Jupyter at OLCF

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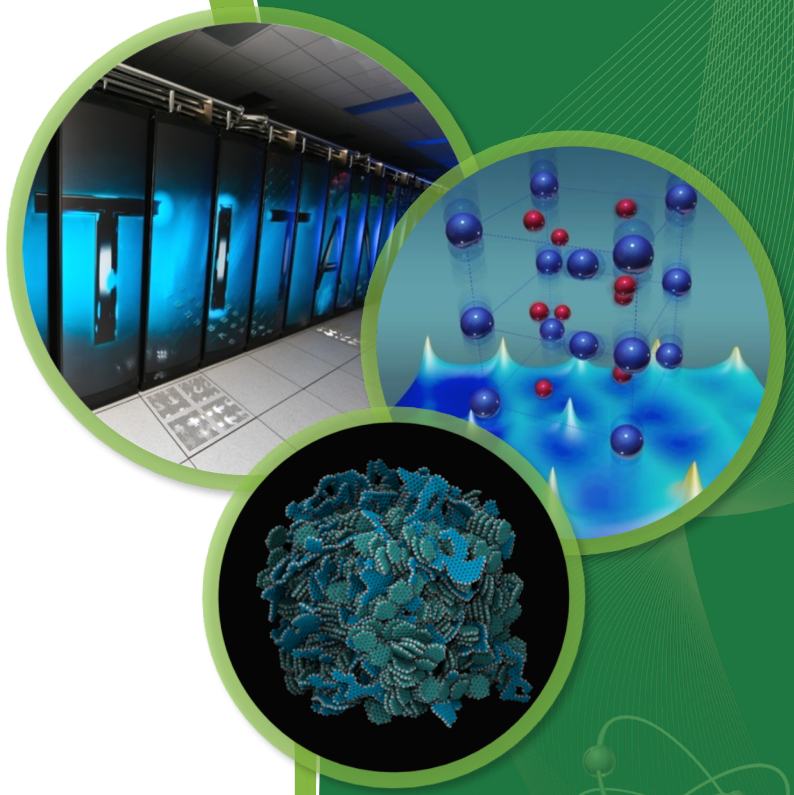
HPC Engineer - User Assistance



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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

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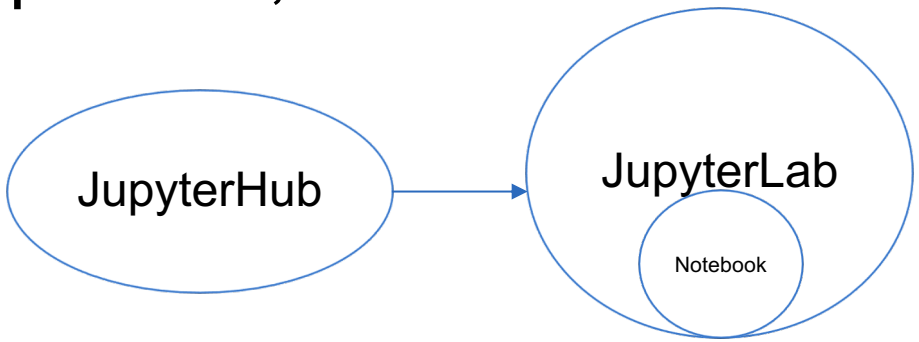
General, high-level, overview of Jupyter

- **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.



