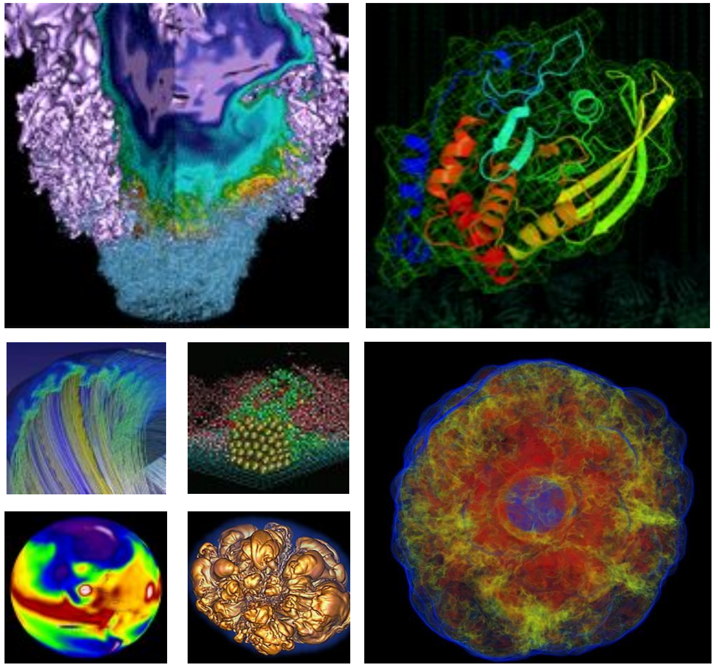
Python and Jupyter at NERSC

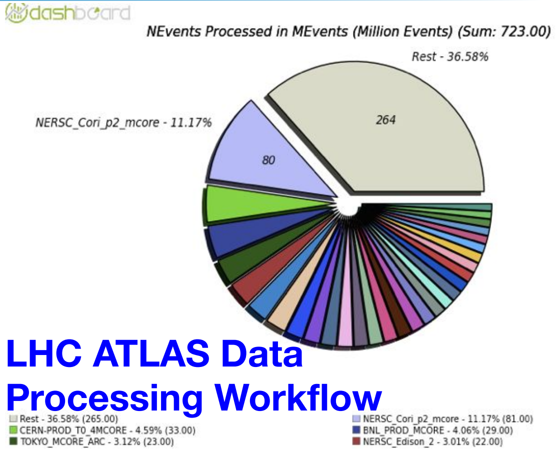


Rollin Thomas
Data Architect
Data and Analytics Services, NERSC

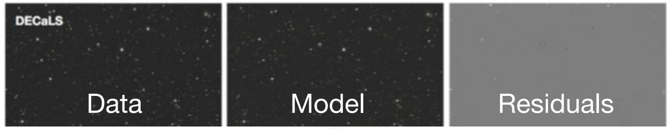
New User Training, 2019-06-21

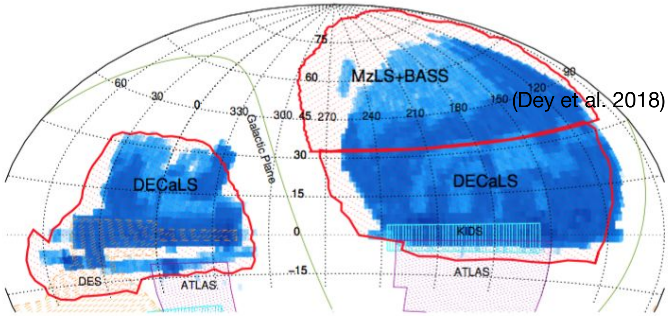
Science via Python@NERSC

Powering Workflows to Understand Properties of Materials



LHC ATLAS Data Processing Workflow



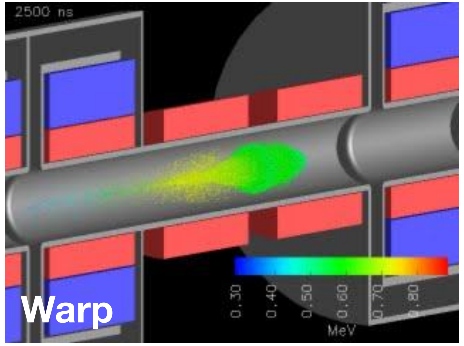


(Dey et al. 2018)

