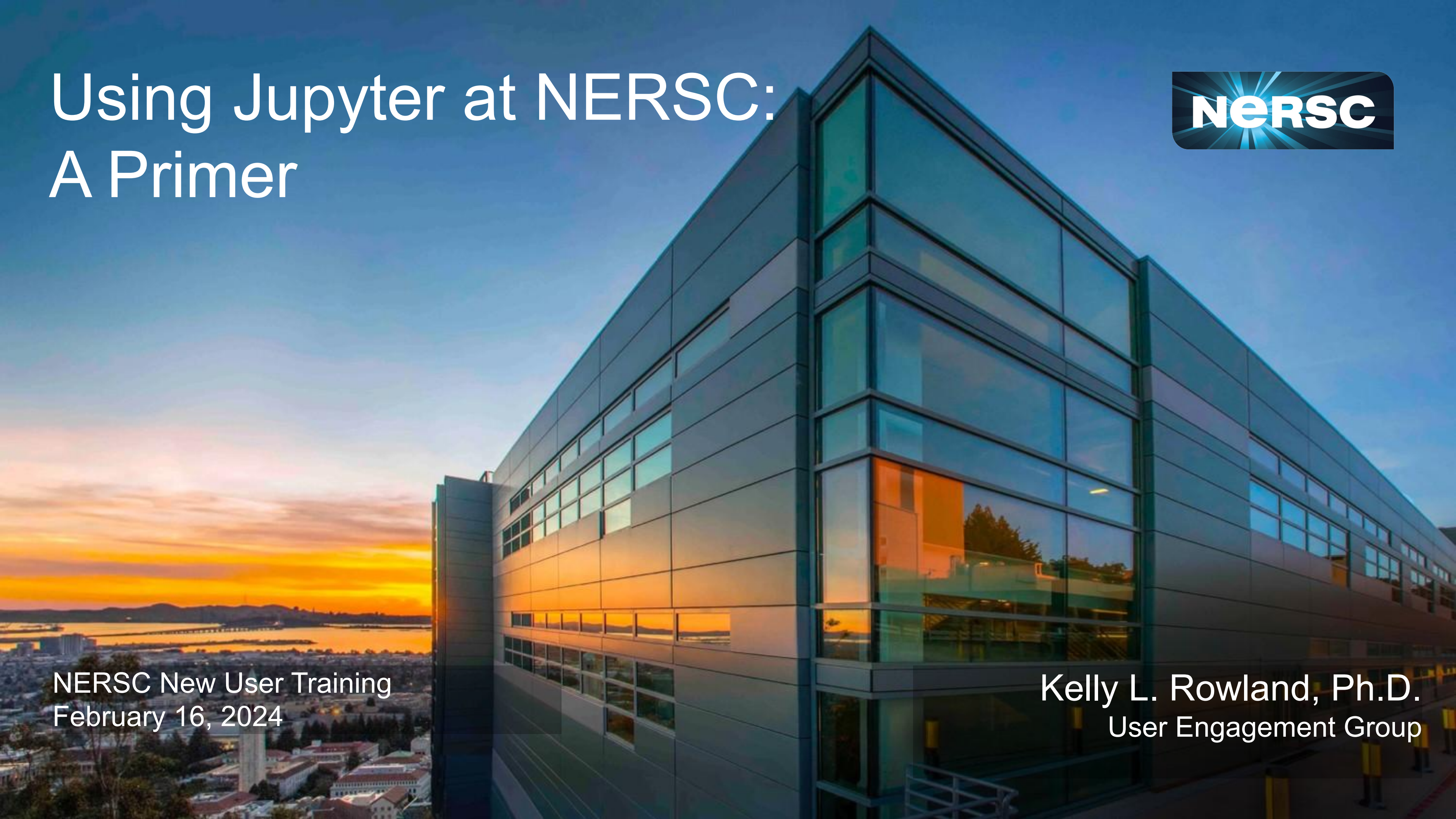

Using Jupyter at NERSC: A Primer

NERSC New User Training
February 16, 2024

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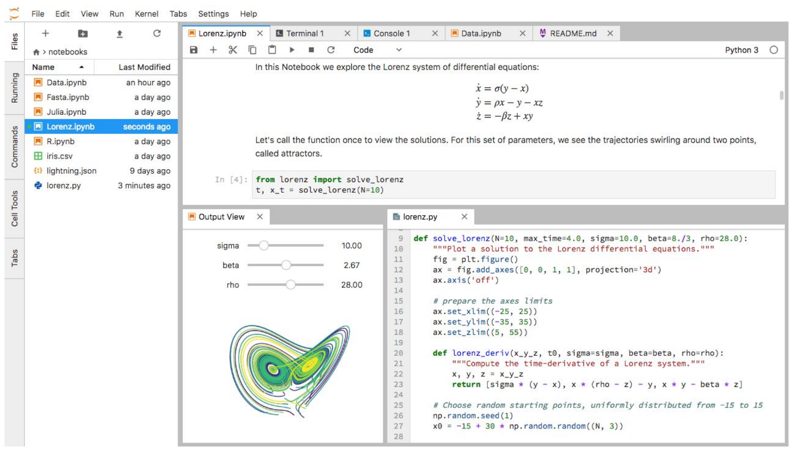
User Engagement Group

What is Jupyter?