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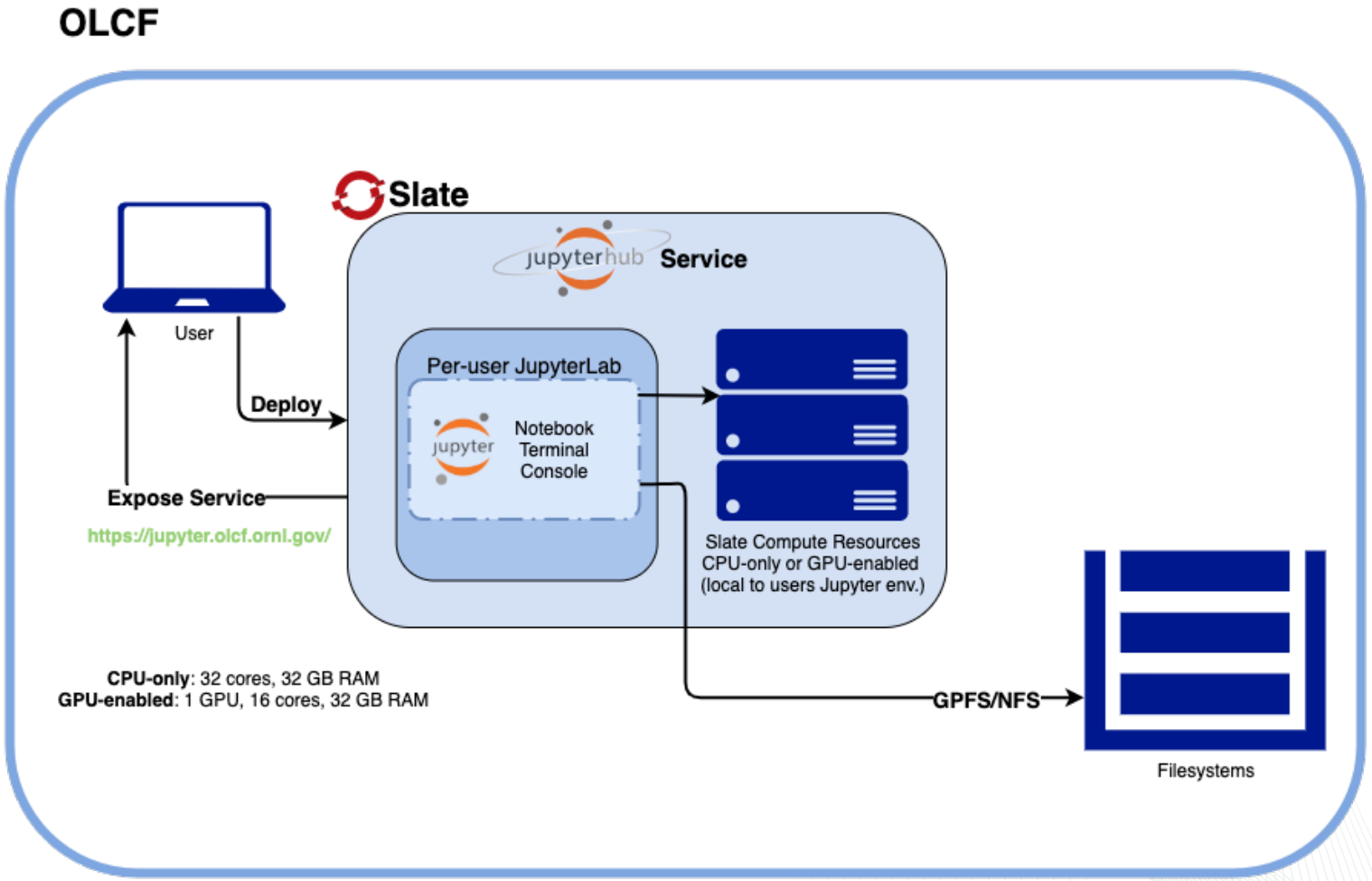
General, high-level, overview of Jupyter @ OLCF (current state)

