cleanup, etc.)
  - Automatically locates physical locations for both workflow tasks and data
- A workflow engine (DAGMan)
  - Executes the workflow on local or distributed resources (HPC, clouds)
  - Task executables are wrapped with *pegasus-kickstart* and managed by Condor *schedd*
- Provenance and execution traces are collected and stored
- Traces and DB can be mined for performance and overhead information

Generating executable workflows

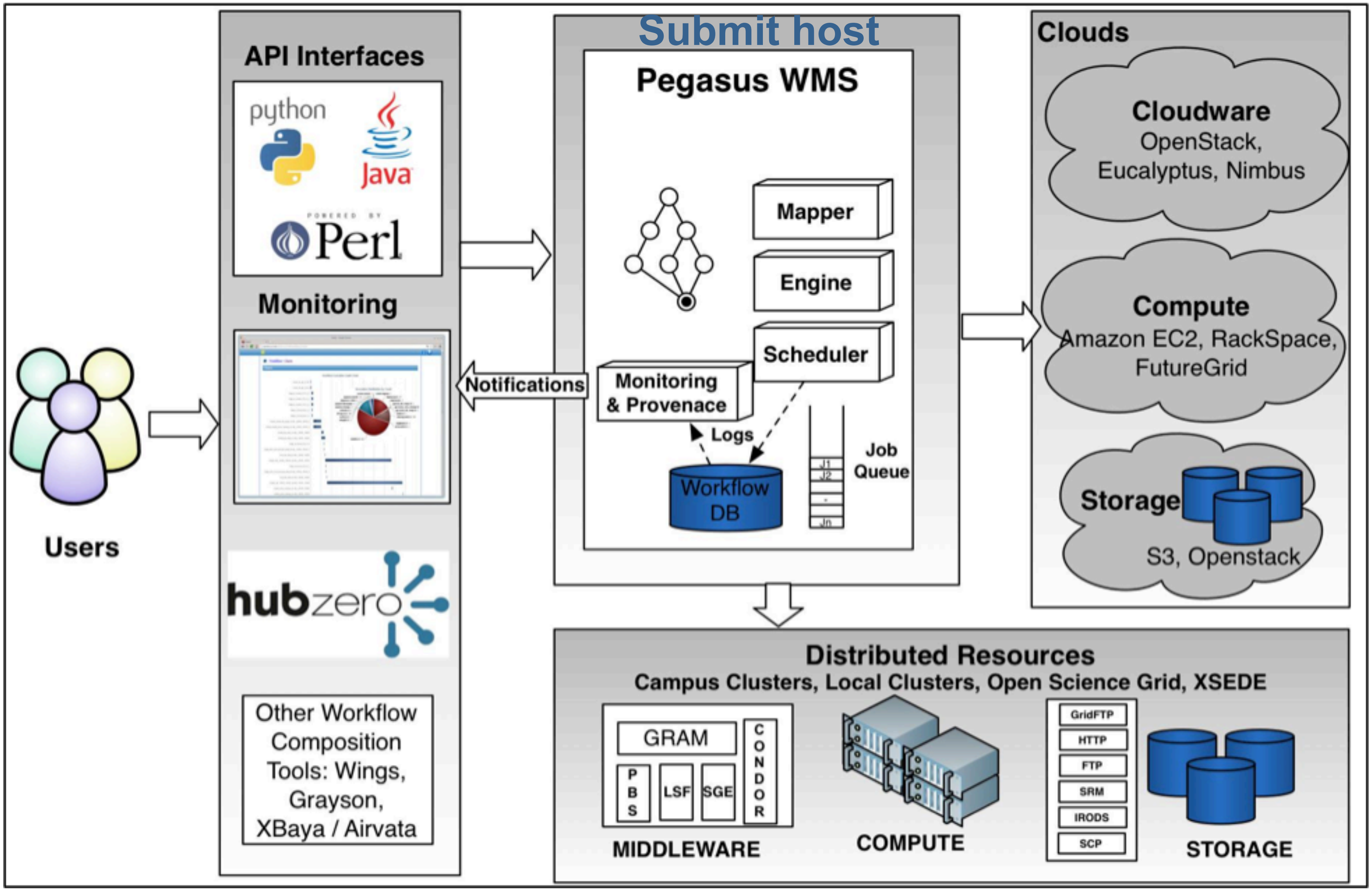
APIs for workflow specification (DAX--- DAG in XML)