- At NERSC, we say "Jupyter" in reference to a collection of many things
    - Access shareable Jupyter "notebooks" via JupyterHub
- What can I put in a Jupyter notebook?
    - Live code
    - Equations
    - Visualizations
    - Narrative text
    - Interactive widgets
- What applications would I use a notebook for?
    - Data cleaning and data transformation
    - Numerical simulation
    - Statistical modeling
    - Data visualization
    - Machine learning
    - Workflows and analytics frameworks



Name	Last Modified
Data.ipynb	an hour ago
Fasta.ipynb	a day ago
Julia.ipynb	a day ago
Lorenz.ipynb	seconds ago
R.ipynb	a day ago
iris.csv	a day ago
lightning.json	9 days ago
lorenz.py	3 minutes ago

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

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

Let's call the function once to view the solutions. For this set of parameters, we see the trajectories swirling around two points, called attractors.

```
In [4]: from lorenz import solve_lorenz
        t, x_t = solve_lorenz(N=10)
```

```
def solve_lorenz(N=10, max_time=4.0, sigma=10.0, beta=8./3, rho=28.0):
    """Plot a solution to the Lorenz differential equations."""
    fig = plt.figure()
    ax = fig.add_axes([0, 0, 1, 1], projection='3d')
    ax.axis('off')

    # prepare the axes limits
    ax.set_xlim((-25, 25))
    ax.set_ylim((-35, 35))
    ax.set_zlim((5, 55))

    def lorenz_deriv(x_y_z, t0, sigma=sigma, beta=beta, rho=rho):
        """Compute the time-derivative of a Lorenz system."""
        x, y, z = x_y_z
        return [sigma * (y - x), x * (rho - z) - y, x * y - beta * z]

    # Choose random starting points, uniformly distributed from -15 to 15
    np.random.seed(1)
    x0 = -15 + 30 * np.random.random((N, 3))

```

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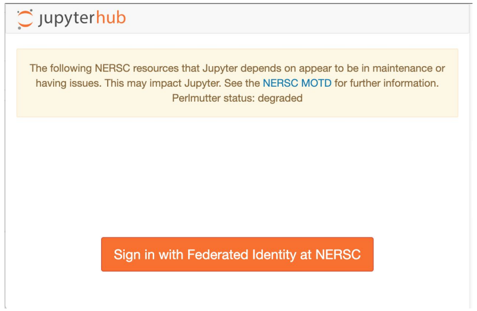
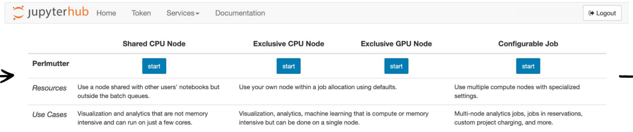
U.S. DEPARTMENT OF ENERGY | Office of Science

How Do I Use Jupyter at NERSC?

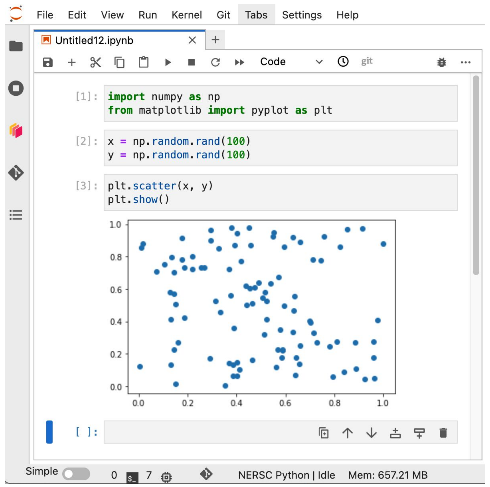
- https://jupyter.nersc.gov



The following NERSC resources that Jupyter depends on appear to be in maintenance or having issues. This may impact Jupyter. See the NERSC MOTD for further information.
Perlmutter status: degraded



	Shared CPU Node	Exclusive CPU Node	Exclusive GPU Node	Configurable Job
Perlmutter	start	start	start	start
Resources	Use a node shared with other users' notebooks but outside the batch queues.	Use your own node within a job allocation using defaults.		Use multiple compute nodes with specialized settings.
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.		Multi-node analytics jobs, jobs in reservations, custom project charging, and more.



```
[1]: import numpy as np
     from matplotlib import pyplot as plt

[2]: x = np.random.rand(100)
     y = np.random.rand(100)

[3]: plt.scatter(x, y)
     plt.show()

[ ]:
```