- 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



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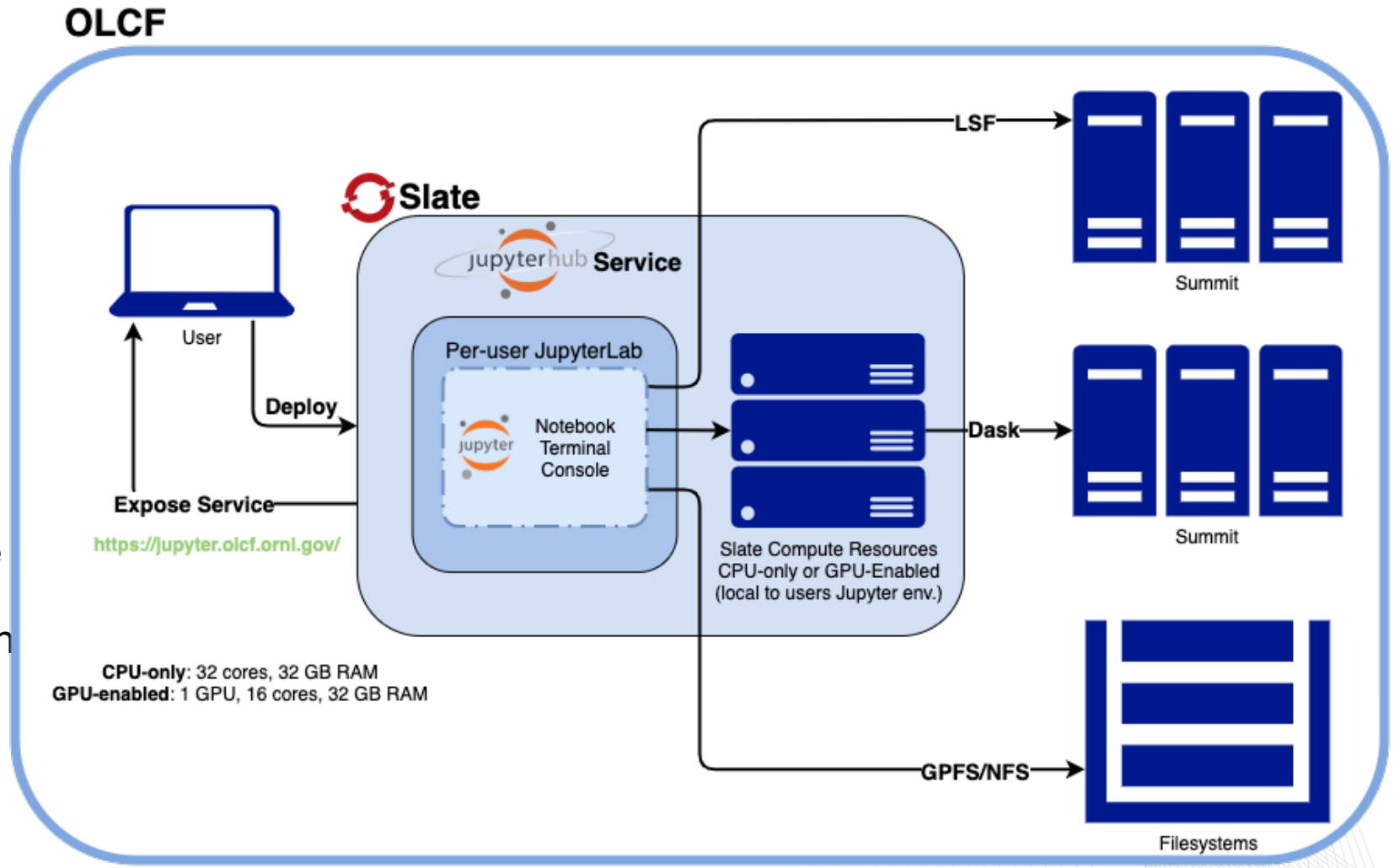
General, high-level, overview of Jupyter @ OLCF (future state)

- 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



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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”)

```
[2]: !conda env list

# conda environments:
#
                         /autofs/nccs-svm1_proj/stf007/rprout/dask_test
                         /autofs/nccs-svm1_proj/stf007/rprout/openslide-test
blazing-sql              /ccs/home/rprout/.conda/envs/blazing-sql
clone-py3.7.1            /ccs/home/rprout/.conda/envs/clone-py3.7.1
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

[ ]:
```