Java, Perl, Python



Abstract Workflow

Executable Workflow



Users

API Interfaces

python

Java

Powered by Perl

Monitoring

hubzero

Other Workflow Composition Tools: Wings, Grayson, XBaya / Airvata

Notifications

Submit host

Pegasus WMS

Mapper

Engine

Scheduler

Monitoring & Provenace

Logs

Workflow DB

Job Queue

J1

J2

Jn

Clouds

Cloudware

OpenStack, Eucalyptus, Nimbus

Compute

Amazon EC2, RackSpace, FutureGrid

Storage

S3, Openstack

Distributed Resources

Campus Clusters, Local Clusters, Open Science Grid, XSEDE

GRAM

PBS

LSF

SGE

CONDOR

MIDDLEWARE

COMPUTE

GridFTP

HTTP

FTP

SRM

IRODS

SCP

STORAGE

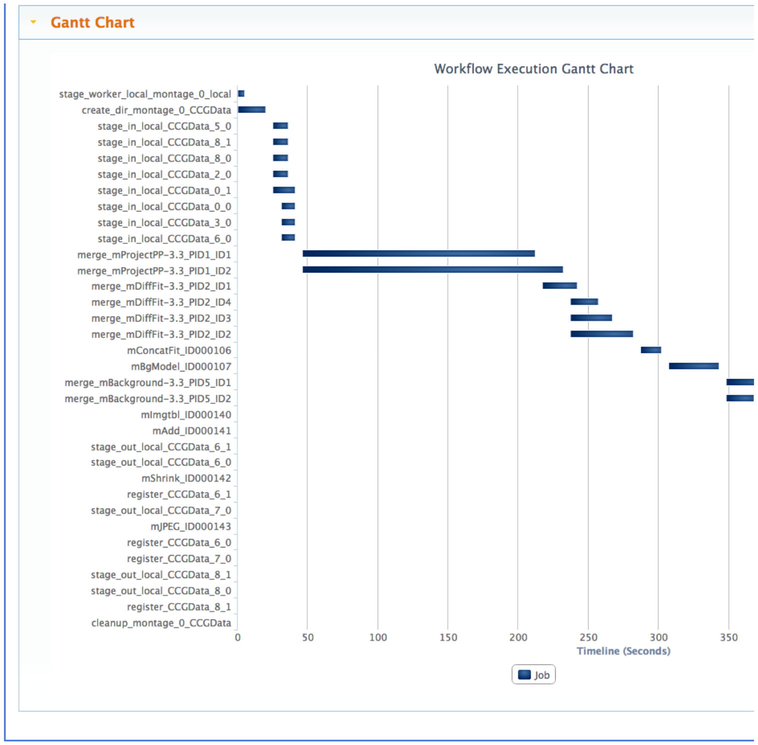
Pegasus-kickstart

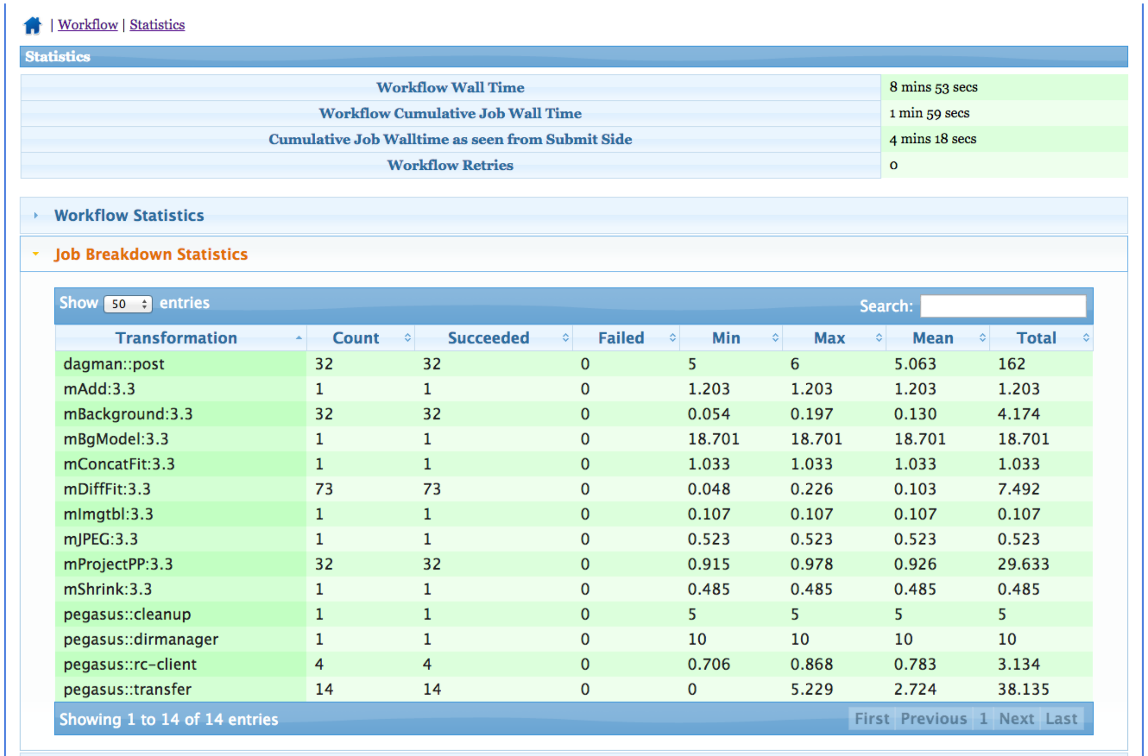
- Lightweight C based executable to launch jobs
- Captures job runtime provenance and logs it as a XML record
- Following information is captured about each job on all supported platforms
  - exit code with which the job it launched exited
  - start time and duration of the job
  - hostname and IP address of the host the job ran on
  - stdout and stderr of the job
  - arguments with which it launched the job
  - directory in which the job was launched
  - environment that was set for the job before it was launched

Pegasus-kickstart with extra tracing enabled

- Captures extra tracing information (optional) on Linux based hosts
- Traces each process that the job launches
  - Using LD_PRELOAD library interposition (faster, less accurate),
  - ptrace() system call interposition (slower, more accurate)
- Collects, for each process in process tree
  - peak memory usage (resident set size, and vm size)
  - total I/O read and write,
  - runtime,
  - start and end time
  - Pid
  - all files accessed (total read and write per file)
- Traces also include DAGMan and Condor logs (release of jobs to the scheduling system, sending jobs to remote resources, etc..)