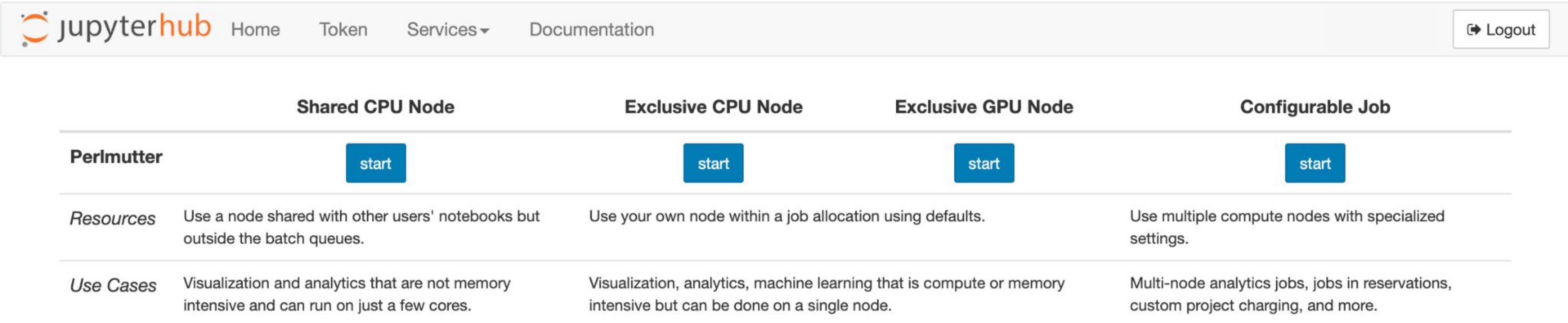
Authenticate   Choose   Go!

How Do I Choose a Notebook Server to Spawn?

Shared CPU:
Notebook on one of 40 login nodes
Same Python env as SSH login
Can submit jobs via !sbatch

Exclusive CPU/GPU:
Notebook in job allocation
CPU node or GPU node
Uses NERSC hours

Configurable Job:
Notebook in job allocation
CPU node(s) or GPU node(s)
Uses NERSC hours
Can be used in reservations



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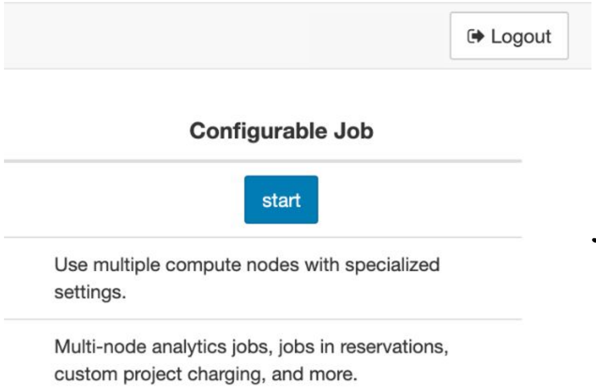
Shared = other users and processes on the same node