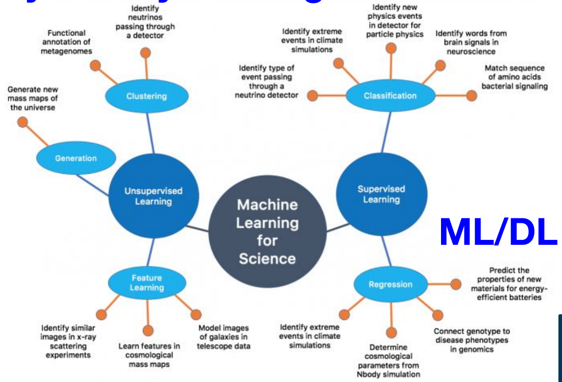
Sky Survey Catalogs for Cosmology

NBODYKIT

Modeling Dark Matter and Dark Energy



PIC Code for Plasmas and High Current Particle Beams


Machine Learning for Science
Unsupervised Learning
Supervised Learning
Clustering
Generation
Feature Learning
Classification
Regression
Functional annotation of metagenomes
Identify neutrinos passing through a detector
Generate new mass maps of the universe
Identify type of event passing through a neutrino detector
Identify extreme events in climate simulations
Identify new physics events in detector for particle physics
Identify words from brain signals in neuroscience
Match sequence of amino acids bacterial signaling
Predict the properties of new materials for energy-efficient batteries
Identify similar images in x-ray scattering experiments
Learn features in cosmological mass maps
Model images of galaxies in telescope data
Identify extreme events in climate simulations
Determine cosmological parameters from Nbody simulation
Connect genotype to disease phenotypes in genomics

ML/DL

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NERSC Python Documentation

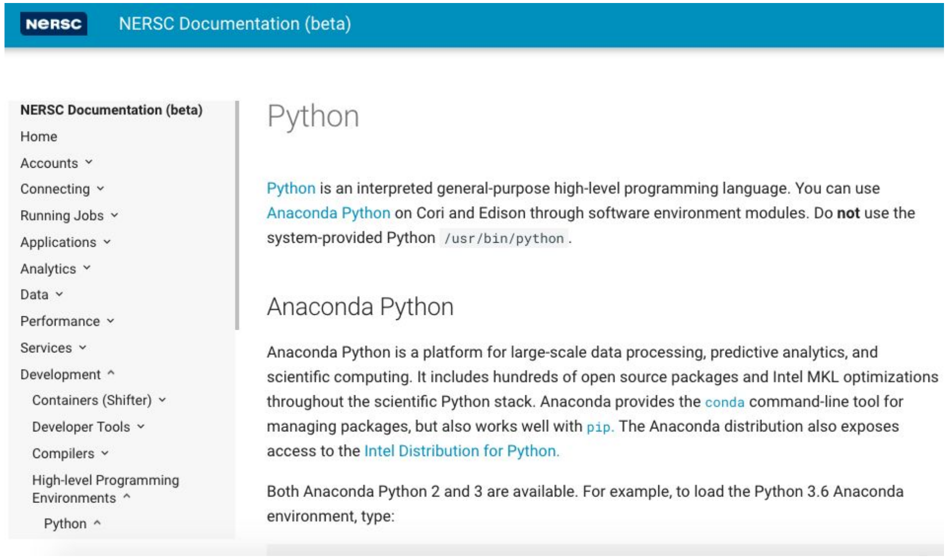
Good docs advise on how to use Python at NERSC.

Updates are ~continuous.
[Main page.]

Frequently Asked Questions
[FAQ page.]
Suggest new questions!

Advice/gotchas for KNL users
[KNL page.]

