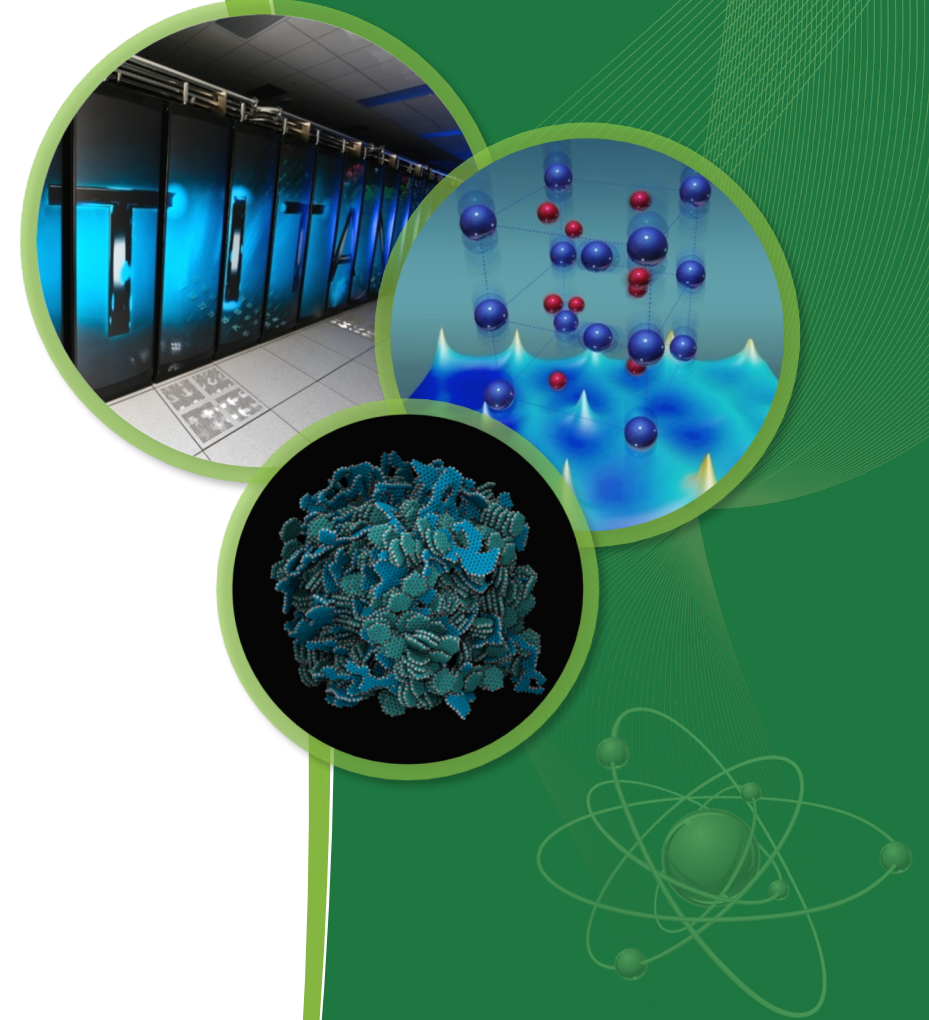


# Jupyter at OLCF

Ryan Prout

HPC Engineer - User Assistance

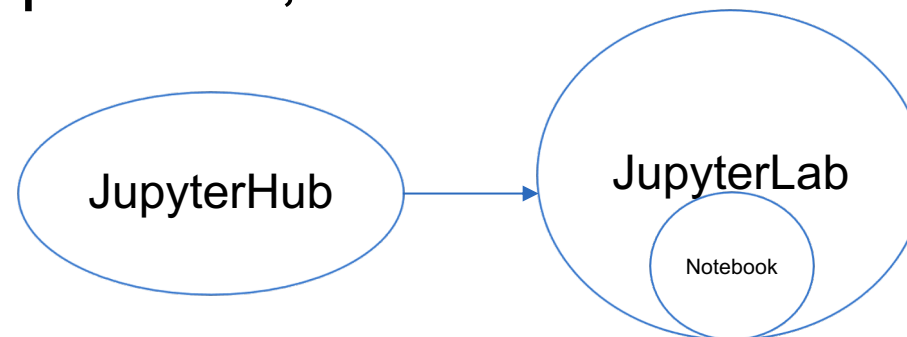


# Agenda For Today

- General, high-level, overview of Jupyter
- General, high-level, overview of Jupyter @ OLCF
  - Current State
  - Future State
- Software environments
- How to get started using Jupyter @ OLCF
- Questions/Discussion