Exclusive and configurable = compute nodes just for your notebook and processes

Configurable Job Settings

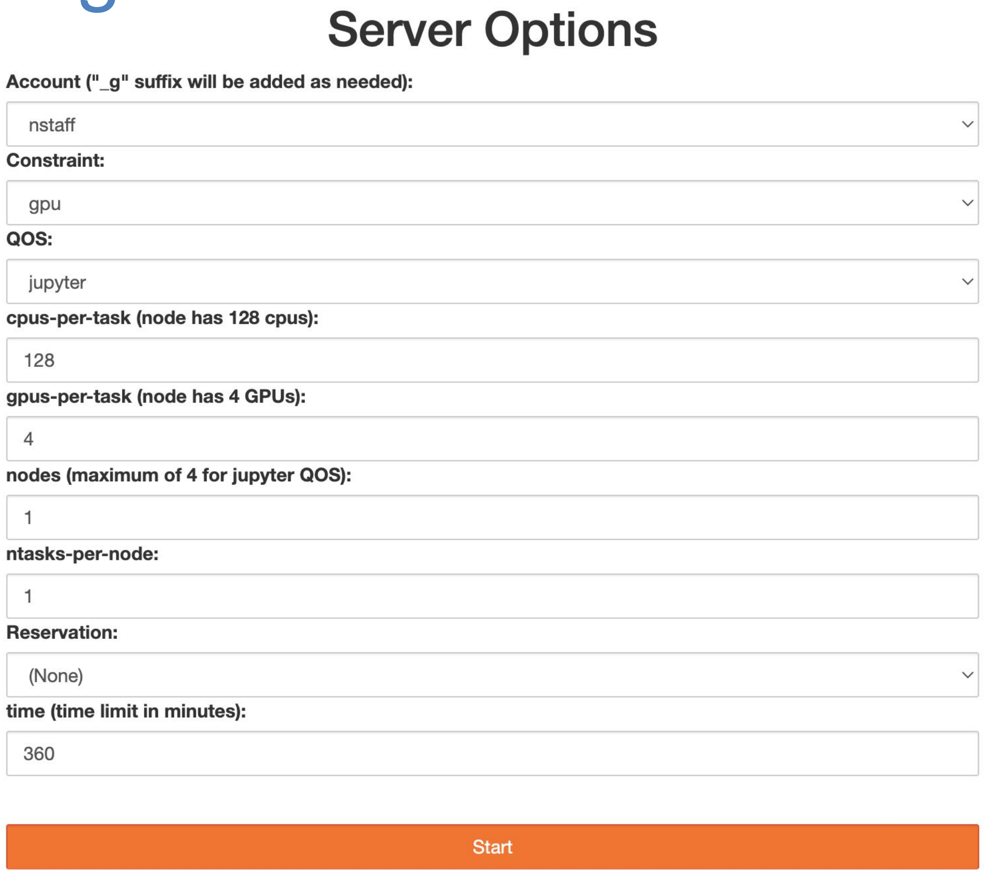


Configurable Job

Use multiple compute nodes with specialized settings.

Multi-node analytics jobs, jobs in reservations, custom project charging, and more.

→



Server Options

Account ("_g" suffix will be added as needed): nstaff

Constraint: gpu

QOS: jupyter

cpus-per-task (node has 128 cpus): 128

gpus-per-task (node has 4 GPUs): 4

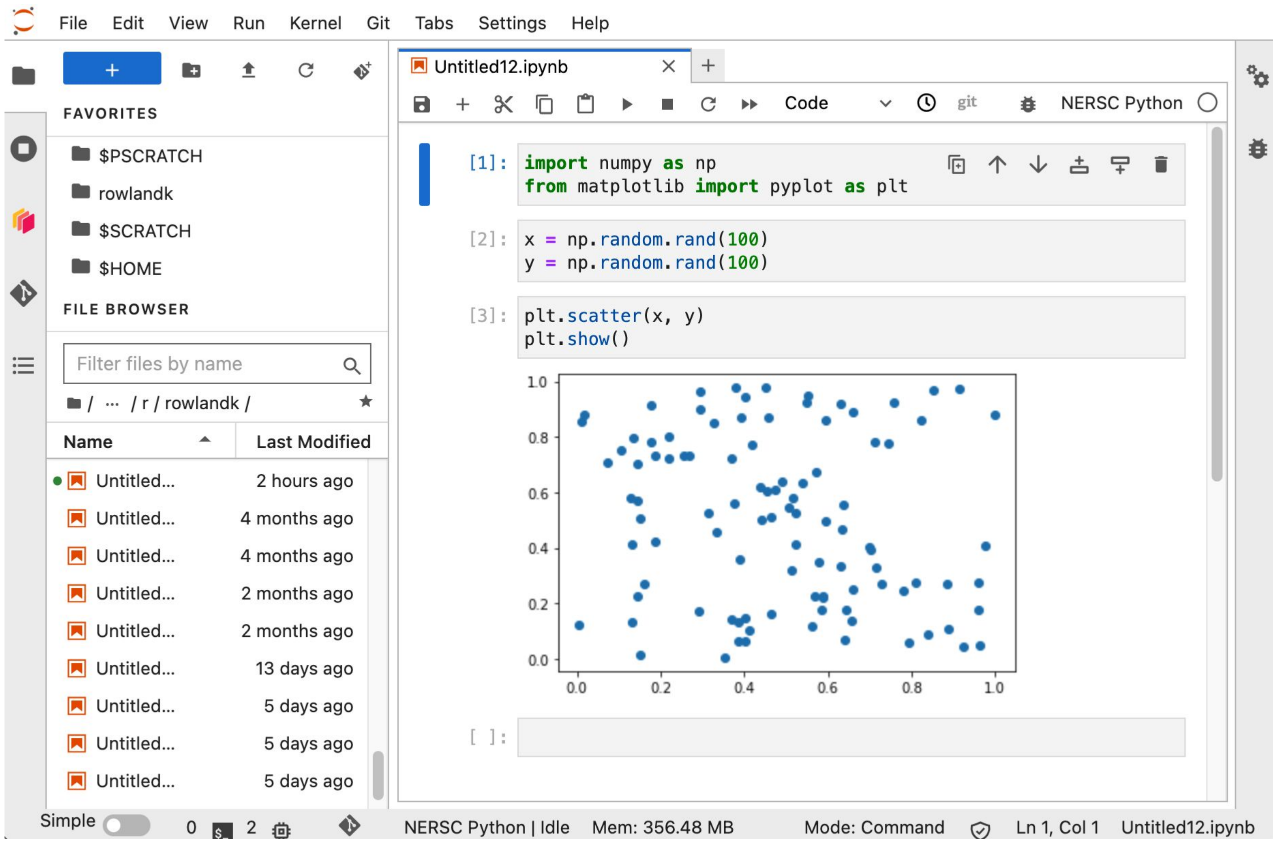
nodes (maximum of 4 for jupyter QOS): 1

ntasks-per-node: 1

Reservation: (None)