- Create your own conda environments on NFS/GPFS, from JuptyerLab.
  - ”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**: *JuptyerLab runs on x86 hardware (underlying Slate hardware). Environments are not directly compatible between Slate, Summit, and Andes.*

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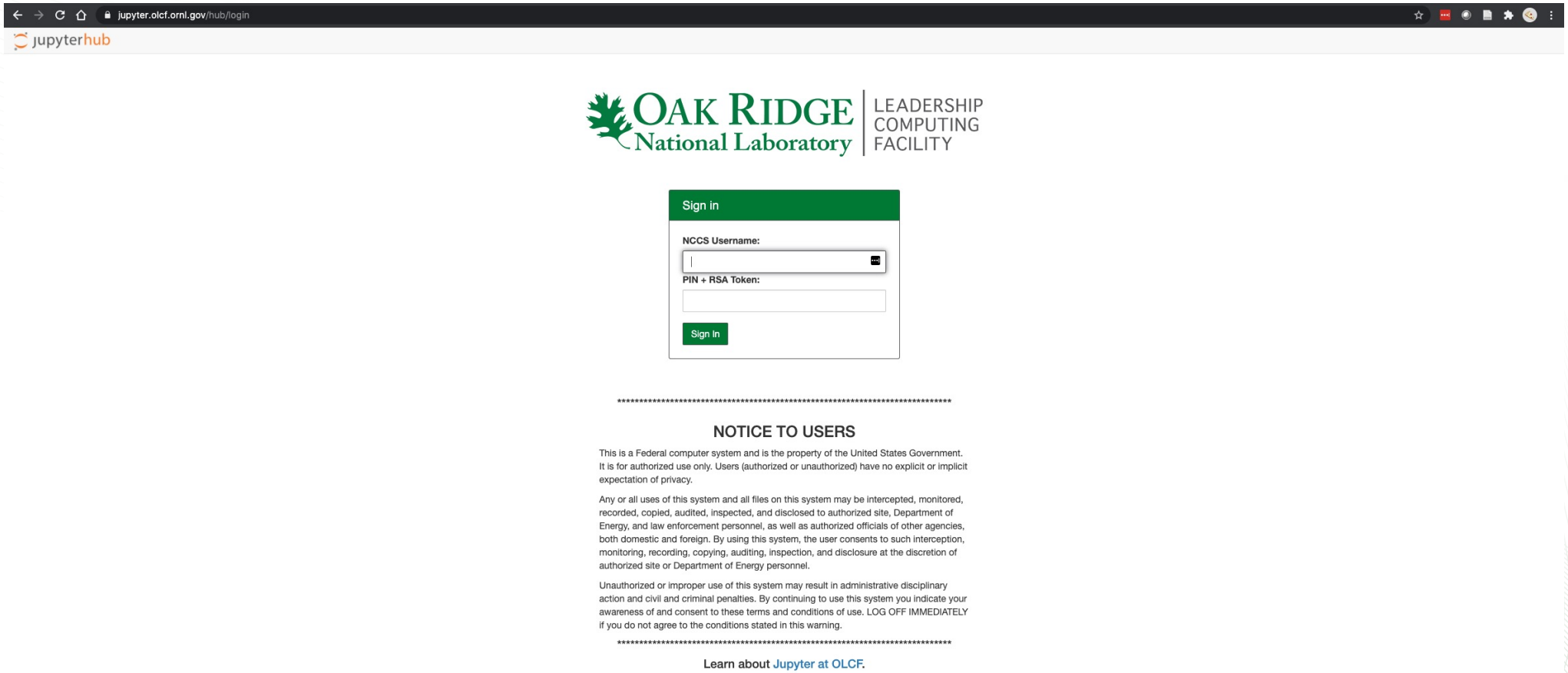
How to get started with Jupyter @ OLCF

