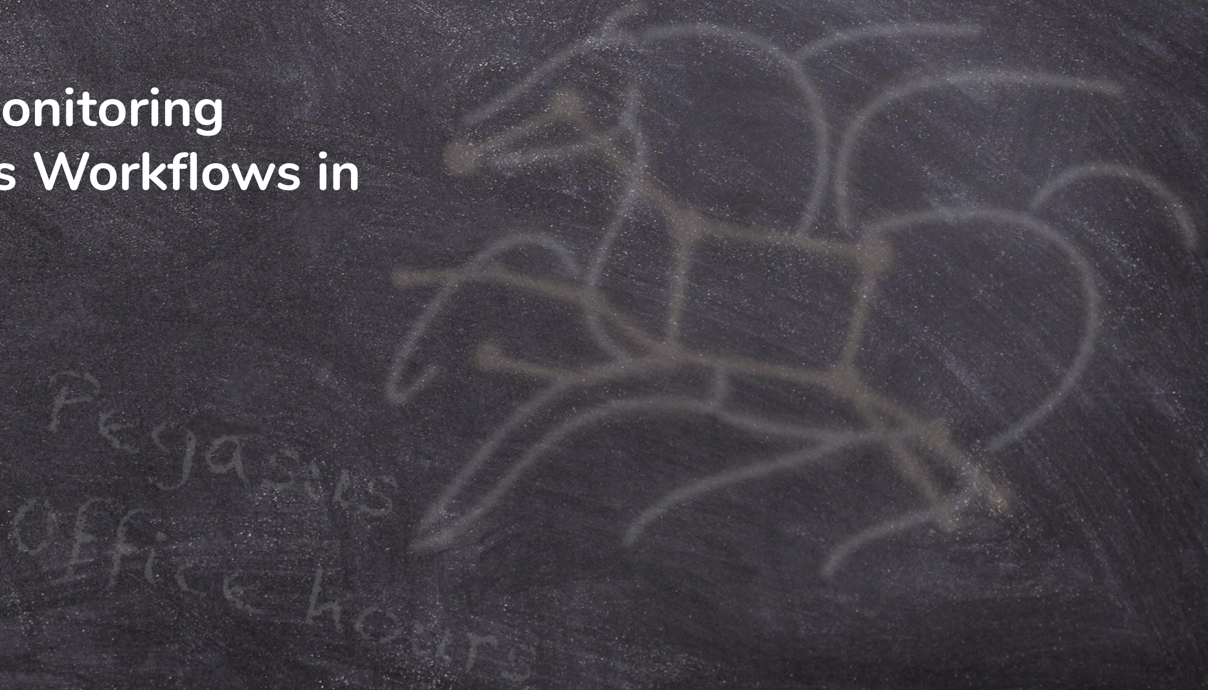
Data Collection and Monitoring Across Heterogeneous Workflows in Pegasus

Ryan Tanaka
tanaka@isi.edu



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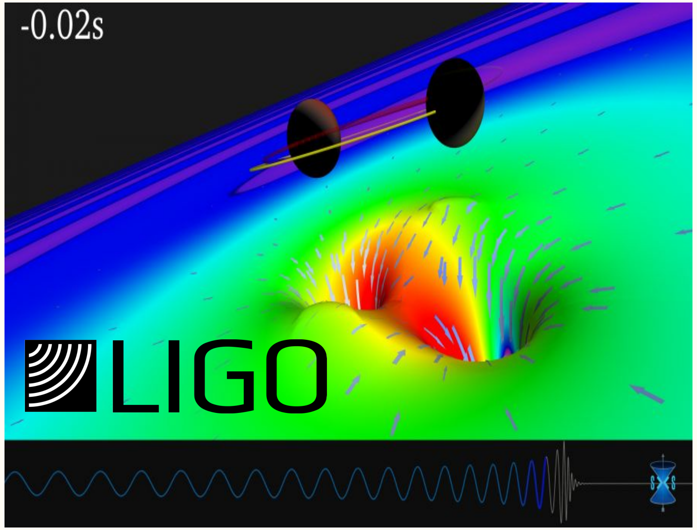
https://pegasus.isi.edu/

Background: Gravitational Waves, Workflows, LIGO

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

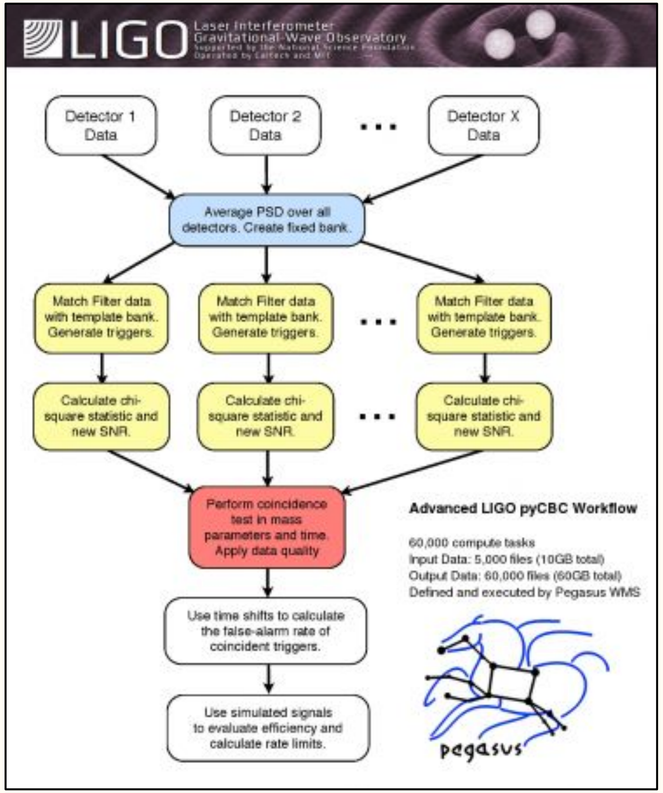
Background: Gravitational Waves, Workflows, LIGO

Advanced PyCBC Workflows:

- 60,000 compute tasks
- 5,000 input files (10GB total)
- 60,000 output files (60GB total)
- Post run analysis

Challenges:

- Error analysis on workflows of this scale
- Monitoring across multiple runs, users, and submit machines


