

Developing Pegasus Workflows via Jupyter Notebooks

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Jupyter Notebooks

From Jupyter.org:

The Jupyter Notebook is an open-source web application that allows you to create and share documents that contain live code, equations, visualizations and narrative text. Uses include: data cleaning and transformation, numerical simulation, statistical modeling, data visualization, machine learning, and much more.

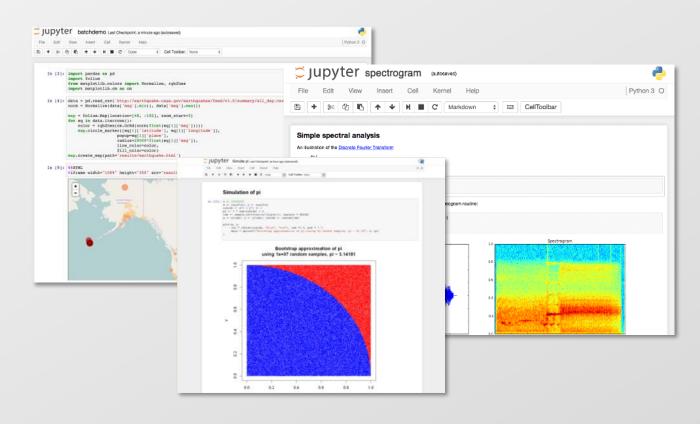
Key Advantages

Collaboration
Easy access to resources
Building blocks
Reproducibility

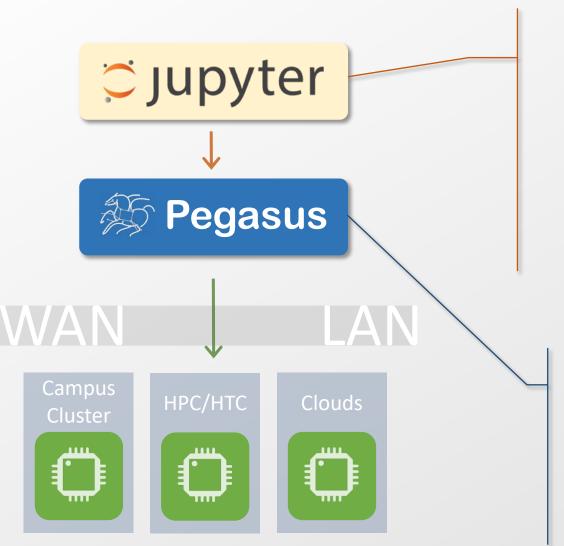
Examples

LIGO Gravitational Wave Data Satellite Imagery Analysis 12 Steps to Navier-Stokes Computer Vision Machine Learning