Workflow Monitoring Dashboard – *pegasus-dashboard*





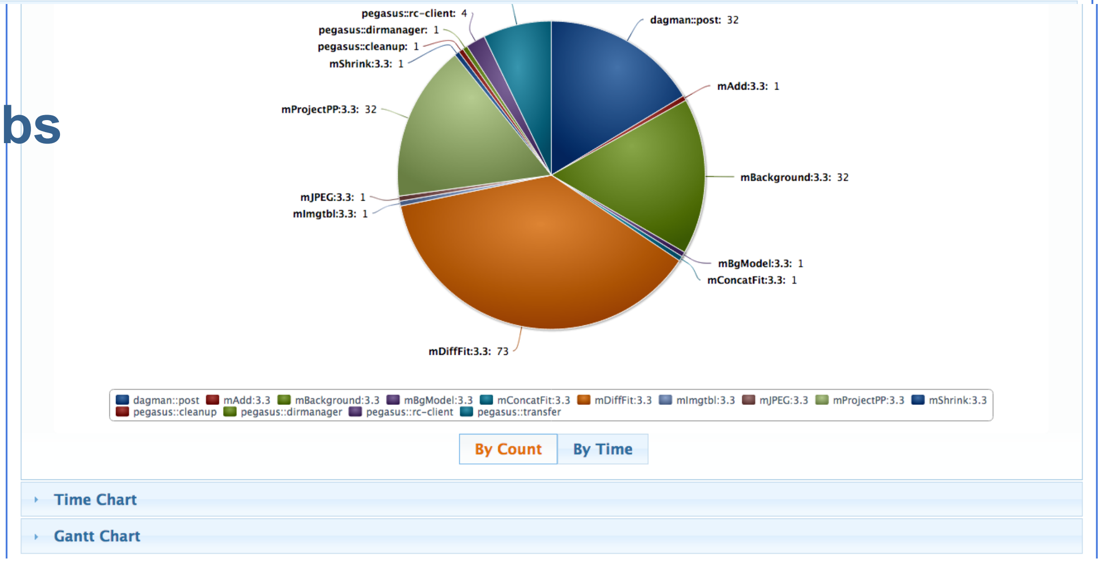
Statistics

Workflow Wall Time	8 mins 53 secs
Workflow Cumulative Job Wall Time	1 min 59 secs
Cumulative Job Walltime as seen from Submit Side	4 mins 18 secs
Workflow Retries	0

Transformation	Count	Succeeded	Failed	Min	Max	Mean	Total
dagman::post	32	32	0	5	6	5.063	162
mAdd:3.3	1	1	0	1.203	1.203	1.203	1.203
mBackground:3.3	32	32	0	0.054	0.197	0.130	4.174
mBgModel:3.3	1	1	0	18.701	18.701	18.701	18.701
mConcatFit:3.3	1	1	0	1.033	1.033	1.033	1.033
mDiffFit:3.3	73	73	0	0.048	0.226	0.103	7.492
mImgtbl:3.3	1	1	0	0.107	0.107	0.107	0.107
mJPEG:3.3	1	1	0	0.523	0.523	0.523	0.523
mProjectPP:3.3	32	32	0	0.915	0.978	0.926	29.633
mShrink:3.3	1	1	0	0.485	0.485	0.485	0.485
pegasus::cleanup	1	1	0	5	5	5	5
pegasus::dirmanager	1	1	0	10	10	10	10
pegasus::rc-client	4	4	0	0.706	0.868	0.783	3.134
pegasus::transfer	14	14	0	0	5.229	2.724	38.135

Showing 1 to 14 of 14 entries

Status, statistics, timeline of jobs



USC Viterbi
School of Engineering

Overview of the Community Resources

www.workflowarchive.org

- **Execution Traces** of a range of real workflow applications
- **Synthetic Workflow Generator** produces realistic workflows based on profiles extracted from execution traces (astronomy, gravitational-wave physics, bioinformatics, earthquake science)
- **Workflow Simulator** mimics the execution of synthetic workflows on realistic infrastructures