LIGO
Laser Interferometer Gravitational-Wave Observatory
Supported by the National Science Foundation
Operated by Caltech and MIT
Detector 1 Data
Detector 2 Data
Detector X Data
Average PSD over all detectors. Create fixed bank.
Match Filter data with template bank. Generate triggers.
Calculate chi-square statistic and new SNR.
Perform coincidence test in mass parameters and time. Apply data quality
Use time shifts to calculate the false-alarm rate of coincident triggers.
Use simulated signals to evaluate efficiency and calculate rate limits.
Advanced LIGO pyCBC Workflow
60,000 compute tasks
Input Data: 5,000 files (10GB total)
Output Data: 60,000 files (60GB total)
Defined and executed by Pegasus WMS
pegasus

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

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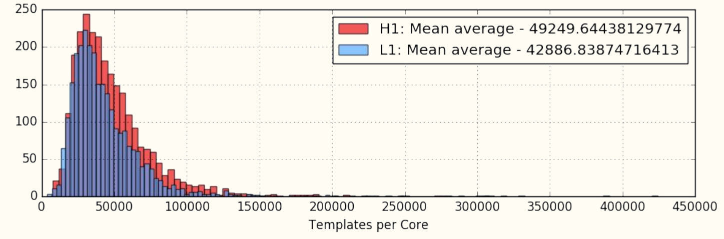

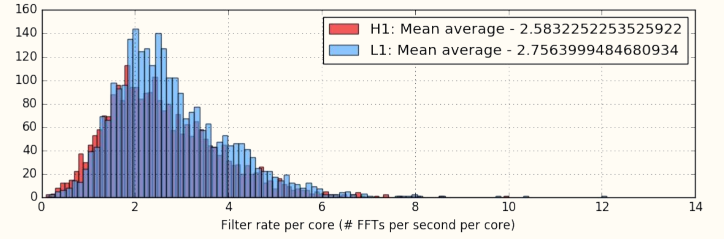

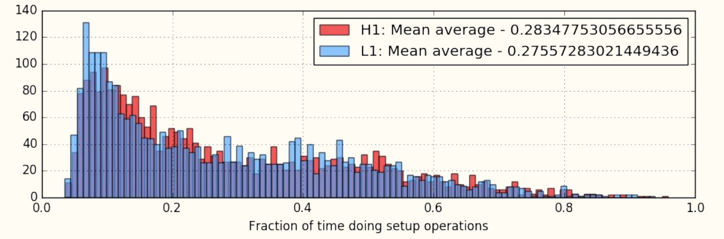

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Background: Empowering LIGO Researchers

CIF21 DIBBs: Domain-Aware Management of Heterogeneous Workflows

Active Data Management for Gravitational-Wave Science

PI: Duncan Brown[1], Co-PIs: Peter Couvares[2] Ewa Deelman[3], Jian Qin[1] NSF Award ACI-1443047

1 Syracuse University. 2 LIGO Caltech, 3 USC Information Sciences Institute.

Goals:

- Develop new data management techniques in Pegasus
- Improve data access for LIGO researchers
- Enhance Pegasus workflow monitoring capabilities
- Enable LIGO researchers to conduct analysis across multiple PyCBC pipeline runs

Background: Empowering LIGO Researchers

Outcomes:

- Developed Pegasus extensions to capture runtime provenance metadata
- Data storage Solutions
  - relational datastore linked to a single PyCBC run
  - Elasticsearch persisting data across multiple PyCBC runs
- Browser based monitoring/analytics solutions
  - Kibana: query/explore Elasticsearch data via a browser
  - Grafana: dashboard for viewing workflow runs at varying levels of granularity

Outline

- ~~Background~~
- **Data collection pipeline**
- Getting started
- Demo

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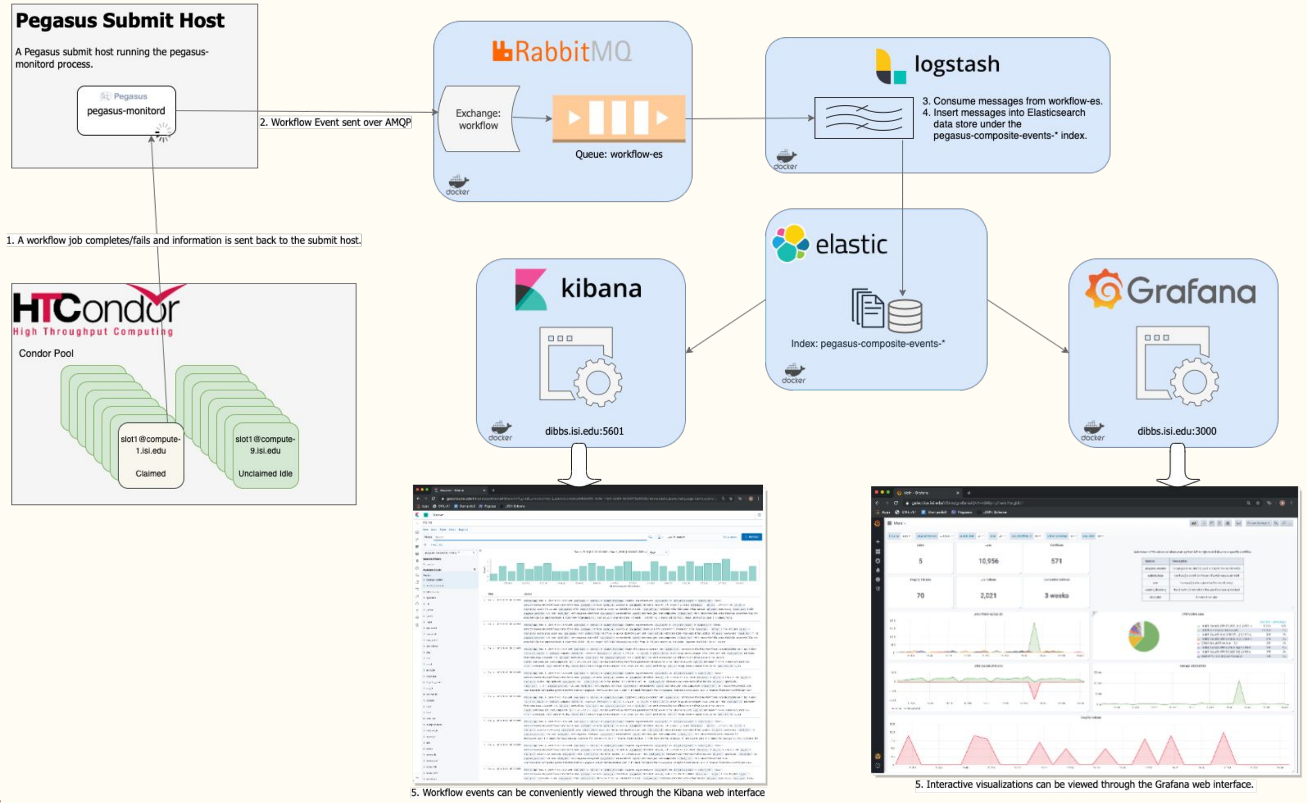
Data Collection Pipeline: Overview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A Pegasus submit host running the pegasus-monitord process.
Pegasus
pegasus-monitord
2. Workflow Event sent over AMQP
RabbitMQ
Exchange: workflow
Queue: workflow-es
docker
logstash
3. Consume messages from workflow-es.
4. Insert messages into Elasticsearch data store under the pegasus-composite-events-* index.
1. A workflow job completes/fails and information is sent back to the submit host.
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High Throughput Computing
Condor Pool
slot1@compute-1.isi.edu
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elastic
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dibbs.isi.edu:5601
Grafana
dibbs.isi.edu:3000
5. Workflow events can be conveniently viewed through the Kibana web interface
5. Interactive visualizations can be viewed through the Grafana web interface.