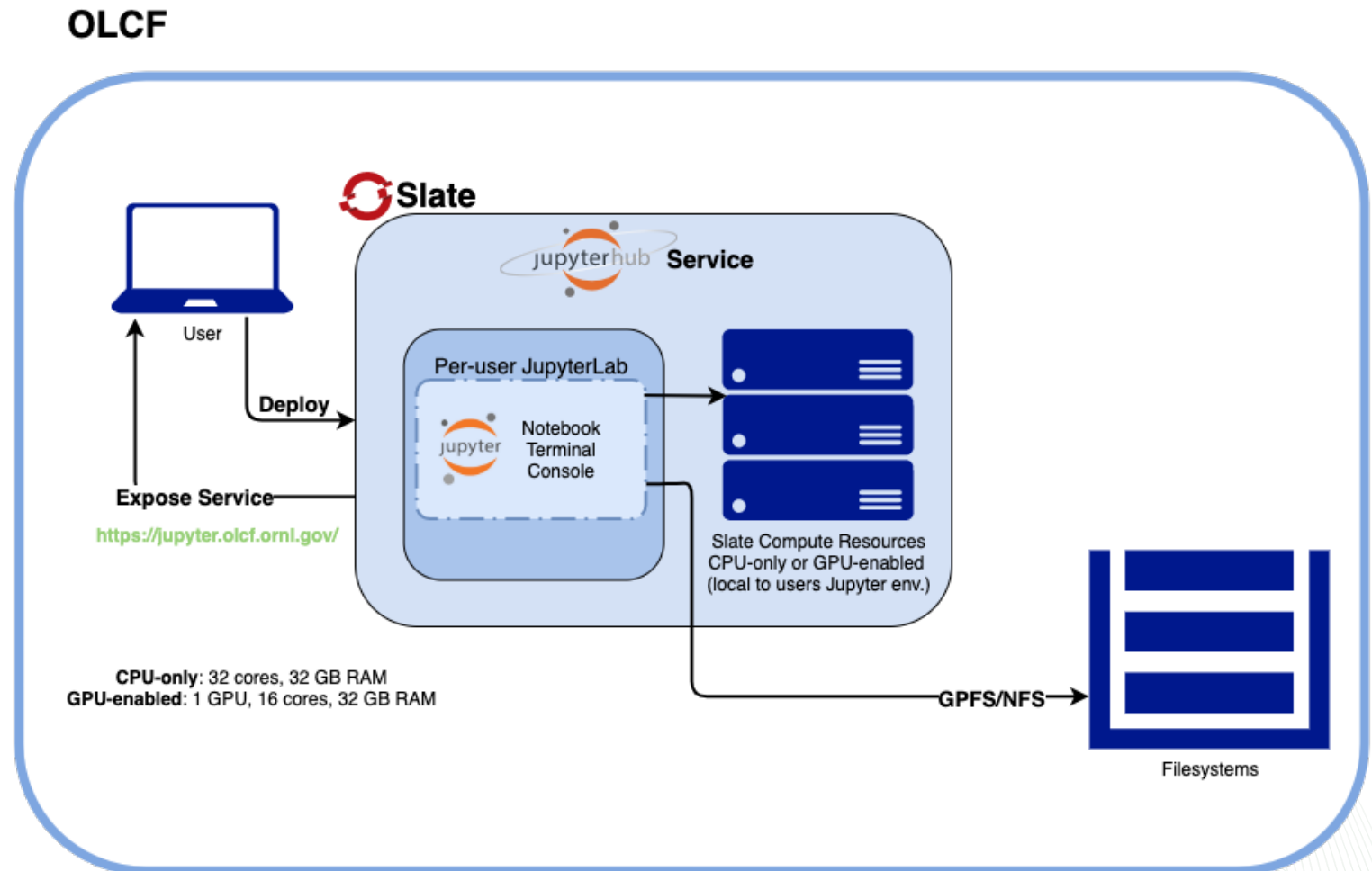
# General, high-level, overview of Jupyter

- **JupyterHub** - Brings the power of notebooks to groups of users. Enables computational environments and resources without the burden of installation of and maintenance (for users).
- **JupyterLab** – Next-generation web-based user interface for Jupyter. This is launched by JupyterHub – each user gets a JupyterLab environment.
- **Jupyter Notebooks** - Document within the JupyterLab interface that allows live code, equations, visualizations and narrative text.