Workflow Traces Archive

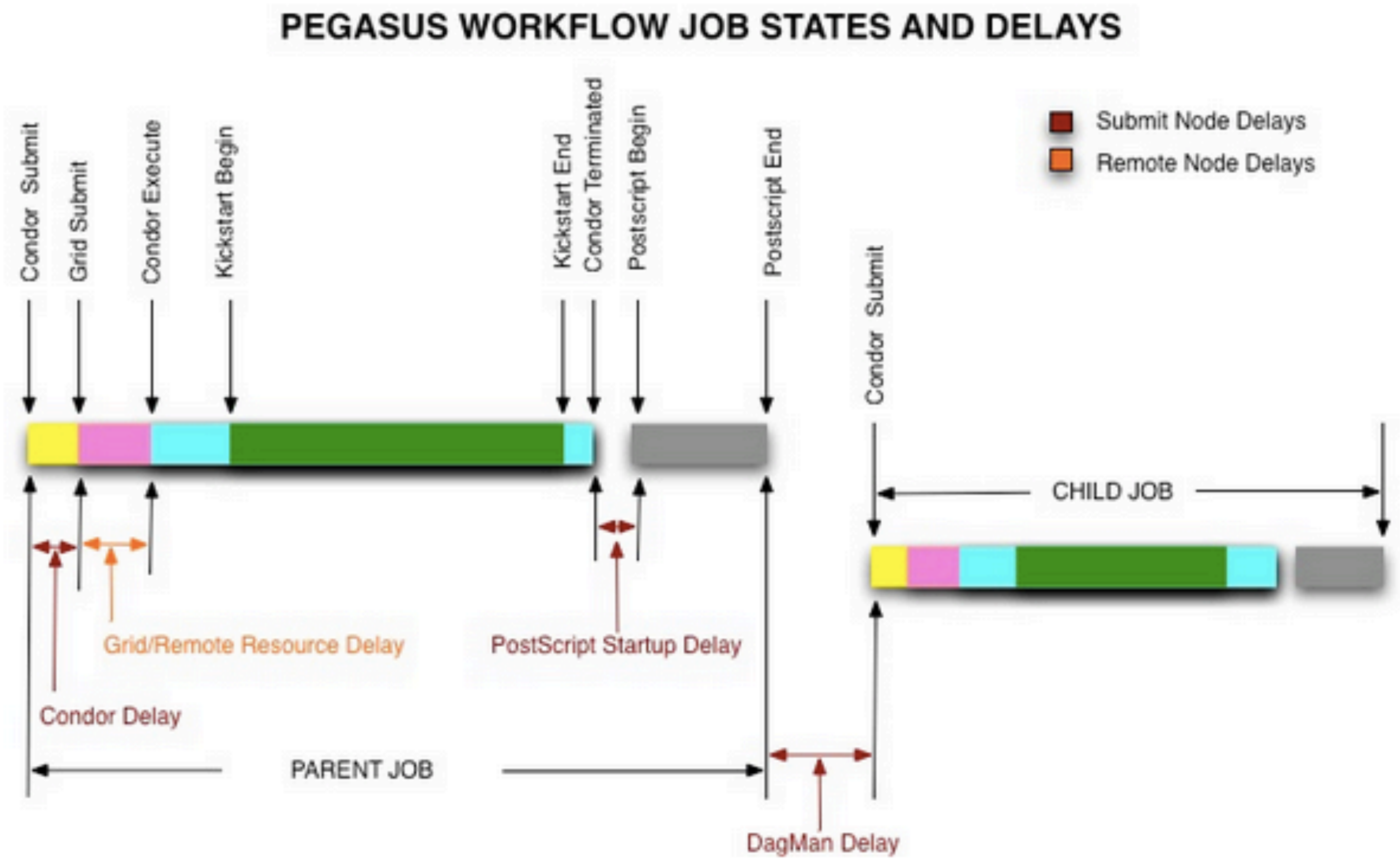
- **Workflow Gallery currently has 11 workflow applications, most with multiple runs**

```
08/24 12:24:55 submitting: condor_submit -a dag_node_name' '=' 'stage_in_remote_usc_1 -a
+DAGManJobId' '=' '11443 -a DAGManJobId' '=' '11443 -a submit_event_notes' '=' 'DAG' 'Node:'
'stage_in_remote_usc_1 -a +DAGParentNodeNames' '='
'"create_dir_61HE2AAXX_2_HSB_135_S1C_R_0_usc" stage_in_remote_usc_1.sub
08/24 12:24:55 From submit: Submitting job(s).
08/24 12:24:55 From submit: Logging submit event(s).
08/24 12:24:55 From submit: 1 job(s
08/24 12:24:55    assigned Condor I
08/24 12:24:55 Submitting Condor N
08/24 12:24:55 submitting: condor_s
+DAGManJobId' '=' '11443 -a DAGM
'stage_in_remote_usc_2 -a +DAGPa
'"create_dir_61HE2AAXX_2_HSB_1
08/24 12:24:55 From submit: Submit
08/24 12:24:55 From submit: Loggin
08/24 12:24:55 From submit: 1 job(s
08/24 12:24:55    assigned Condor I
08/24 12:24:55 Submitting Condor N
```

DAGMan, Condor, Pegasus logs, submit files, stdout, stderr

```
1314221995 Sam
1314221995 SamToMrf_SamToMrf-0-1 EXECUTE 11602.0 usc 7200 159
1314221995 SamToBam_SamToBam-26-1 EXECUTE 11600.0 usc 7200 157
1314222155 SamToBam_SamToBam-27-1 JOB_TERMINATED 11601.0 usc
1314222155 SamToBam_SamToBam-27-1 JOB_SUCCESS 0 usc 7200 158
1314222155 SamToBam_SamToBam-27-1 POST_SCRIPT_STARTED 11601
1314222160 SamToBam_SamToBam-27-1 POST_SCRIPT_TERMINATED 1
1314222160 SamToBam_SamToBam-27-1 POST_SCRIPT_SUCCESS 0 usc
1314222166 stage_out_remote_usc_5_1 SUBMIT 11605.0 usc - 162
1314222176 stage_out_remote_usc_5_1 GLOBUS_SUBMIT 11605.0 usc - 1
1314222176 stage_out_remote_usc_5_1 GRID_SUBMIT 11605.0 usc - 162
1314222176 stage_out_remote_usc_5_1 EXECUTE 11605.0 usc - 162
```