Data Collection Pipeline: Data Flow

Sequence of Events:

1. Workflow job completes and information sent to pegasus-monitord
2. Workflow event sent over AMQP to RabbitMQ message queue
3. Logstash consumes message from queue
4. Logstash inserts event under pegasus-composite-even-* index in Elasticsearch data store
5. Data Exploration/Visualization
    a. Workflow events viewable through Kibana
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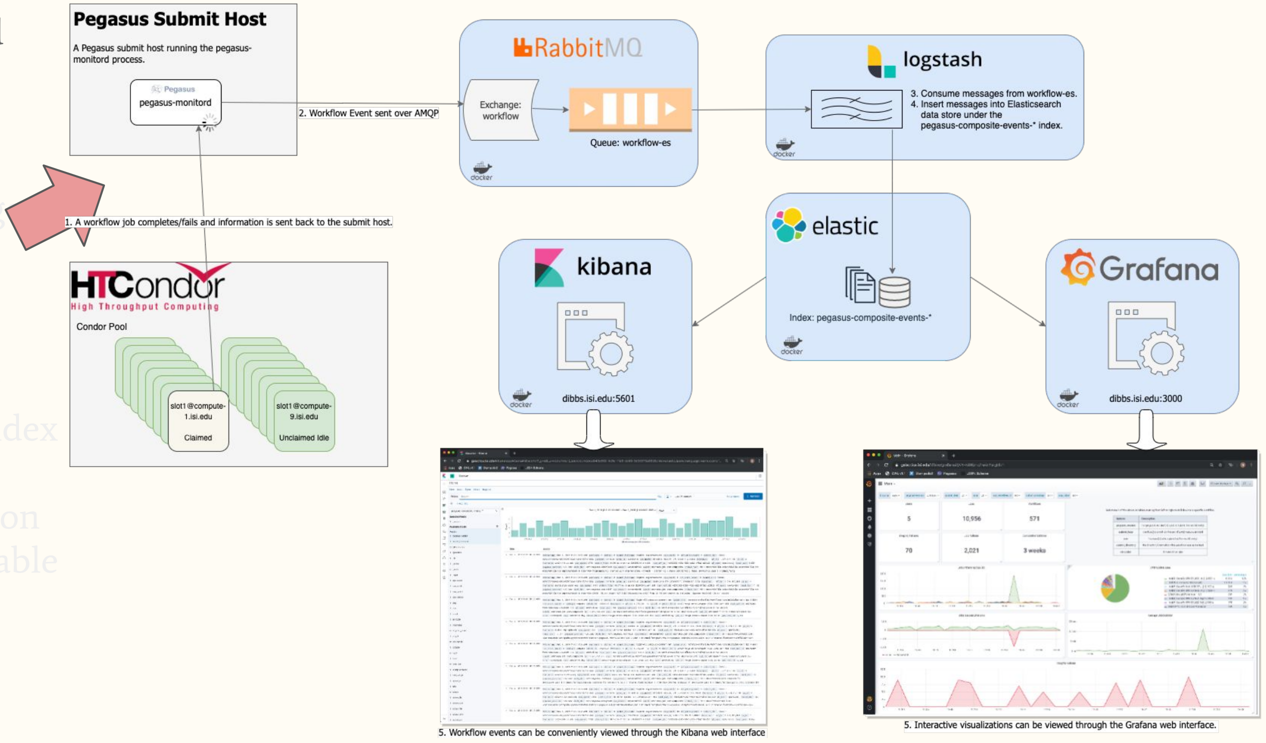