## General, high-level, overview of Jupyter @ OLCF (current state)

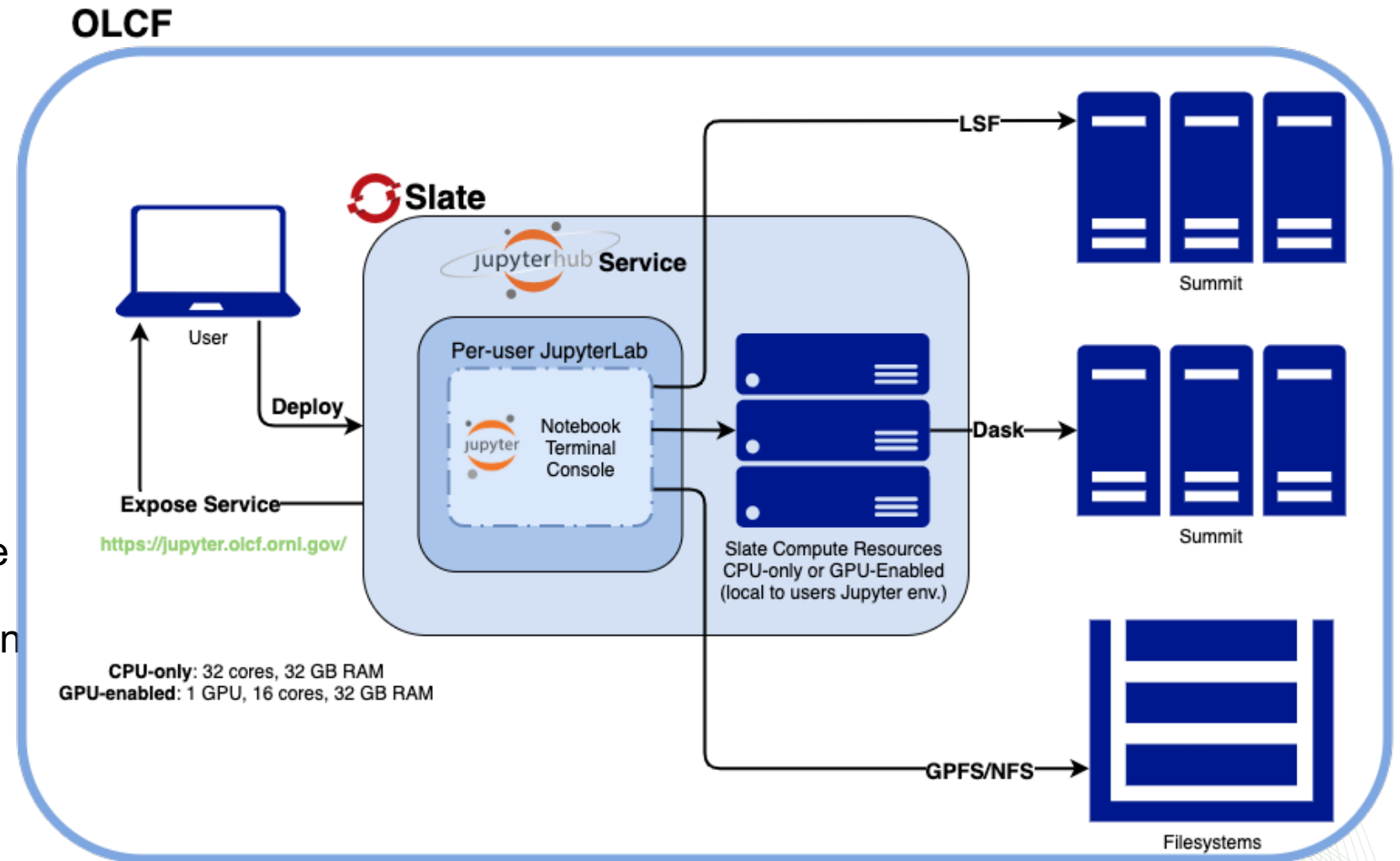
- JupyterHub is a “Slate” service (OLCF’s cloud-native platform – uses OpenShift)
- Service is exposed via the web
- Each user gets a JupyterLab environment, running with their NCCS UID
- CPU-only or GPU-enabled JupyterLab
- Jupyter’s local resources are from Slate’s underlying hardware (Not Summit)
- NCCS Filesystem access