Advice on [optimizing Python.]



Python

Python is an interpreted general-purpose high-level programming language. You can use Anaconda Python on Cori and Edison through software environment modules. Do **not** use the system-provided Python `/usr/bin/python`.

Anaconda Python

Anaconda Python is a platform for large-scale data processing, predictive analytics, and scientific computing. It includes hundreds of open source packages and Intel MKL optimizations throughout the scientific Python stack. Anaconda provides the `conda` command-line tool for managing packages, but also works well with `pip`. The Anaconda distribution also exposes access to the Intel Distribution for Python.

Both Anaconda Python 2 and 3 are available. For example, to load the Python 3.6 Anaconda environment, type:

New site: docs.nersc.gov

Use Environment Modules

Environment modules:

Environment modules project:

http://modules.sourceforge.net/

Always* “module load python”

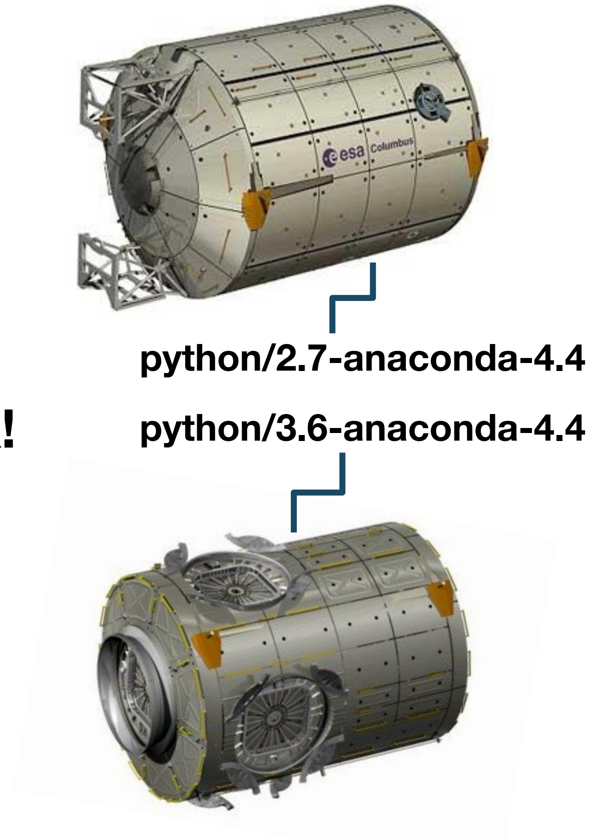
Do not use /usr/bin/python.

Using #!/usr/bin/env python is OK!

What is there?

module avail python

* Unless you install your own somehow.
(Totally fine, see later in the talk.)



NERSC's Python is Anaconda

NERSC's builds of Python on Cori have been retired for a while.

Modules Now Leverage Anaconda Python

- **Distro for large-scale data analytics and scientific computing.**
- **Handy package management and deployment (conda tool).**
- **Conda environments replace virtualenv.**

Hundreds of useful packages (400+ already installed)

- **Threaded Intel MKL comes for free.**
- **Now with some ML tools too.**
- **Additional "channels" and you can still use pip.**

https://docs.anaconda.com/anaconda/

They are monolithic; with some add-on modules (h5py-parallel).

NERSC Python Modules

Recommended environment modules at NERSC for Python users:

```
module load python/2.7-anaconda-4.4
module load python/3.6-anaconda-4.4
```

Default Python is 2.7 up to no later than 6 months from now:

```
module load python
[= module load python/2.7-anaconda-4.4]
```

Conda Environments

Conda makes it easy to create tailored environments with the packages you need.

```
module load python/3.6-anaconda-4.4
conda create -n myenv python=2 numpy
[installation outputs]
source activate myenv
```

And pip is OK to use too. Note, "--no-cache-dir" is handy

Don't bother with --user, just pip in your conda env.