https://unidata.github.io/online-python-training/introduction.html

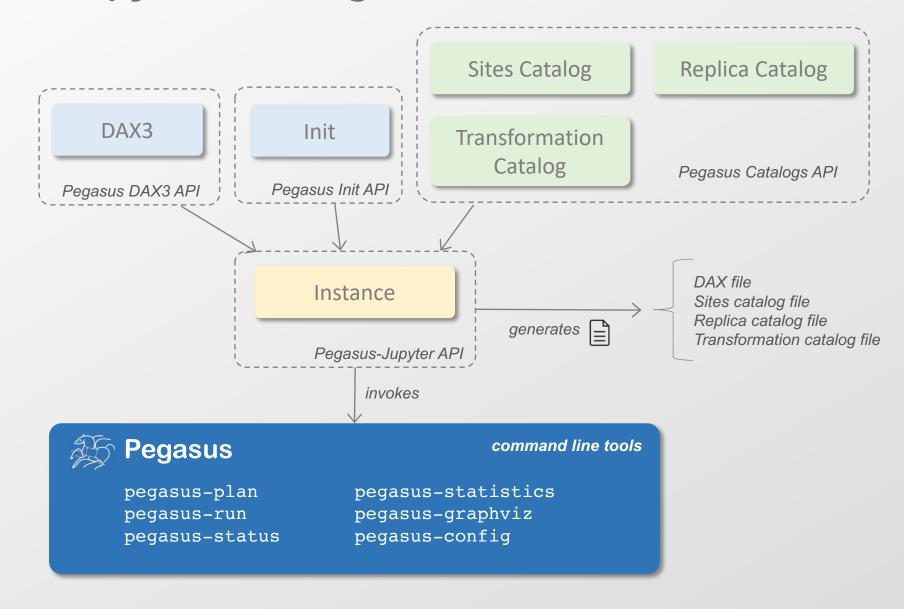


Running Pegasus workflows with Jupyter



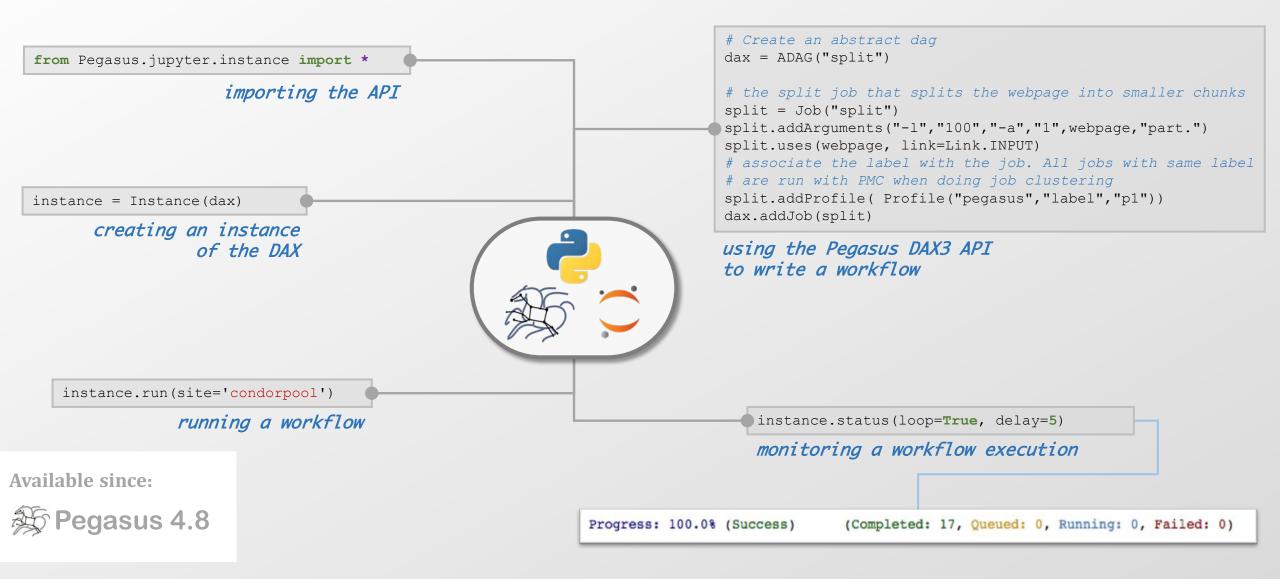
```
File for submitting this DAG to Condor
                                              : split-0.dag.condor.sub
Log of DAGMan debugging messages
                                              : split-0.dag.dagman.out
Log of Condor Library output
                                              : split-0.dag.lib.out
Log of Condor Library error messages
                                              : split-0.dag.lib.err
Log of the life of condor_dagman itself
                                              : split-0.dag.dagman.log
Your database is compatible with Pegasus version: 4.7.0
Submitting to condor split-0.dag.condor.sub
Submitting job(s).
1 job(s) submitted to cluster 1068.
Your workflow has been started and is running in the base directory:
  /Users/silva/Downloads/split-submit-host-2017-03-27T10:17:45/submit/silva/pegasus/split/run0002
*** To monitor the workflow you can run ***
  pegasus-status - I /Users/silva/Downloads/split-submit-host-2017-03-27T10:17:45/submit/silva/pegasus/split/run0002
```

Pegasus - Jupyter Integration Overview





Pegasus-Jupyter Python API



Additional capabilities...

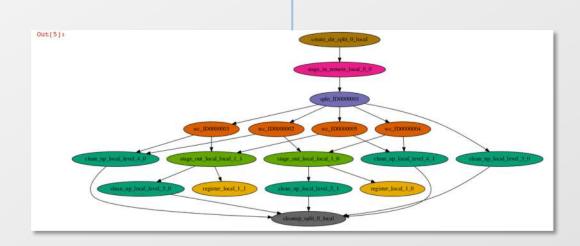
```
wf_image_exe = instance.view(abstract=False)
# IPython package for visualizing images
from IPython.display import Image
Image(wf_image_exe)
```

visualizing the workflow

instance.statistics()

collect statistics

Workflow Wall Time: 47 min, 23 secs



Available since:



```
# creating a site catalog. A local site is automatically created
sites_catalog = SitesCatalog()

# adding a site with some profile characteristics
sites_catalog.add_site('condorpool', Arch.X86_64, OSType.LINUX)
sites_catalog.add_profile('condorpool', Namespace.ENV, 'JAVA_HOME', '/usr/local/jre')
dax.set_sites_catalog(sites_catalog)
```

create catalogs: site, replica, and transformation



Requirements

Pegasus submit node

```
Python 2.7 or higher (Jupyter requires version 2.7+)
Java 1.8 or higher
Pegasus 4.8.0 or higher
<a href="https://pegasus.isi.edu/downloads/">https://pegasus.isi.edu/downloads/</a>
Jupyter
<a href="http://jupyter.org/install.html">http://jupyter.org/install.html</a>
```

JupyterHub

Due to the strict requirement of **Python 3** for running the multi-user hub, our API requires the Python **future package** in order to be compatible with Python 3.



https://pypi.python.org/pypi/future





References

Documentation

https://pegasus.isi.edu/documentation/jupyter.php

API Reference

Instance: https://pegasus.isi.edu/documentation/python/instance.html
Catalogs:
 https://pegasus.isi.edu/documentation/python/sites_catalog.html

https://pegasus.isi.edu/documentation/python/replica_catalog.html
https://pegasus.isi.edu/documentation/python/transformation_catalog.html

Example Tutorial Notebook

Distributed with Pegasus releases (since 4.8)

Also available in the Pegasus Tutorial VM (https://pegasus.isi.edu/downloads/)

Instructions

https://pegasus.isi.edu/documentation/jupyter-example.php





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

Pegasus Online Office Hours

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

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

HipChat





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Thank You

Questions?

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Meet our team



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