## General, high-level, overview of Jupyter @ OLCF (future state)

- Extends current state to integrate with Summit
- Job submission from users Jupyter environment (*being tested in our development environment*)
- Jupyter's local resources are still from Slate's underlying hardware (but job submission is enabled)
- Dask workload distribution onto Summit



# Software Environments

- Provided “base” conda environments in JupyterLab
  - Pytorch
  - TensorFlow
  - NumPy
  - Pandas
  - .....
  - GPU lab has CUDA11, CuPy, and CuDNN

(take a look for full package list with “conda list”)

- Create your own conda environments on NFS/GPFS, from JupyterLab.
  - “conda env list” will show you *all* your environments (whether built on Summit, Andes, or JupyterLab)
    - “/opt/conda” path denotes the environments local to your Slate-based JupyterLab
    - “/ccs/\*” and “/gpfs/\*” are environments built by user (either from Summit, Andes, or JupyterLab)
  - **NOTE:** *JupyterLab runs on x86 hardware (underlying Slate hardware). Environments are not directly compatible between Slate, Summit, and Andes.*

```
[2]: !conda env list

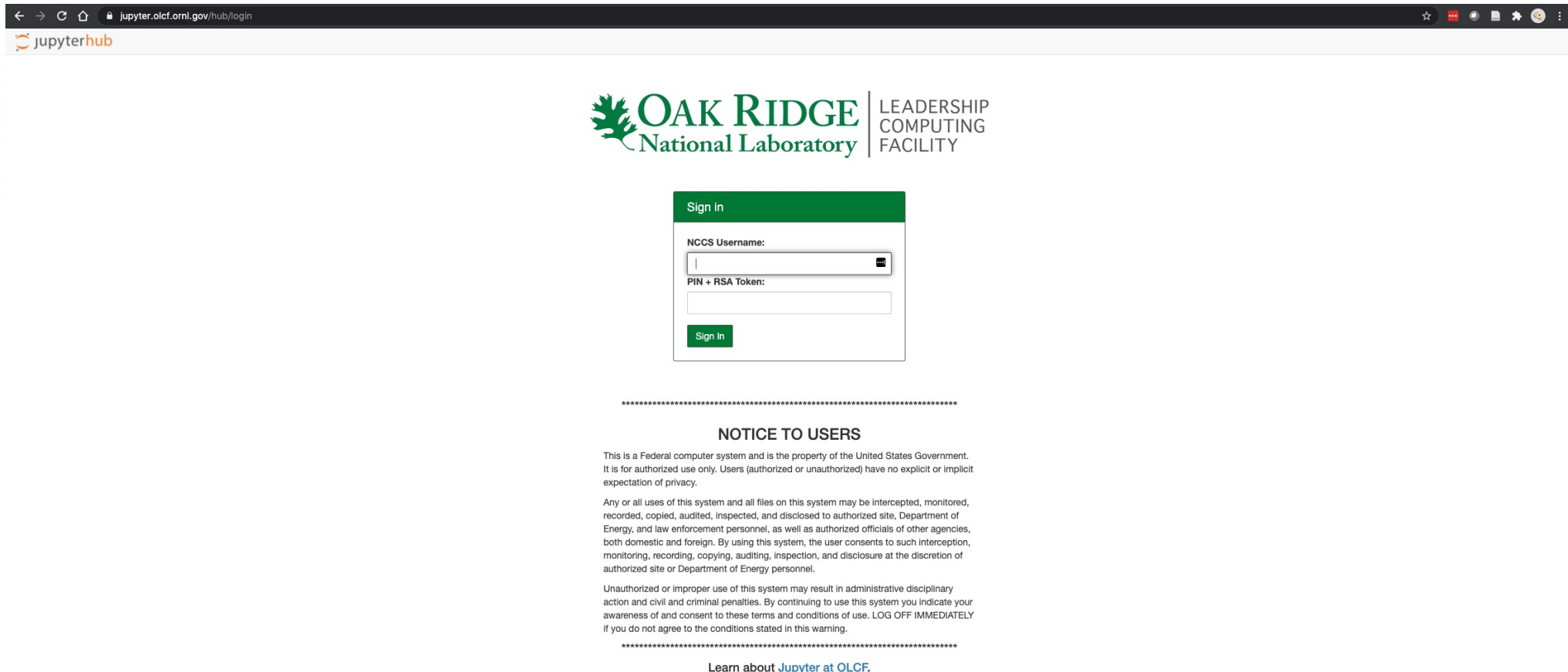
# conda environments:
#
blazing-sql      /autofs/nccs-svm1_proj/stf007/rprout/dask_test
clone-py3.7.1    /autofs/nccs-svm1_proj/stf007/rprout/openslide-test
dask_dev         /ccs/home/rprout/.conda/envs/dask_dev
jupyter_dask_test /ccs/home/rprout/.conda/envs/jupyter_dask_test
jupyter_lab      /ccs/home/rprout/.conda/envs/jupyter_lab
                 /ccs/proj/stf007/13322/rapids
                 /ccs/proj/stf007/rprout/base-env-clone
                 /ccs/proj/stf007/rprout/dask_test
                 /ccs/proj/stf007/rprout/phonopy-andes
                 /ccs/proj/stf007/rprout/slate-env-clone
                 /ccs/proj/stf007/rprout/slate-test-env
                 /ccs/proj/stf007/rprout/xarray-test
                 /gpfs/alpine/stf007/scratch/rprout/open-ce-clone
                 /gpfs/alpine/stf007/scratch/rprout/py3.7_base_clone

base             * /opt/conda
cuda11dev        /opt/conda/envs/cuda11dev
```