Doing Things Yourself

Project-wide Anaconda installation, e.g. at
/global/common/software/<project-name>

```
module unload python
unset PYTHONSTARTUP

wget https://repo.continuum.io/miniconda/Miniconda2-latest-Linux-x86_64.sh
/bin/bash Miniconda2-latest-Linux-x86_64.sh -b -p $PREFIX
source $PREFIX/bin/activate
    <or export PATH=$PREFIX/bin:$PATH>
conda install basemap yt…
```

Doing Things Yourself

Building your own mpi4py or parallel h5py?

Do not conda install ...

Do not pip install ...

Link to Cray MPICH, using compiler wrappers

```
wget https://bitbucket.org/mpi4py/mpi4py/downloads/mpi4py-3.0.0.tar.gz
tar zxvf mpi4py-3.0.0.tar.gz
cd mpi4py-3.0.0
module swap PrgEnv-intel PrgEnv-gnu
python setup.py build --mpicc=$(which cc)
python setup.py install
```

Parallelism with Python

Within a node:

- Use OpenMP-threaded math libs.
- Multiprocessing is OK too.

Multi-node parallelism:

- Best supported by mpi4py.
- Dask, PySpark work too.

Hybrid parallelism:

- Best route is mpi4py + threaded math libs.

Handling MPI with mpi4py

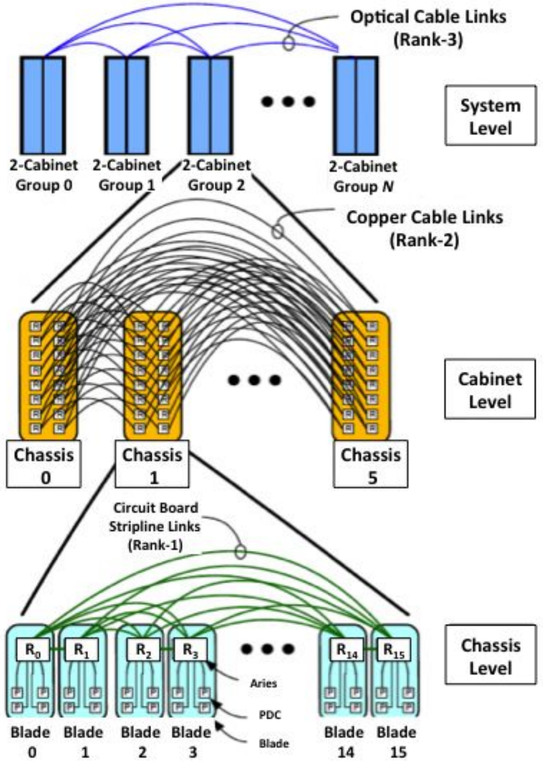
Cluster parallelism with MPI via mpi4py:

- MPI-1/2/3 specification support
- OO interface ~ MPI-2 C++ bindings
- Point-to-point and collectives
- Picklable Python objects & buffers

Build mpi4py & dependents with Cray MPICH:

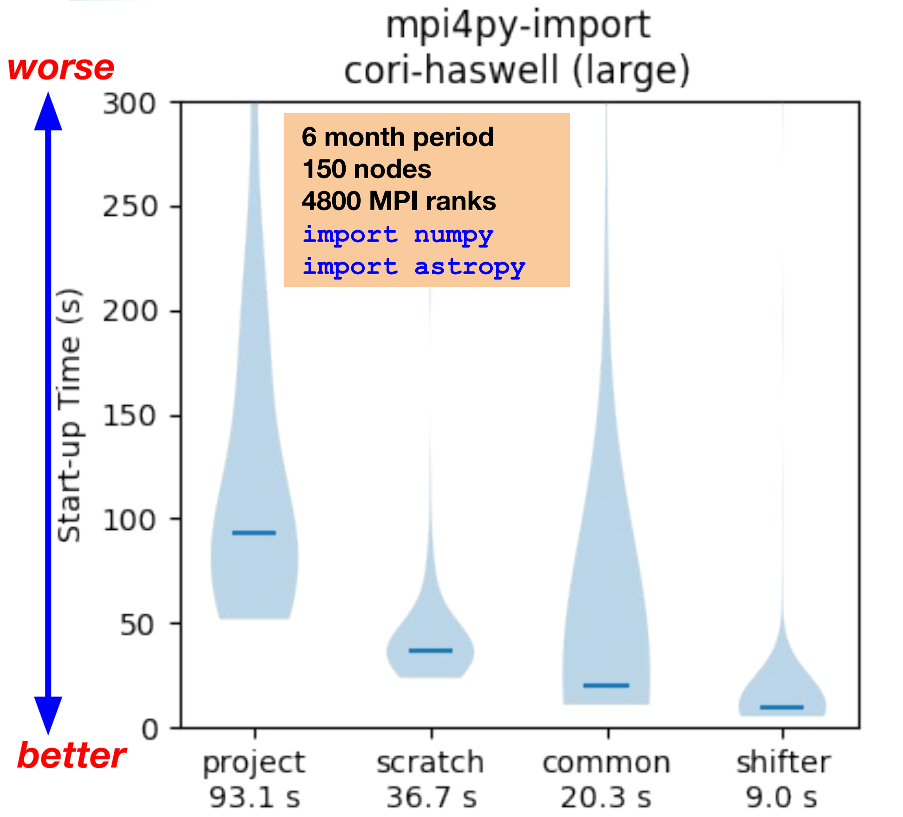
```
python setup.py build --mpicc=cc
python setup.py install
```

Cray-provided Compiler wrapper



Cori Aries Interconnect

Python “Slow Launch” at Scale



6 month period
150 nodes
4800 MPI ranks

```
import numpy
import astropy
```

[Median launch time incl. MPI_Init()]

Python’s import is metadata intensive,
⇒ catastrophic contention at scale
⇒ *it matters where you install your env*

Project (GPFS):
For sharing large data files

Scratch (Lustre):
OK, but gets purged periodically!

Common (GPFS):
RO w/Cray DVS client-side caching
Open to users now, was only staff

Shifter (Docker Containers):
Metadata lookup only on compute
Storage on compute is RAM disk
ldconfig when you build image

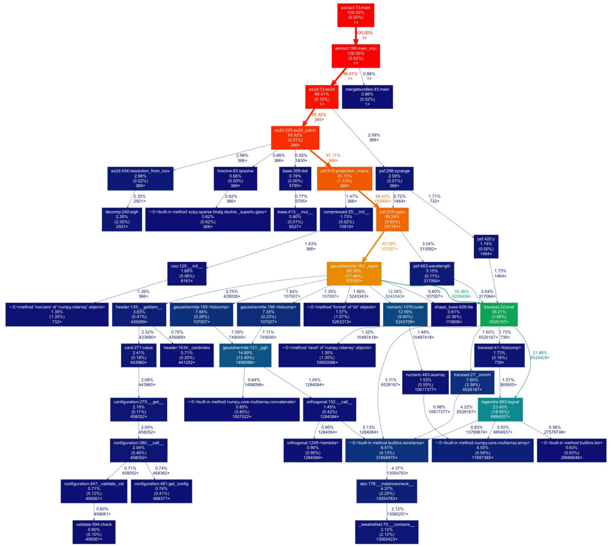
Profiling, Debugging

Ye olde stand-bye, `print()`!

```
srun -u python -u <script-name> …
```

Unbuffer both srun and python.

Can be a lot of messy output to parse.



Good for general exploration (standard lib):

- cProfile plus snakeviz or gprof2dot
- MPI processes? [see an example here]

Good for a deeper dive on one function (package):

- line_profiler

High-performance instrumented timer (mixed-language, MPI, package):