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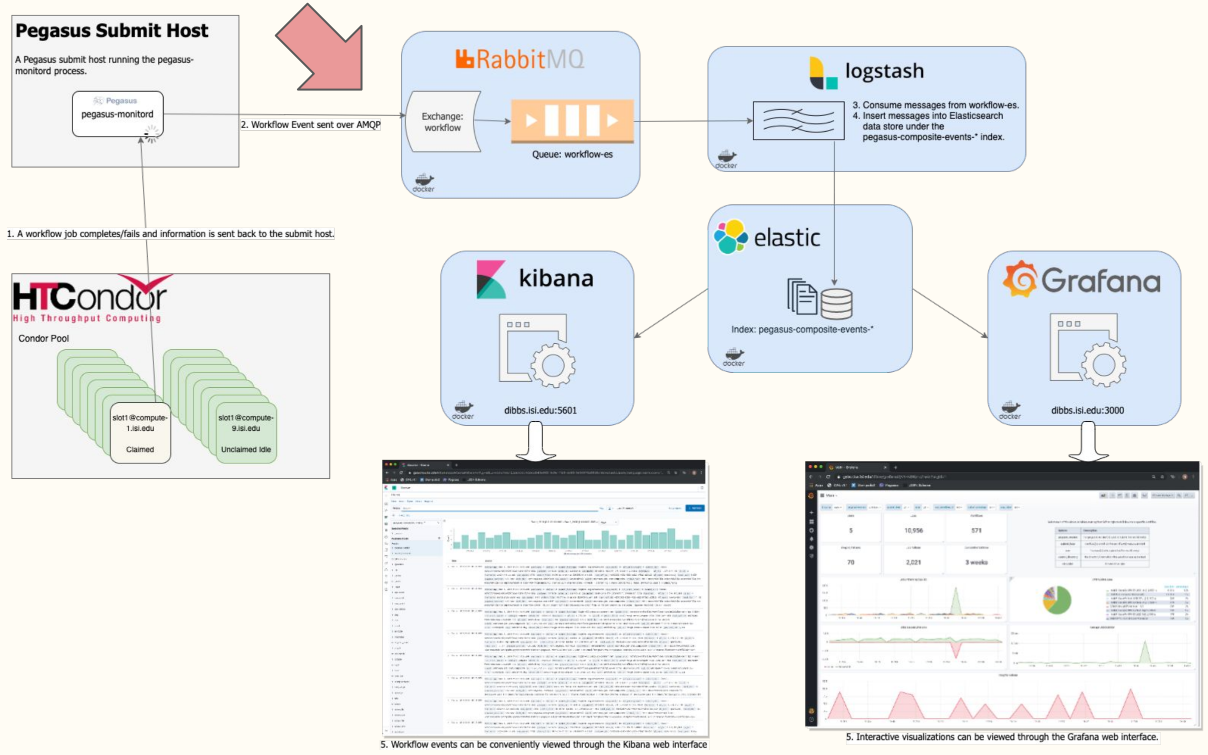
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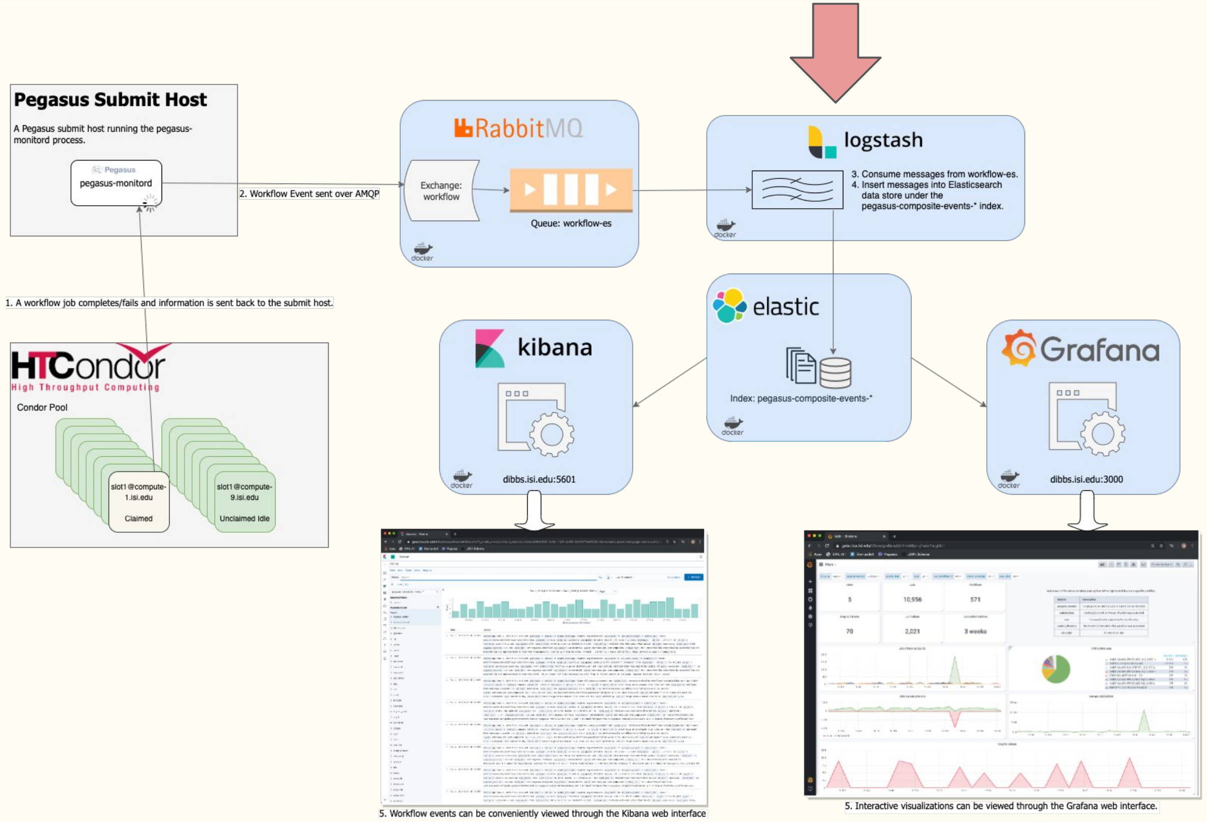
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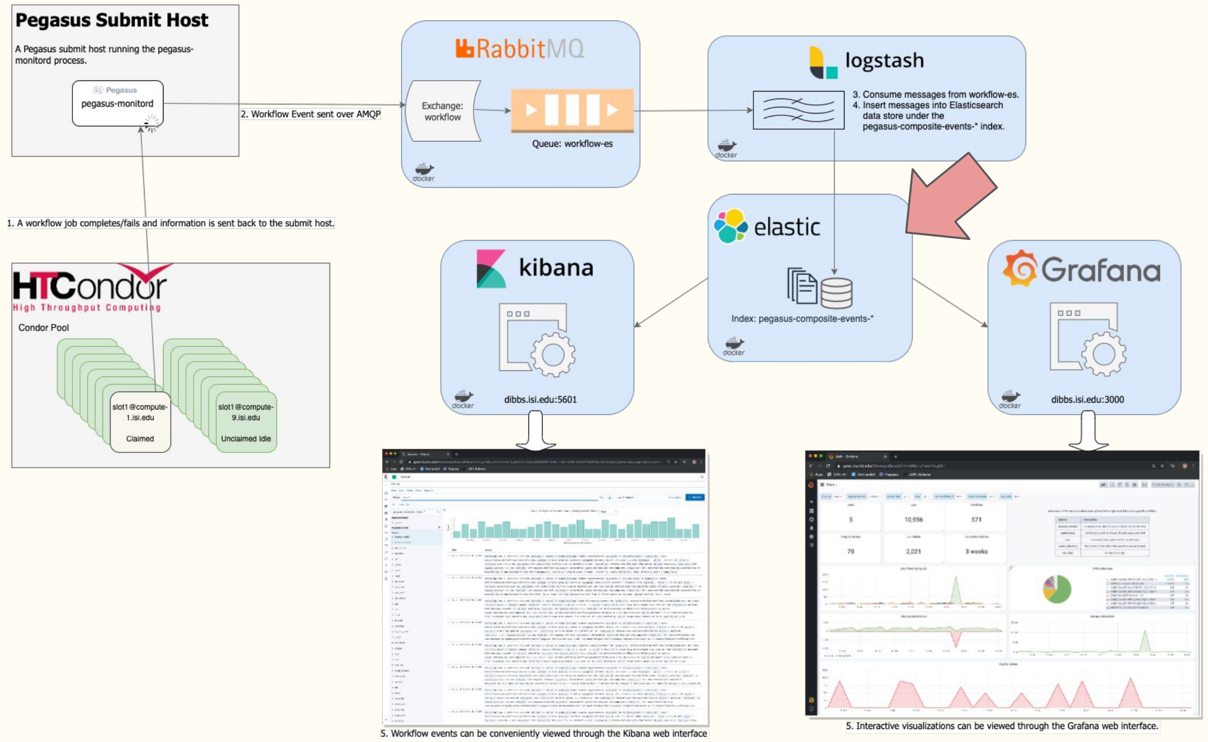
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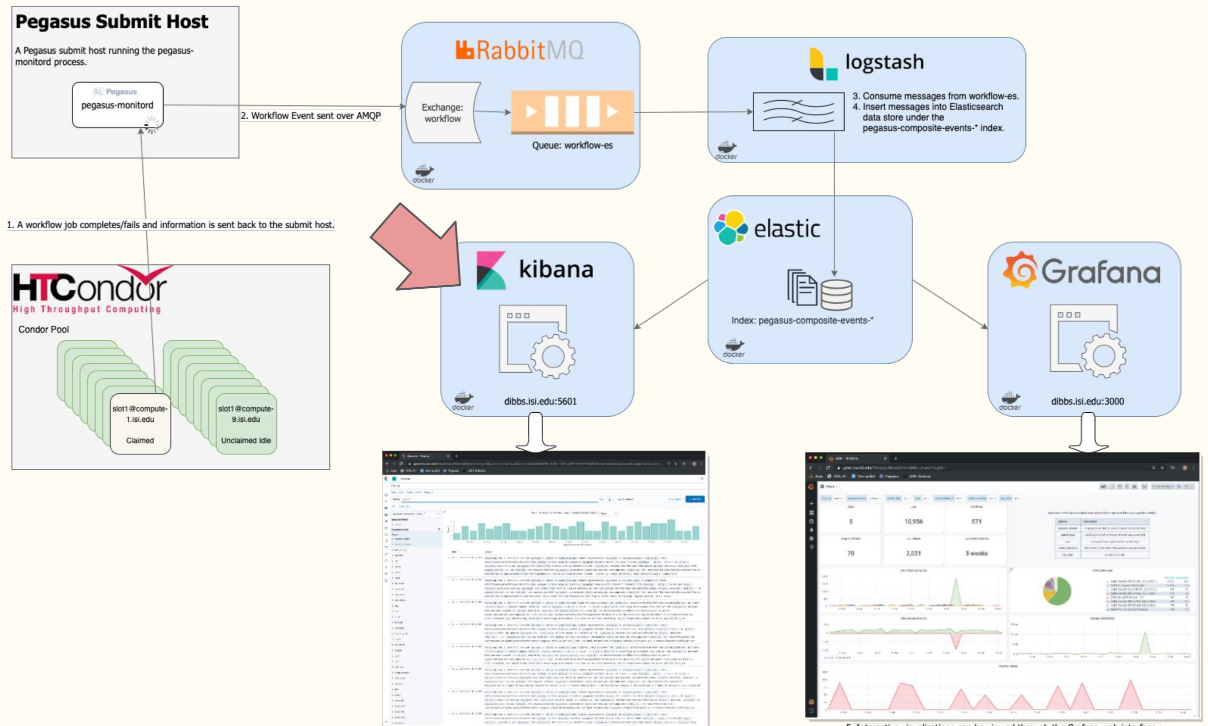
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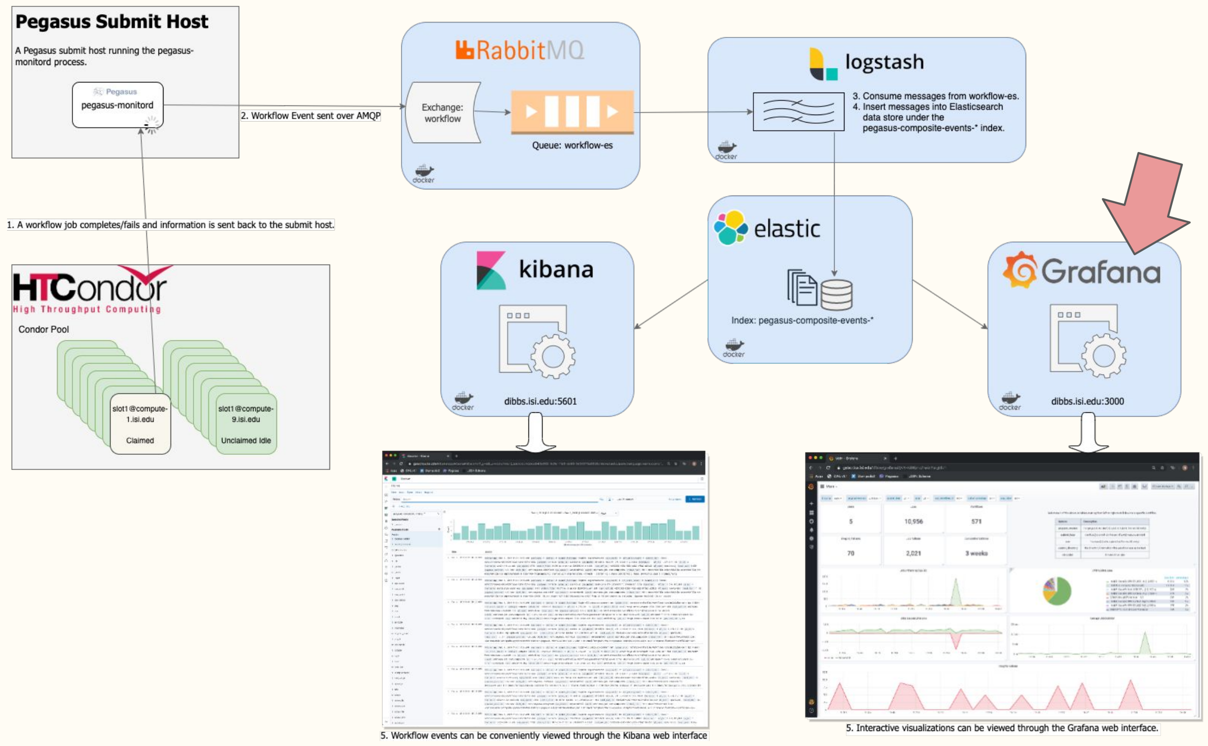