Traces include information about system overheads



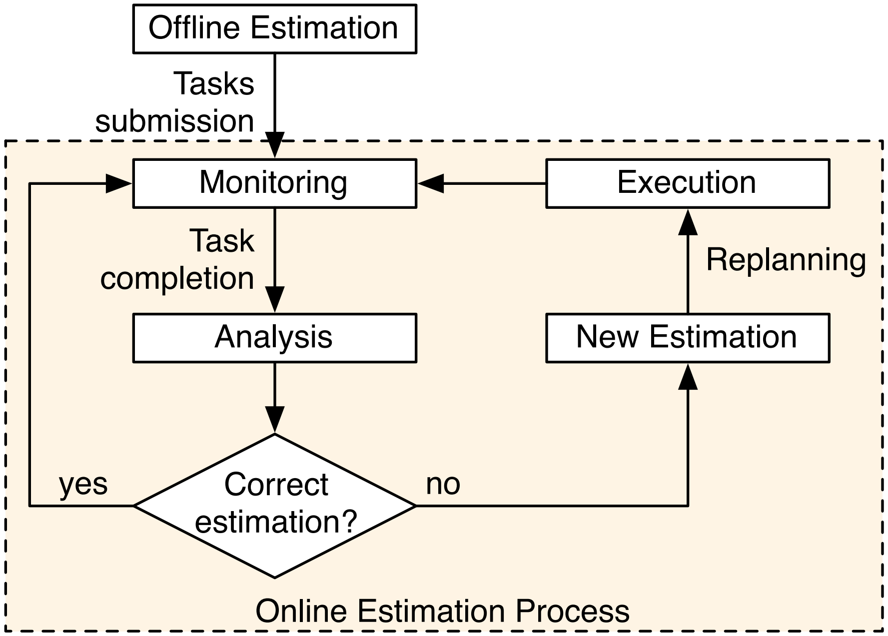
Tools to calculate job statistics

Task Type	Count	Runtime(s)	IO Read (MB)	IO Write (MB)	Memory Peak(MB)	CPU Utilization(%)
mProjectPP	2102	1.73	2.05	8.09	11.81	86.96
mDiffFit	6172	0.66	16.56	0.64	5.76	28.39
mConcatFit	1	143.26	1.95	1.22	8.13	53.17
mBgModel	1	384.49	1.56	0.10	13.64	99.89
mBackground	2102	1.72	8.36	8.09	16.19	8.46
mImgtbl	17	2.78	1.55	0.12	8.06	3.48
mAdd	17	282.37	1102	775.45	16.04	8.48
mShrink	16	66.10	412	0.49	4.62	2.30
mJPEG	1	0.64	25.33	0.39	3.96	77.14

Table 1. Execution profile of the Montage workflow, averages calculated

Workflow Resource Usage Prediction

- Profile and Characterize Workflow Execution
  - I/O, runtime, memory usage, and CPU utilization
  - Predict task runtime, e.g. using correlations based techniques
  - Predict resource usage (disk space, memory consumption) using an online estimation process

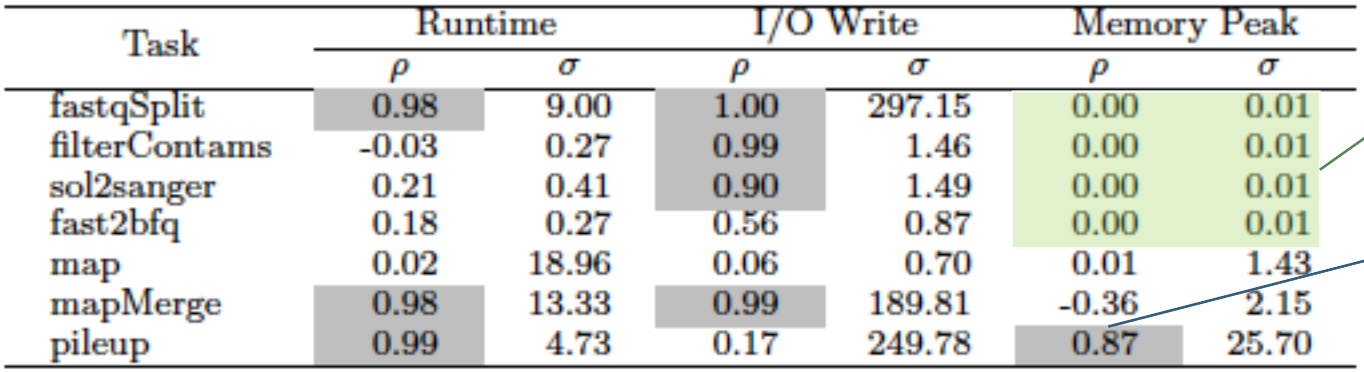


DOE project: dV/dt Accelerating the Rate of Progress towards Extreme Scale Collaborative Science

Automatic Workflow Characterization

- Characterize tasks based on their estimation capability
  - **Runtime, I/O write, memory peak ➔ estimated from I/O read**

- Use correlation statistics to identify statistical relationships between parameters
  - High correlation values yield accurate estimations, **Estimation based on the ratio: parameter/input data size**
  - Low correlation: use mean value