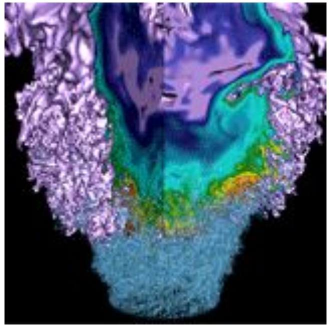
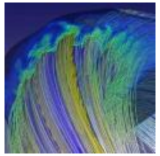
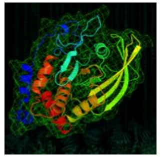
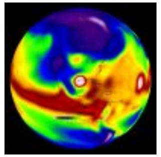
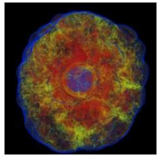
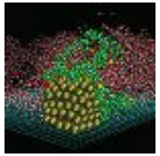
- TiMemory

High-performance tools (mixed-language, MPI):

- Intel VTune (some collection methods) on Intel Python, and Tau

https://docs.nersc.gov/development/high-level-environments/python/profiling-python/

Jupyter at NERSC

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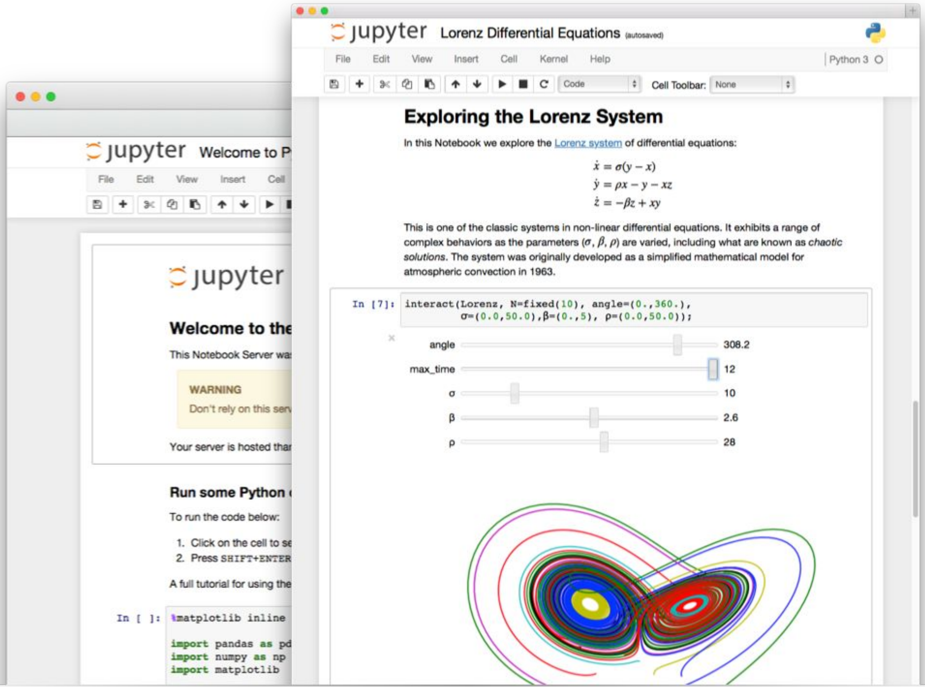
Using Jupyter at NERSC

Jupyter Notebook: “Literate Computing.”
Code, text, equations, viz in a narrative.

Use JupyerHub for Jupyter at NERSC.

https://jupyter.nersc.gov/
- **Cori Shared CPU Node:**
  - **Launches notebooks on Cori**
  - **Can see Cori $SCRATCH**
  - **Same Python env as ssh login**
  - **Can submit jobs via `%sbatch`**
- **Spin Shared CPU Node:**
  - **External to Cori**
  - **Can’t see $SCRATCH**
  - **But can see /project, $HOME**



Welcome to the
This Notebook Server wa
WARNING
Don't rely on this serv
Your server is hosted tha
Run some Python
To run the code below:
1. Click on the cell to se
2. Press SHIFT+ENTER
A full tutorial for using the

```
In [ ]: %matplotlib inline

        import pandas as pd
        import numpy as np
        import matplotlib
```

Exploring the Lorenz System

In this Notebook we explore the Lorenz system of differential equations:

$$\dot{x} = \sigma(y - x)$$
$$\dot{y} = \rho x - y - xz$$
$$\dot{z} = -\beta z + xy$$