time (time limit in minutes): 360

JupyterLab Interface



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Untitled...	5 days ago
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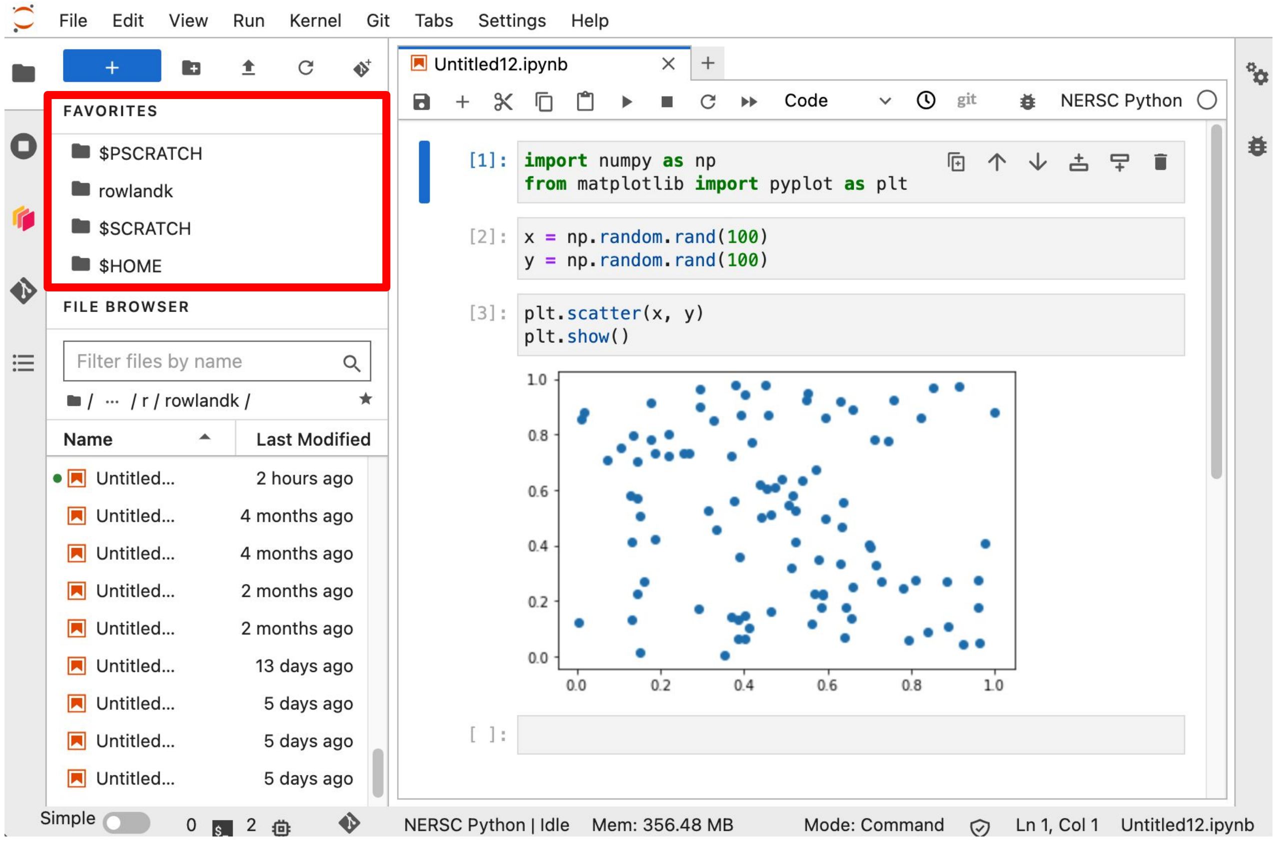
     plt.show()