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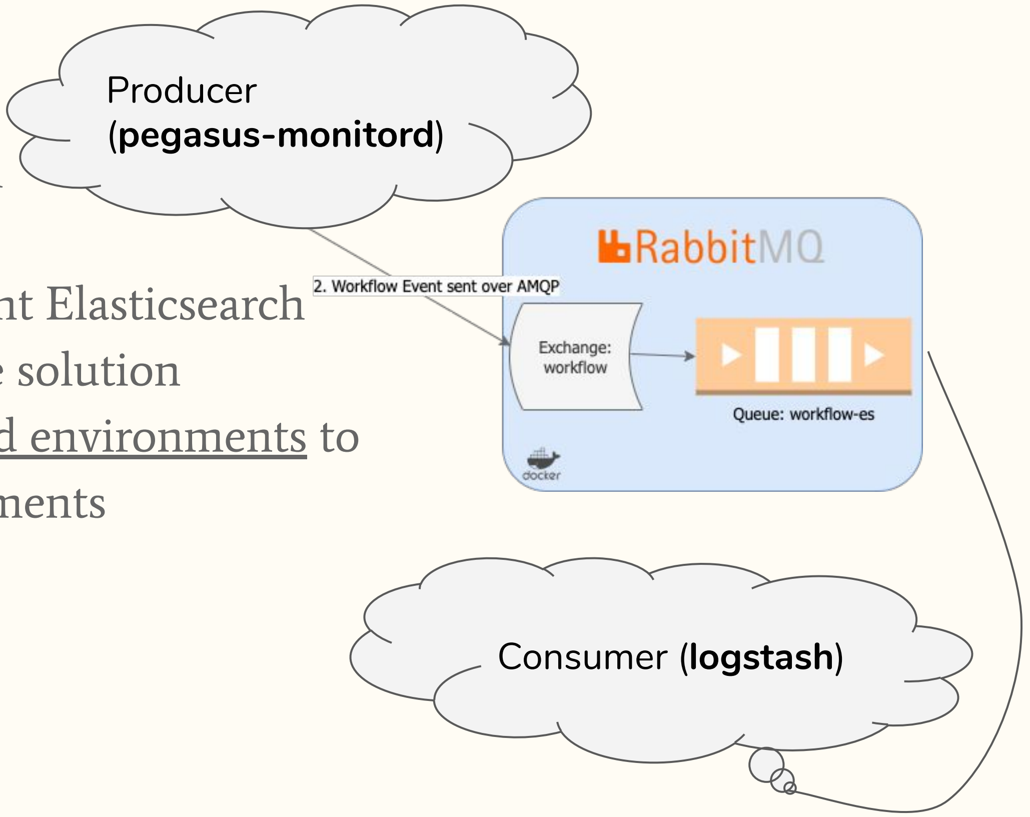
Data Collection Pipeline: RabbitMQ