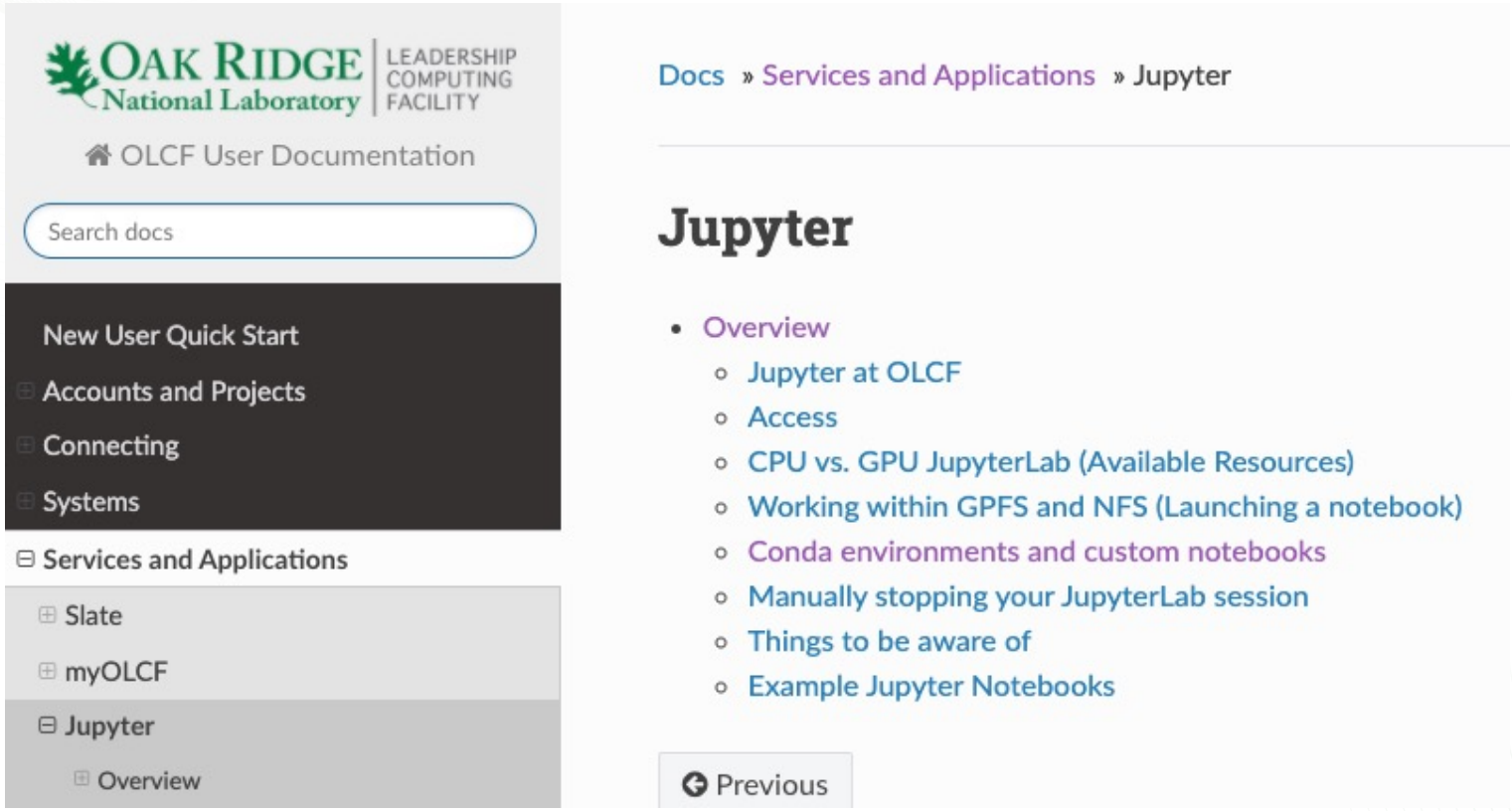
- Login (requires active access to an NCCS project):

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



- Explore the docs:

https://docs.olcf.ornl.gov/services_and_applications/jupyter/index.html



Jupyter Table-Top Breakout Session Today!

12-1PM

Bring your ideas and questions ☺

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