Task	Runtime		I/O Write		Memory Peak	
	ρ	σ	ρ	σ	ρ	σ
fastqSplit	0.98	9.00	1.00	297.15	0.00	0.01
filterContams	-0.03	0.27	0.99	1.46	0.00	0.01
sol2sanger	0.21	0.41	0.90	1.49	0.00	0.01
fast2bfq	0.18	0.27	0.56	0.87	0.00	0.01
map	0.02	18.96	0.06	0.70	0.01	1.43
mapMerge	0.98	13.33	0.99	189.81	-0.36	2.15
pileup	0.99	4.73	0.17	249.78	0.87	25.70

Constant values

Correlated if $\rho > 0.8$

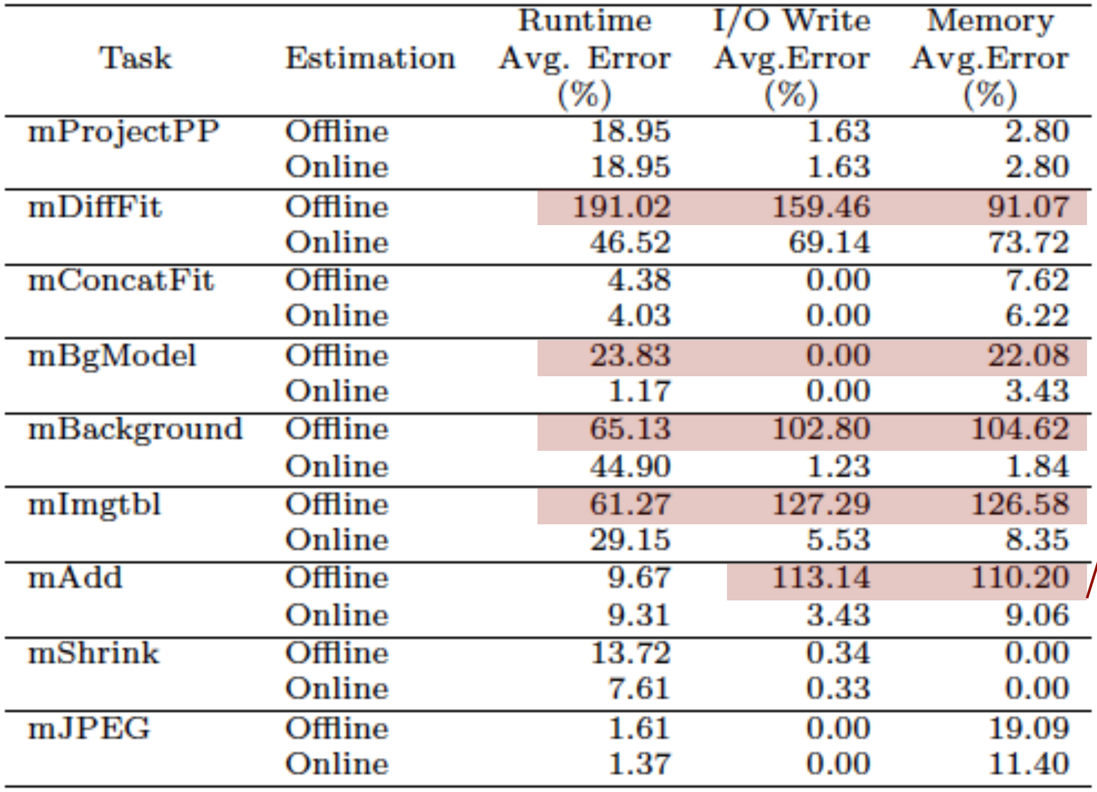
Epigenomics workflow

Task Characterization/Execution

- Understand the resource needs of a task
- Establish expected values and limits for task resource consumption
- Launch tasks on the correct resources
- Monitor task execution and resource consumption, interrupt tasks that reach resource limits
- Possibly re-launch tasks on different resources

- Task characterization needs to be an online process
- **New DOE project to improve the modeling of workflow behavior including data handling (Vetter, Tierney, Mandal, Carothers) “Predictive Modeling and Diagnostic Monitoring of Extreme Science Workflows;”**

Results: Average Estimation Errors - Montage



Task	Estimation	Runtime Avg. Error (%)	I/O Write Avg.Error (%)	Memory Avg.Error (%)
mProjectPP	Offline	18.95	1.63	2.80
	Online	18.95	1.63	2.80
mDiffFit	Offline	191.02	159.46	91.07
	Online	46.52	69.14	73.72
mConcatFit	Offline	4.38	0.00	7.62
	Online	4.03	0.00	6.22
mBgModel	Offline	23.83	0.00	22.08
	Online	1.17	0.00	3.43
mBackground	Offline	65.13	102.80	104.62
	Online	44.90	1.23	1.84
mImgtbl	Offline	61.27	127.29	126.58
	Online	29.15	5.53	8.35
mAdd	Offline	9.67	113.14	110.20
	Online	9.31	3.43	9.06
mShrink	Offline	13.72	0.34	0.00
	Online	7.61	0.33	0.00
mJPEG	Offline	1.61	0.00	19.09
	Online	1.37	0.00	11.40

Poor output data estimations leads to a chain of estimation errors in scientific workflows

Offline Process
Avg. Runtime Error: 43%
Avg. I/O Write Error: 56%
Avg. Memory Error: 53%

Online Process
Avg. Runtime Error: 18%
Avg. I/O Write Error: 9%
Avg. Memory Error: 13%