- Lightweight message broker
- Relevant advantages
  - Promotes decoupling between producer/consumers
    - You can swap out/augment Elasticsearch with another data storage solution
  - Can be deployed in distributed environments to meet high availability requirements

    https://www.rabbitmq.com/



Data Collection Pipeline: ELK Stack

Elasticsearch:

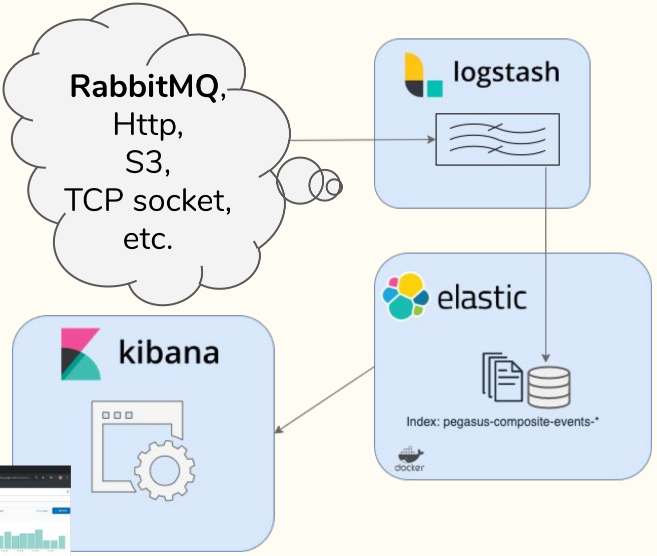
- distributed , RESTful search and analytics engine
- Log analytics, application performance monitoring, infrastructure metrics

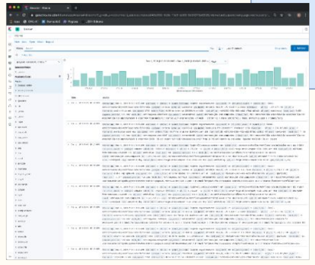
Logstash:

- Service that can aggregate and process data from various sources and insert it to elasticsearch

Kibana:

- Data visualization and exploration

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https://www.elastic.co/what-is/elk-stack