This is one of the classic systems in non-linear differential equations. It exhibits a range of complex behaviors as the parameters (σ, β, ρ) are varied, including what are known as *chaotic solutions*. The system was originally developed as a simplified mathematical model for atmospheric convection in 1963.

```
In [7]: interact(Lorenz, N=fixed(10), angle=(0.,360.),
                 σ=(0.0,50.0),β=(0.,5), ρ=(0.0,50.0));
```

angle	308.2
max_time	12
σ	10
β	2.6
ρ	28

Your Own Jupyter-dev Kernel

Most common Jupyter question:

"How do I take a conda environment and turn it into a Jupyter kernel?"

Several ways to accomplish this, here's the easy one.

```
 $ module load python
 $ conda create -n myenv python=3.6
 $ source activate myenv
(myenv) $ conda install ipykernel <other-packages>...
(myenv) $ python -m ipykernel install --user --name myenv-jupyter
```

This creates a "kernelspec" file.

Point your browser to jupyter-dev.nersc.gov.
(You may need to restart your notebook server via control panel).
Kernel "myenv-jupyter" should be present in the kernel list.

The kernelspec File

```
(myenv) rthomas@cori01:~> cat \
    $HOME/.local/share/jupyter/kernels/myenv-jupyter/kernel.json
{
 "argv": [
  "/global/homes/r/rthomas/.conda/envs/myenv/bin/python",
  "-m",
  "ipykernel_launcher",
  "-f",
  "{connection_file}"
 ],
 "display_name": "myenv-jupyter",
 "language": "python"
}
```

Additional Customization

```
{
 "argv": [
  "/global/homes/r/rthomas/.conda/envs/myenv/bin/python",
  "-m",
  "ipykernel_launcher",
  "-f",
  "{connection_file}"
 ],
 "display_name": "myenv-jupyter",
 "language": "python",
 "env": {
  "PATH": …,
  "LD_LIBRARY_PATH": …,
 }
}
```

Additional Customization

```
{
 "argv": [
  "/global/homes/r/rthomas/jupyter-helper.sh",
  "-f",
  "{connection_file}"
 ],
 "display_name": "myenv-jupyter2",
 "language": "python",
}
```

Meanwhile, in jupyter-helper.sh:

```
#!/bin/bash
export SOMETHING=123
module load texlive
exec python -m ipykernel "$@”
```

A Shifter Kernelspec

```
{
  "argv": [
    "shifter",
    "--image=continuumio/anaconda3:latest",
    "/opt/conda/bin/python",
    "-m",
    "ipykernel_launcher",
    "-f",
    "{connection_file}"
  ],
  "display_name": "my-shifter-kernel",
  "language": "python"
}
```

