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
How Do I Use Jupyter at NERSC?

- [https://jupyter.nersc.gov](https://jupyter.nersc.gov)
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

### Perlmutter

<table>
<thead>
<tr>
<th>Resources</th>
<th>Shared CPU Node</th>
<th>Exclusive CPU Node</th>
<th>Exclusive GPU Node</th>
<th>Configurable Job</th>
</tr>
</thead>
<tbody>
<tr>
<td>Use Cases</td>
<td>Use a node shared with other users’ notebooks but outside the batch queues.</td>
<td>Use your own node within a job allocation using defaults.</td>
<td>Use multiple compute nodes with specialized settings.</td>
<td>Multi-node analytics jobs, jobs in reservations, custom project charging, and more.</td>
</tr>
<tr>
<td>Use Cases</td>
<td>Visualization and analytics that are not memory intensive and can run on just a few cores.</td>
<td>Visualization, analytics, machine learning that is compute or memory intensive but can be done on a single node.</td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

- 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

Start
JupyterLab Interface
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
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
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

● 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

This creates a “kernelspec” file
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

```json
{
  "argv": [
    "/global/homes/u/user/.conda/envs/myenv/bin/python",
    "-m",
    "ipykernel_launcher",
    "-f",
    "{connection_file}"
  ],
  "display_name": "myenv-jupyter",
  "language": "python",
  "env": {
    "PATH": ...
  }
}
```
Additional Customization - Kernel Helper Script

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

Meanwhile, in kernel-helper.sh:

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

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

```json
{
  "argv": [
    "shifter",
    "--image=continuumio/anaconda3:latest",
    "/opt/conda/bin/python",
    "-m",
    "ipykernel_launcher",
    "-f",
    "{connection_file}"
  ],
  "display_name": "my-shifter-kernel",
  "language": "python"
}
```
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
[I 2023-06-12 14:20:17.036 SingleUserLabApp kernelmanager:321] Starting buffering for fcb31e09-6a2a-427e-aaf8-f15d1a443bda:fbe5d17f-91a2-49d7-bf22-1da23dc8ef4b
[I 2023-06-12 14:20:17.111 SingleUserLabApp kernelmanager:321] Starting buffering for fac60c02-f294-4a49-b711-89501fefcfe8:006691d0-c3c5-480c-aacb-ffde01ab6169
[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
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!