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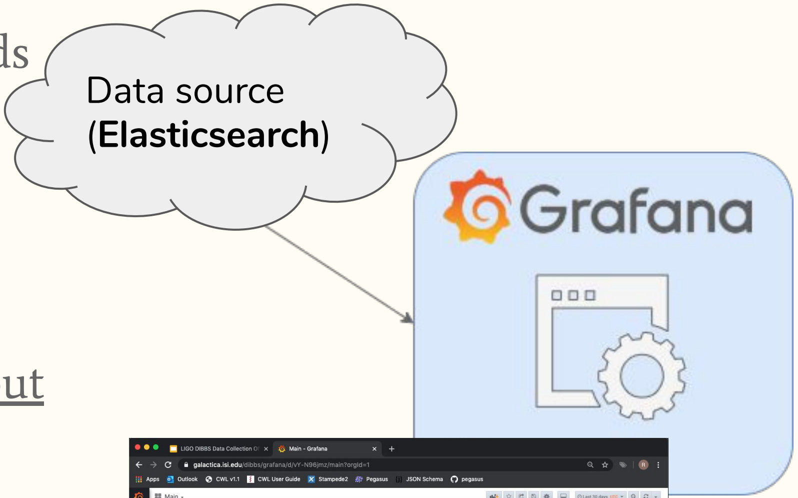
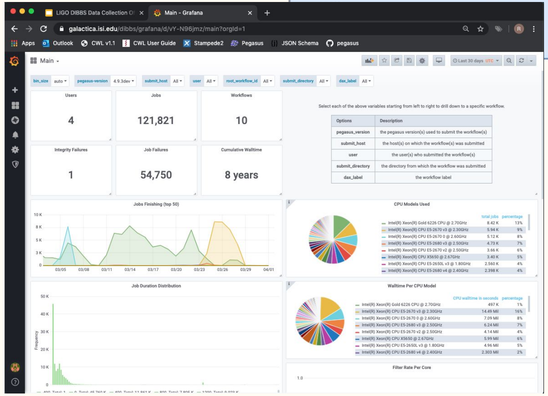
Data Collection Pipeline: Grafana

- Customizable browser based dashboards
- Support for multiple data sources
  - Elasticsearch
  - MySql
  - Etc.
- Enable data sharing across teams without exposing database

  https://grafana.com/





galactica.isi.edu/dibbs/grafana/d/vY-N96jmz/main?orgId=1

bin_size: auto · pegasus-version: 4.9.3dev · submit_host: All · user: All · root_workflow_id: All · submit_directory: All · dax_label: All

Users	Jobs	Workflows
4	121,821	10

Integrity Failures	Job Failures	Cumulative Walltime
1	54,750	8 years

Select each of the above variables starting from left to right to drill down to a specific workflow.

Options	Description
pegasus_version	the pegasus version(s) used to submit the workflow(s)
submit_host	the host(s) on which the workflow(s) was submitted
user	the user(s) who submitted the workflow(s)
submit_directory	the directory from which the workflow was submitted
dax_label	the workflow label

CPU Models Used

	total jobs	percentage
Intel(R) Xeon(R) Gold 6226 CPU @ 2.70GHz	8.42 K	13%
Intel(R) Xeon(R) CPU E5-2670 v3 @ 2.30GHz	5.94 K	9%
Intel(R) Xeon(R) CPU E5-2670 0 @ 2.60GHz	5.12 K	8%
Intel(R) Xeon(R) CPU E5-2680 v3 @ 2.50GHz	4.73 K	7%
Intel(R) Xeon(R) CPU E5-2670 v2 @ 2.50GHz	3.66 K	6%
Intel(R) Xeon(R) CPU X5650 @ 2.67GHz	3.40 K	5%
Intel(R) Xeon(R) CPU E5-2650L v3 @ 1.80GHz	2.560 K	4%
Intel(R) Xeon(R) CPU E5-2680 v4 @ 2.40GHz	2.398 K	4%

Walltime Per CPU Model

	CPU walltime in seconds	percentage
Intel(R) Xeon(R) Gold 6226 CPU @ 2.70GHz	497 K	1%
Intel(R) Xeon(R) CPU E5-2670 v3 @ 2.30GHz	14.49 Mil	16%
Intel(R) Xeon(R) CPU E5-2670 0 @ 2.60GHz	7.09 Mil	8%
Intel(R) Xeon(R) CPU E5-2680 v3 @ 2.50GHz	6.24 Mil	7%
Intel(R) Xeon(R) CPU E5-2670 v2 @ 2.50GHz	4.14 Mil	4%
Intel(R) Xeon(R) CPU X5650 @ 2.67GHz	5.99 Mil	6%
Intel(R) Xeon(R) CPU E5-2650L v3 @ 1.80GHz	4.96 Mil	5%
Intel(R) Xeon(R) CPU E5-2680 v4 @ 2.40GHz	2.303 Mil	2%

Data Collection Pipeline: How We Use It

Deployment:

- 3 node elasticsearch cluster on 3 VMs
- Single logstash instance in docker
- Single RabbitMQ instance

Usage:

- Also stores OSG data, system data
- Projects:
    - Panorama 360: Performance Data Capture and Analysis for End-to-end Scientific Workflows (https://panorama360.github.io/)
    - IRIS: Integrity Introspection For Scientific Workflows (http://nrig.renci.org/project/iris-integrity-introspection-for-scientific-workflows/)

Outline

- ~~Background~~
- ~~Data collection pipeline~~
- **Getting started**
- Demo

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Getting Started: Prerequisites

Requirements:

- Host with a static ip (dibbs.isi.edu in this example)
  - Following ports unused:
    - 5673 <- RabbitMQ
    - 15672 <- RabbitMQ
    - 9200 <- Elasticsearch
    - 9600 <- Logstash
    - 5601 <- Kibana
    - 3000 <- Grafana
- Docker v17.02+
- Docker Compose v3.5

Getting Started: Up and Running

Clone Repository (https://github.com/pegasus-isi/dibbs-data-collection-setup):

```
git clone https://github.com/pegasus-isi/dibbs-data-collection-setup.git
```

Grant Read/Write Access Permissions:

- dibbs-data-collection-setup/**elasticsearch**/data
- dibbs-data-collection-setup/**grafana**/data
- dibbs-data-collection-setup/**kibana**/data
- dibbs-data-collection-setup/**rabbitmq**/data