- Online strategy counterbalances the propagation of estimation errors

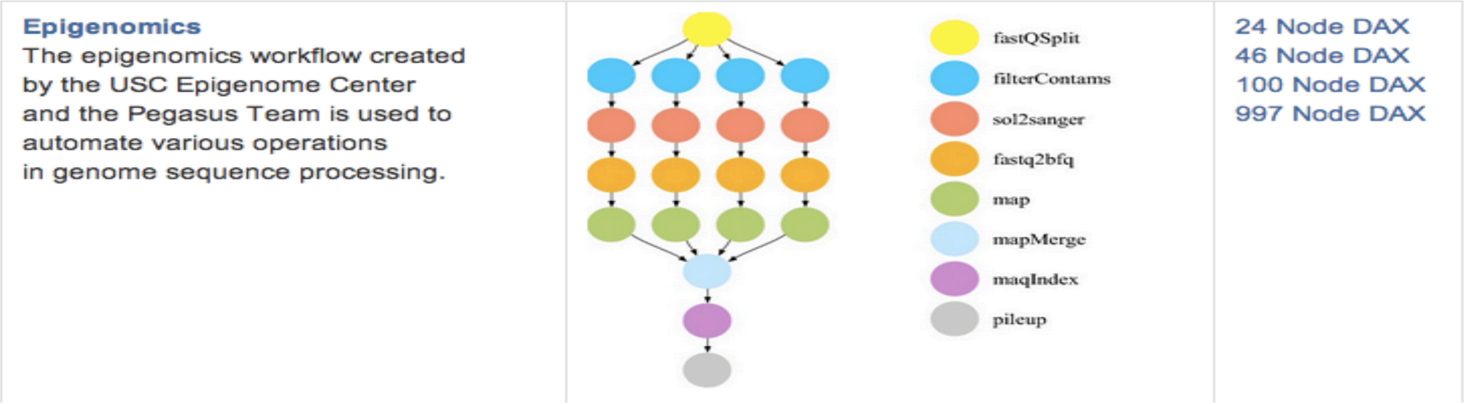
Workflow Generator Toolkit

Allows to explore more application configurations

- Uses randomization and parameter sweeps to create different workflow instances
  - Generate task runtimes and data sizes based on patterns observed in execution profiles.
  - Generate workflow structure based on the targeted application: pipelines, data distribution, aggregation, or redistribution
    - Montage: number of inputs is based on the degree square of the final image, e.g.
- Outputs DAX (DAG in XML) files that can be used by Workflow Simulators

Workflow Generator Toolkit

- Inputs: the size of the workflow in number of jobs, or the input data size, or a scaling factor
- Inputs are combined with probability distributions of file sizes and runtimes from real executions of the workflow, to generate random values that are used in constructing the synthetic workflow.
- Generators have application-specific code and parameters that are designed to reproduce the structure and characteristics of the application.
- **Currently supports 20 workflow applications from astronomy, earth science, bioinformatics, weather, and ocean modeling**
- **Pre-generated workflows: a large collection of synthetic workflow samples is available (5 workflow applications and 2,840 workflow instances)**



Epigenomics

The epigenomics workflow created by the USC Epigenome Center and the Pegasus Team is used to automate various operations in genome sequence processing.

24 Node DAX
46 Node DAX
100 Node DAX
997 Node DAX

Workflow Simulator: WorkflowSim

A workflow simulator for distributed environments

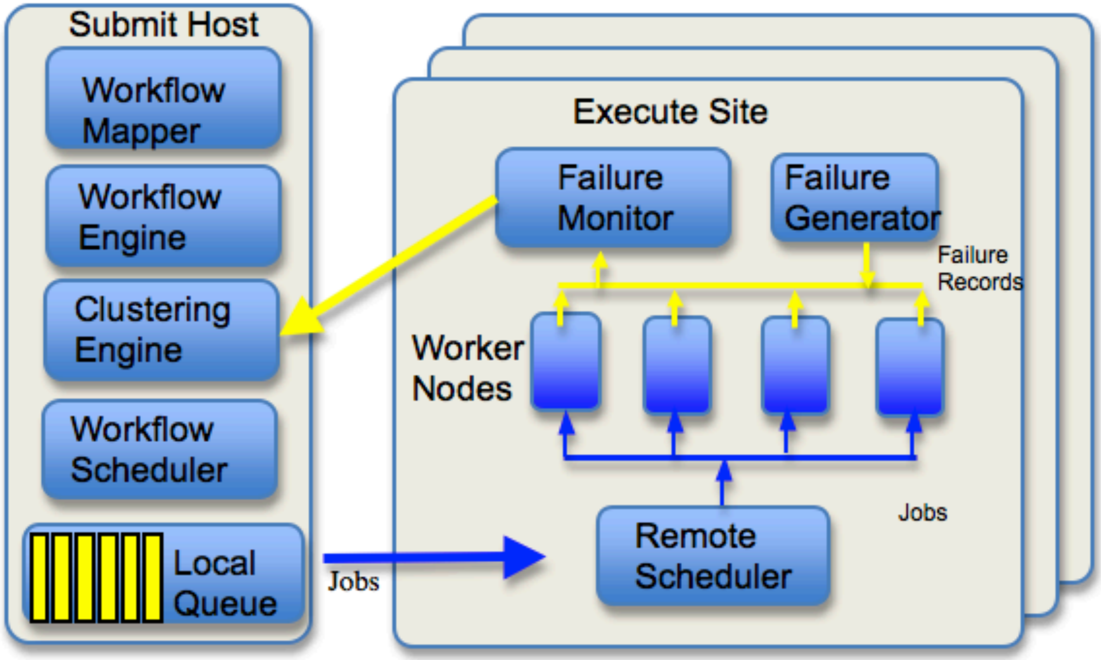
  - Workflow-level support (data dependency) on top of CloudSim
  - Contains a model of system overheads
  - Supports task failures, monitoring, task retry, task clustering

- Can be used to evaluate algorithms and techniques in task scheduling, task clustering, resource provisioning, and data placement etc.
- Input: DAX files from Synthetic Workflow Generator or other DAX generators
- Output: makespan, resource usage, cost, etc.