Image name

Path in the image

Debugging Jupyter Stuff

```
(myenv) rthomas@cori01:~> cat ~/.jupyter.log
```

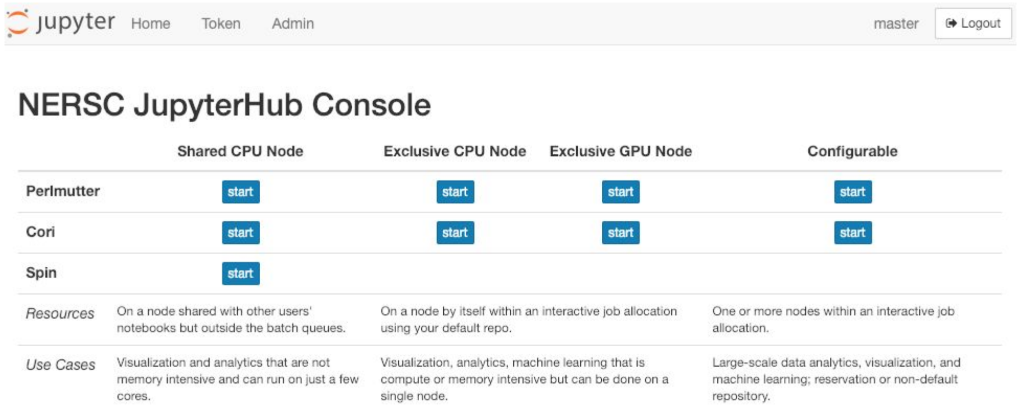
← **YOUR FRIEND**

```
[I 2018-03-19 16:00:08.175 SingleUserNotebookApp manager:40] [nb_conda_kernels] enabled, 5 kernels found
[I 2018-03-19 16:00:08.248 SingleUserNotebookApp extension:53] JupyterLab beta preview extension loaded from
/usr/common/software/python/3.6-anaconda-4.4/lib/python3.6/site-packages/jupyterlab
[I 2018-03-19 16:00:08.248 SingleUserNotebookApp extension:54] JupyterLab application directory is
/global/common/cori/software/python/3.6-anaconda-4.4/share/jupyter/lab
[I 2018-03-19 16:00:09.123 SingleUserNotebookApp handlers:73] [nb_anacondacloud] enabled
[I 2018-03-19 16:00:09.129 SingleUserNotebookApp handlers:292] [nb_conda] enabled
[I 2018-03-19 16:00:09.181 SingleUserNotebookApp __init__:35] ✓ nbpresent HTML export ENABLED
[W 2018-03-19 16:00:09.181 SingleUserNotebookApp __init__:43] ✗ nbpresent PDF export DISABLED: No module
named 'nbbrowserpdf'
[I 2018-03-19 16:00:09.186 SingleUserNotebookApp singleuser:365] Starting jupyterhub-singleuser server
version 0.8.0.rc1
[I 2018-03-19 16:00:09.190 SingleUserNotebookApp log:122] 302 GET /user/rthomas/ →
/user/rthomas/tree/global/homes/r/rthomas? (@128.55.206.24) 0.62ms
[I 2018-03-19 16:00:09.194 SingleUserNotebookApp notebookapp:1445] Serving notebooks from local directory: /
[I 2018-03-19 16:00:09.194 SingleUserNotebookApp notebookapp:1445] 0 active kernels
[I 2018-03-19 16:00:09.194 SingleUserNotebookApp notebookapp:1445] The Jupyter Notebook is running at:
[I 2018-03-19 16:00:09.194 SingleUserNotebookApp notebookapp:1445] http://0.0.0.0:56901/user/rthomas/
[I 2018-03-19 16:00:09.194 SingleUserNotebookApp notebookapp:1446] Use Control-C to stop this server and shut
down all kernels (twice to skip confirmation).
[I 2018-03-19 16:00:09.236 SingleUserNotebookApp log:122] 302 GET /user/rthomas/ →
/user/rthomas/tree/global/homes/r/rthomas? (@::ffff:10.42.245.15) 0.39ms
```

Near Future Jupyter Support

Working on:

- ❖ Expanding resources to support Jupyter
- ❖ New ways to launch parallel workloads managed through Jupyter
- ❖ Expanding JupyterLab interface to:
  - ➢ Track and monitor batch jobs
  - ➢ New viewers



NERSC JupyterHub Console

	Shared CPU Node	Exclusive CPU Node	Exclusive GPU Node	Configurable
Perlmutter	start	start	start	start
Cori	start	start	start	start
Spin	start			
Resources	On a node shared with other users' notebooks but outside the batch queues.	On a node by itself within an interactive job allocation using your default repo.		One or more nodes within an interactive job allocation.
Use Cases	Visualization and analytics that are not memory intensive and can run on just a few cores.	Visualization, analytics, machine learning that is compute or memory intensive but can be done on a single node.		Large-scale data analytics, visualization, and machine learning; reservation or non-default repository.

Python and Jupyter at NERSC

Python & Jupyter: integral elements of NERSC's Data Intensive Science portfolio.

We want users to have a:

familiar	Python environment
productive	Python experience
performant	Python software stack

Always looking for:

New ways to empower Python & data science users.

Feedback, advice, and even help:

https://help.nersc.gov/

rcthomas@lbl.gov

Thank You