Getting Started: Up and Running

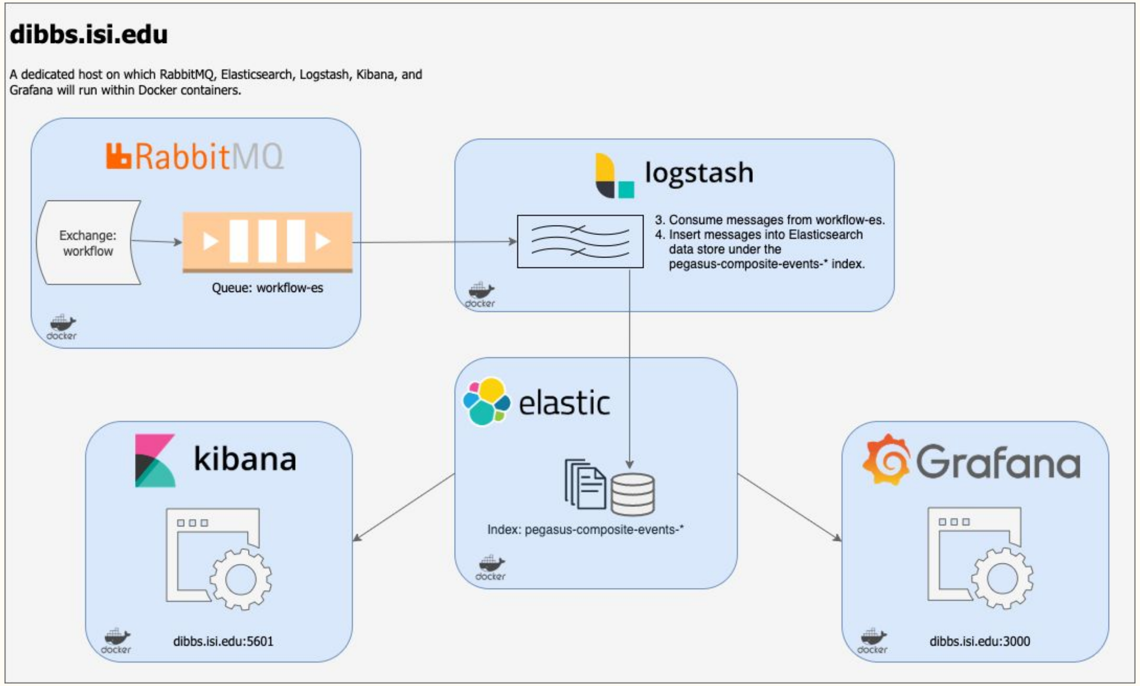
Starting the pipeline:

```
cd dibbs-data-collection-setup
```

```
docker-compose up
```

Access:

- Kibana: dibbs.isi.edu:5602
- Grafana: dibbs.isi.edu:3000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docker

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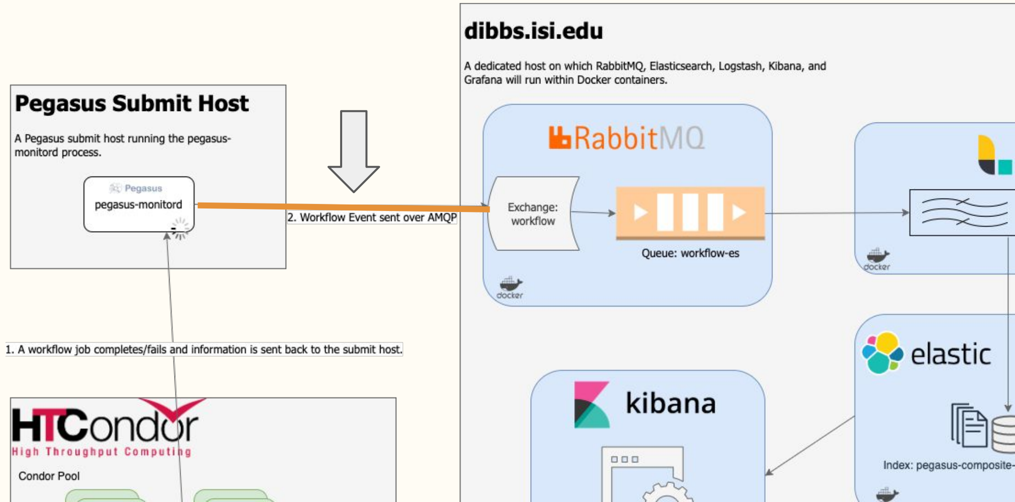
Getting Started: Configuring Pegasus

Say that this setup is running on a host dibbs.isi.edu, then the following must be included in the pegasus configuration file used to run your workflows:

```
pegasus.monitord.encoding = json
pegasus.catalog.workflow.amqp.url = amqp://friend:donatedata@dibbs.isi.edu:5672/prod/workflows
```

**** requires Pegasus 4.9.2+***



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Getting Started: Sending Application Specific Metadata

**** requires Pegasus 4.9.3+***

```
@@@MONITORING_PAYLOAD - START@@@
```

```
{
   “ts”: <long>,
   “monitoring_event”: “metadata”,
   “payload”: [
      {
         “name”: <string>,
         “value”: <scalar|string>
      }
      …
   ]
}
```

```
@@@MONITORING_PAYLOAD - END@@@
```

```
# the start of the marker the monitord will look for in the stdout
echo '@@@MONITORING_PAYLOAD - START@@@'

# a json blurb describing the content following
# the actual content
cat <<EOF
{
    "ts": 1437688574,
    "monitoring_event": "metadata",
    "payload": [
        {
            "name": "num_template_banks",
            "value" : 3
        },
        {
            "name": "event_name",
            "value" : "binary start merger"
        }
    ]
}
EOF

# the end of the marker the monitord will look for in the stdout
echo '@@@MONITORING_PAYLOAD - END@@@'
```

```
"metadata_num_template_banks": 3,
"metadata_event_name": "binary start merger",
```

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- ~~Background~~
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Pegasus est. 2001

Automate, recover, and debug scientific computations

Get Started

Pegasus Website
https://pegasus.isi.edu/

Users Mailing List
pegasus-users@isi.edu

Pegasus Website
pegasus-support@isi.edu

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
office hours

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