Workflow Simulator: WorkflowSim

Components

- Behavior based on Pegasus
  - Workflow Mapper/Compiler, Workflow Engine, Clustering Engine, Workflow Scheduler
- Additional features
  - Failure Generator
  - Failure Monitor
  - System Overheads
  - Monetary Cost



Simulation Usage Examples

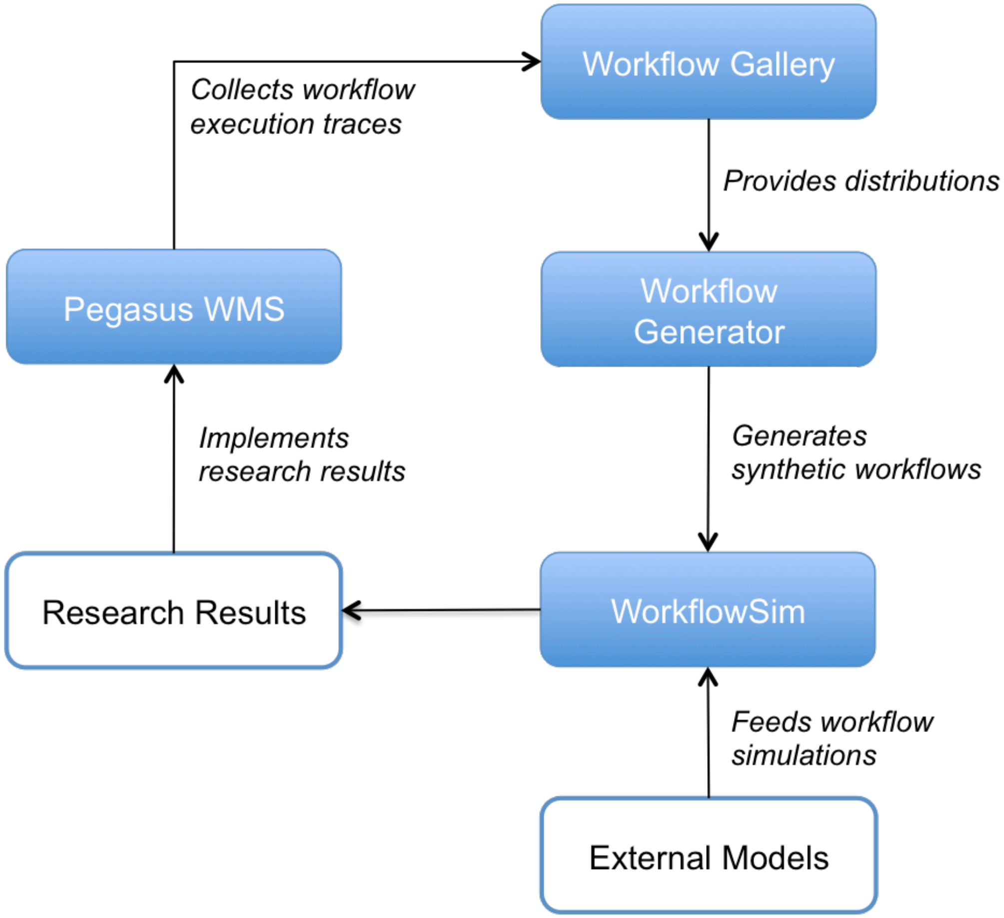
- Balanced Task Clustering: investigate the dependency and runtime imbalance problem in task clustering
  - Used synthetic workflow generator to create a large set of workflow instances

- Fault-Tolerant Task Clustering: improve the task clustering in a faulty environment
  - Relied on the generation of transient failures
  - Synthetic workflows

- Energy-Efficiency: develop an energy consumption model for large-scale infrastructure

Conclusion

- **A collection of tools and data that have enabled research in new methods and systems**
  - Execution traces
  - Synthetic workflow generator
  - Workflow simulator
- **We use these tools to**
  - **Generate traces**
  - **Analyze and profile traces**
  - **Vary system configurations and workflow instances**
  - **Evaluate the results in simulator**
  - **Implement promising approaches in Pegasus**
- **The tools are not limited to the Pegasus community**



Workflow Gallery

Collects workflow execution traces

Provides distributions

Pegasus WMS

Workflow Generator

Implements research results

Generates synthetic workflows

Research Results

WorkflowSim

Feeds workflow simulations

External Models

Current Community Resources
Contributions Welcome!

- **Pegasus Workflow Management System: http://pegasus.isi.edu**
- **Workflow Archive and Workflow Generator: www.workflowarchive.org**
- **WorkflowSim: www.workflowsim.org and https://github.com/WorkflowSim**