[ ]:
```

JupyterLab Interface: NERSC Add-ons

- Favorites
- Bookmark your favorite places on the file systems
- Pre-populated with $HOME and $PSCRATCH
- Add the current directory by clicking the ★ icon



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[ ]:
```
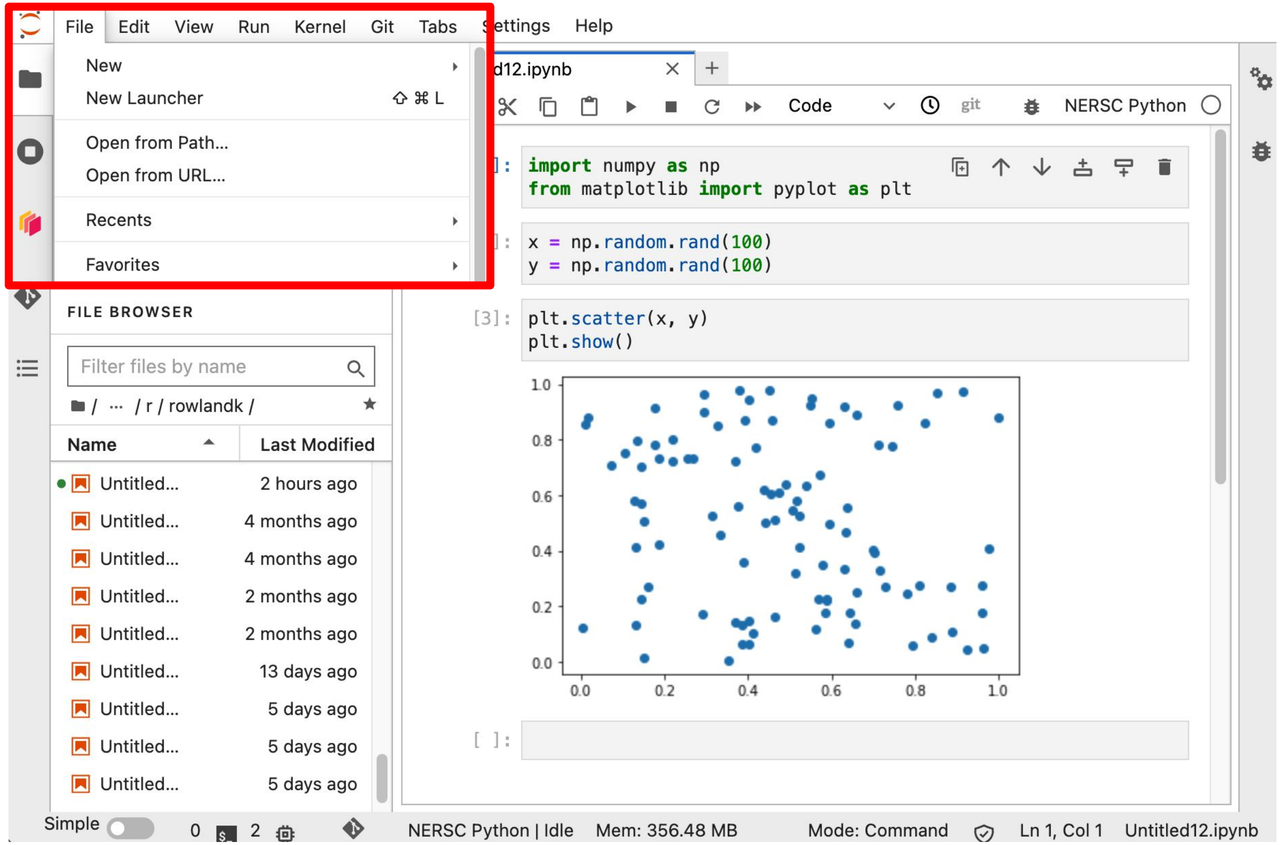

JupyterLab Interface: NERSC Add-ons

- **Open from Path…**
- Jump to anywhere in the file system

- **Recents**
- Recent locations you've visited on the file system



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```
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```

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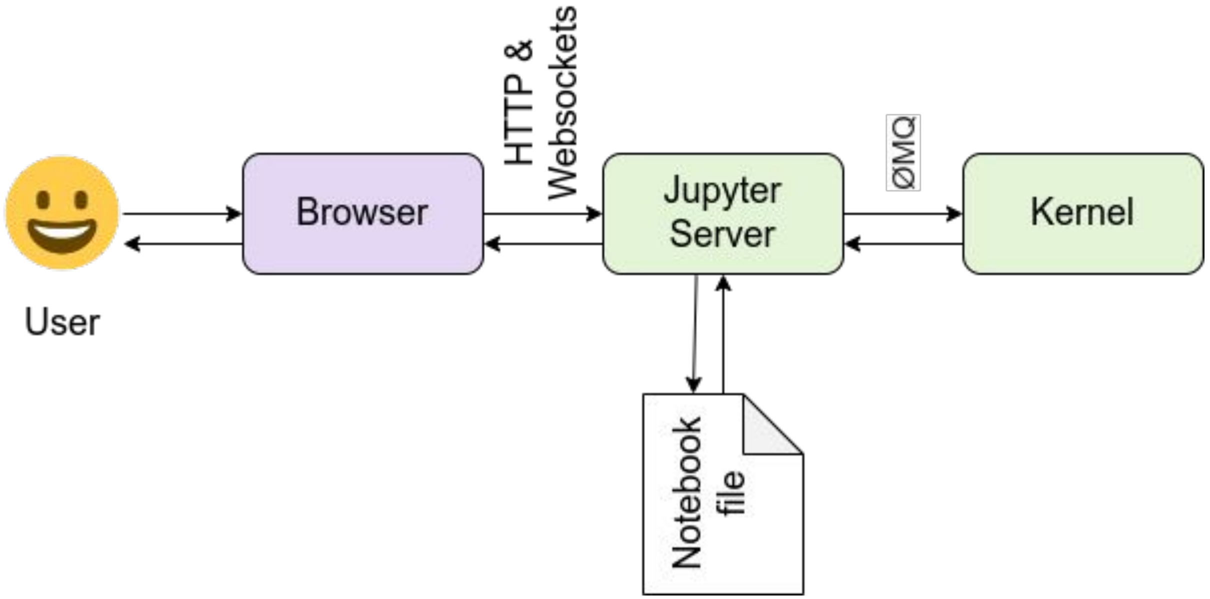
Kernels: How You Compute with Jupyter