# How to get started with Jupyter @ OLCF


- Login (requires active access to an NCCS project):

<https://jupyter.olcf.ornl.gov/>



← → ↻ 🏠 🔒 jupyter.olcf.ornl.gov/hub/login ☆ 🔴 🔊 📄 ⚙️ 👤 ⋮

jupyterhub

 **OAK RIDGE**  
National Laboratory

LEADERSHIP  
COMPUTING  
FACILITY

Sign in

NCCS Username:

PIN + RSA Token:

Sign In

\*\*\*\*\*

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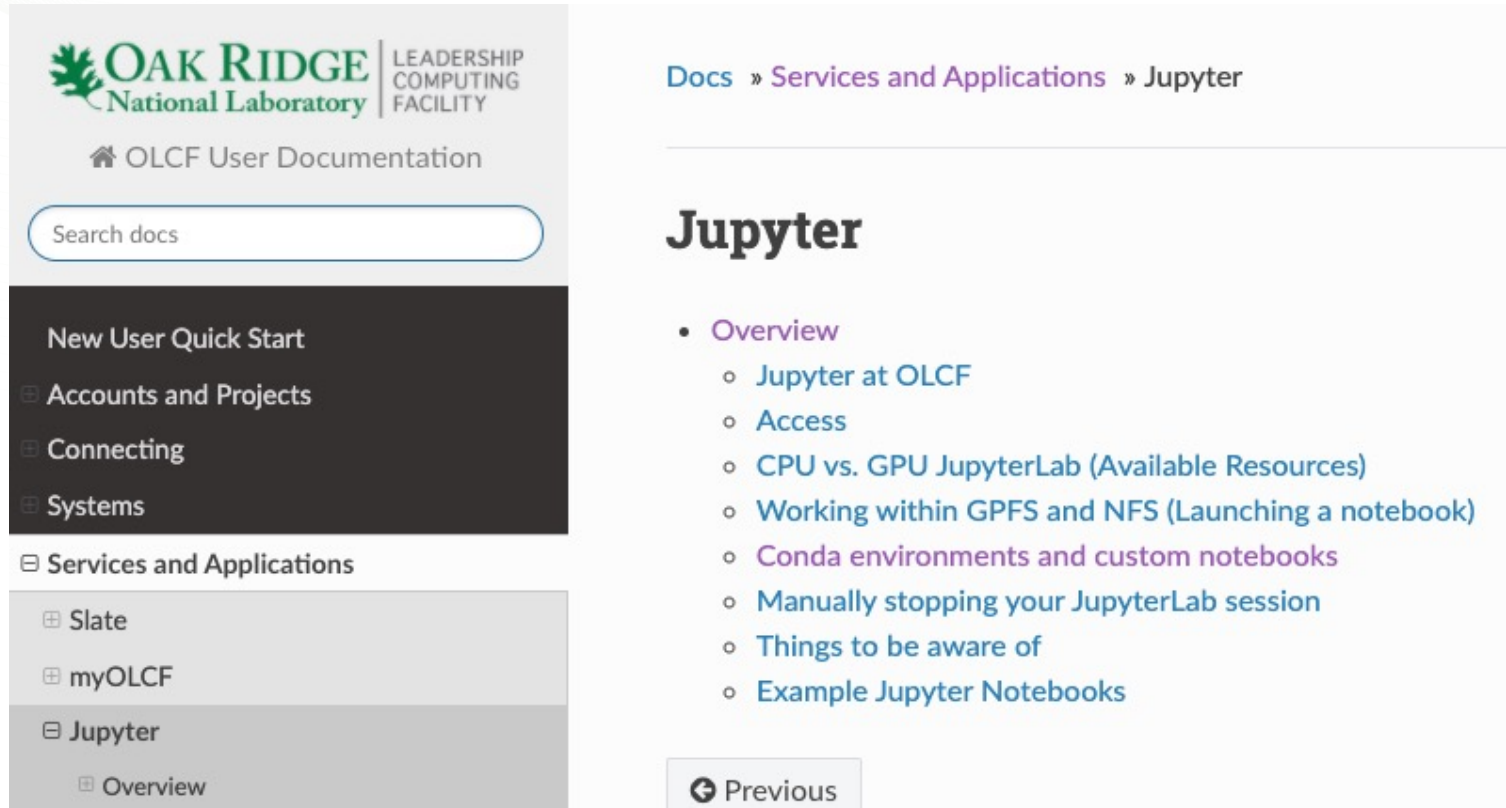
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\*\*\*\*\*

[Learn about Jupyter at OLCF.](#)

- Explore the docs:

[https://docs.olcf.ornl.gov/services\\_and\\_applications/jupyter/index.html](https://docs.olcf.ornl.gov/services_and_applications/jupyter/index.html)



The screenshot displays the OLCF User Documentation website. The header features the Oak Ridge National Laboratory logo and the text 'LEADERSHIP COMPUTING FACILITY'. Below the header is a search bar labeled 'Search docs'. The left sidebar contains a navigation menu with the following items: 'New User Quick Start', 'Accounts and Projects', 'Connecting', 'Systems', 'Services and Applications' (expanded), 'Slate', 'myOLCF', 'Jupyter' (expanded), and 'Overview'. The main content area shows the breadcrumb 'Docs » Services and Applications » Jupyter' and the title 'Jupyter'. A list of links is provided under the heading 'Overview': 'Jupyter at OLCF', 'Access', 'CPU vs. GPU JupyterLab (Available Resources)', 'Working within GPFS and NFS (Launching a notebook)', 'Conda environments and custom notebooks', 'Manually stopping your JupyterLab session', 'Things to be aware of', and 'Example Jupyter Notebooks'. A 'Previous' button is located at the bottom left of the main content area.

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OLCF User Documentation

Search docs

New User Quick Start

- Accounts and Projects
- Connecting
- Systems
- Services and Applications
  - Slate
  - myOLCF
  - Jupyter
    - Overview

Docs » Services and Applications » Jupyter

## Jupyter

- Overview
  - Jupyter at OLCF
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Previous



# **Jupyter Table-Top Breakout Session Today!**

**12-1PM**

**Bring your ideas and questions 😊**