- The kernel is what actually runs your code
- Default kernel is NERSC Python
  - From Python module
- Other kernels also provided
  - Julia, R
  - ML packages
- Bring your own kernel

https://docs.jupyter.org/en/latest/projects/architecture/content-architecture.html

Your Own Jupyter Kernel

- A common Jupyter question:
  - "How do I take a conda environment and use it from Jupyter?"

- Several ways to accomplish this; we recommend:

```
$ module load python
$ conda create -n myenv python=3.9
$ 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.nersc.gov
  - May need to restart notebook server via control panel
- Kernel "myenv-jupyter" should be present in the kernel list

The kernelspec File

```
(myenv) user@login01:~$ cat \
    $HOME/.local/share/jupyter/kernels/myenv-jupyter/kernel.json
{
 "argv": [
  "/global/homes/u/user/.conda/envs/myenv/bin/python",
  "-m",
  "ipykernel_launcher",
  "-f",
  "{connection_file}"
 ],
 "display_name": "myenv-jupyter",
 "language": "python"
}
```

Additional Customization

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

Additional Customization - Kernel Helper Script

```
{
 "argv": [
  "/global/homes/u/user/kernel-helper.sh",
  "-f",
  "{connection_file}"
 ],
 "display_name": "myenv-jupyter2",
 "language": "python",
}
```

The kernel helper script is the most flexible approach for NERSC users since it easily enables use of modules, environment variables, etc.

Meanwhile, in kernel-helper.sh:

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

A Shifter kernelspec File

```
{
  "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 to Python in the image

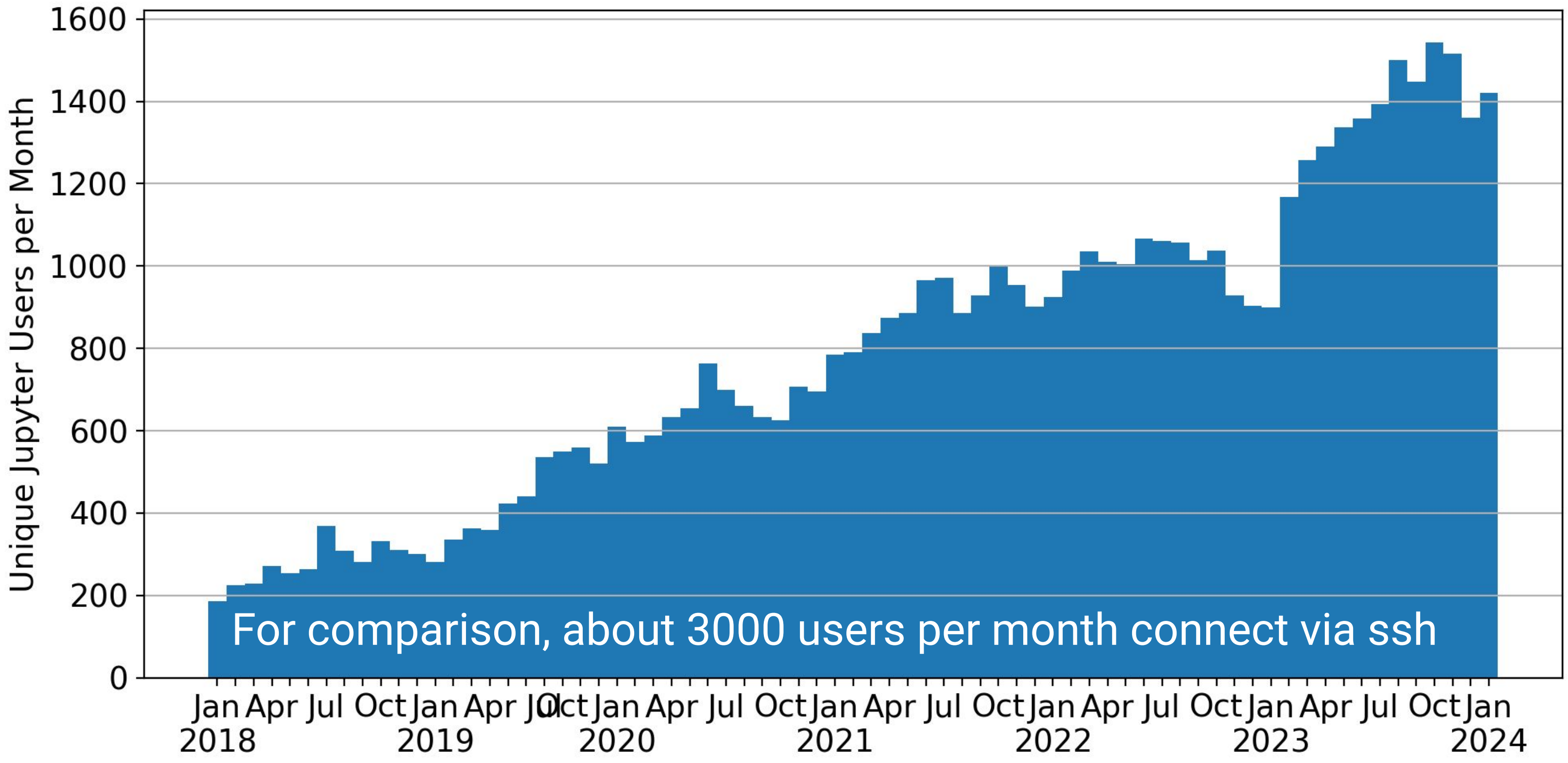
SHIFTER

Debugging Jupyter Issues

```
(myenv) user@login01:~$ cat ~/.jupyter-perlmutter.log
```

```
[IPKernelApp] ERROR | No such comm target registered: jupyter.widget.control
[IPKernelApp] WARNING | No such comm: aa07e0e8-5f78-4899-ab3f-8af339f1318e
[W 2023-06-12 14:20:16.974 SingleUserLabApp zmqhandlers:227] WebSocket ping timeout after 119813 ms.
[I 2023-06-12 14:20:16.977 SingleUserLabApp kernelmanager:321] Starting buffering for
04d30821-f7f4-46c2-a016-ba576b5af07c:74105d47-601c-4d77-8316-c75fdfae4bab
[W 2023-06-12 14:20:17.035 SingleUserLabApp zmqhandlers:227] WebSocket ping timeout after 119874 ms.
[I 2023-06-12 14:20:17.036 SingleUserLabApp kernelmanager:321] Starting buffering for
fcb31e09-6a2a-427e-aaf8-f15d1a443bda:fbe5d17f-91a2-49d7-bf22-1da23dc8ef4b
[W 2023-06-12 14:20:17.110 SingleUserLabApp zmqhandlers:227] WebSocket ping timeout after 119949 ms.
[I 2023-06-12 14:20:17.111 SingleUserLabApp kernelmanager:321] Starting buffering for
fac60c02-f294-4a49-b711-89501fefcfe8:006691d0-c3c5-480c-aacb-ffde01ab6169
[W 2023-06-12 14:20:17.176 SingleUserLabApp zmqhandlers:227] WebSocket ping timeout after 119988 ms.
[I 2023-06-12 14:20:17.177 SingleUserLabApp kernelmanager:321] Starting buffering for
19490e67-80b6-4745-85cb-0d5b8411c959:dc46ed9a-1d6e-4142-a567-c4ad9aa1ea3d
[W 2023-06-12 14:20:17.288 SingleUserLabApp zmqhandlers:227] WebSocket ping timeout after 120040 ms.
[I 2023-06-12 14:20:17.290 SingleUserLabApp handlers:454] Restoring connection for
04d30821-f7f4-46c2-a016-ba576b5af07c:74105d47-601c-4d77-8316-c75fdfae4bab
[I 2023-06-12 14:20:17.291 SingleUserLabApp kernelmanager:321] Starting buffering for
b9cb4f21-1f8c-4917-b7a5-4653b158d87b:230a9755-8454-4f84-a097-041c7e88b5bb
[IPKernelApp] ERROR | No such comm target registered: jupyter.widget.control
[IPKernelApp] WARNING | No such comm: 8844d734-bdf7-4159-b1ab-4534db8105b6
[W 2023-06-12 14:20:17.368 SingleUserLabApp zmqhandlers:227] WebSocket ping timeout after 119844 ms.
```

Jupyter Usage at NERSC



For comparison, about 3000 users per month connect via ssh

Jupyter at NERSC - Summary

- Go to https://jupyter.nersc.gov to use Jupyter at NERSC
- Use a kernelspec to use a conda environment in your notebook
- You can customize those kernelspec files in many ways
- We work on making Jupyter work and work better for you

- Always looking for:
  - New ways to empower Jupyter users
  - Feedback, advice, and even help: https://help.nersc.gov/

Thank you!