

# Breaking Barriers: Accessing HPC Resources Through User-Friendly Interfaces

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# Overview

- JupyterHub
  - What is JupyterHub?
  - How do I access JupyterHub?
  - How do I use JupyterHub?
  - Data Analysis Example
  - HPC Integration (MCC/LCC Demo)
- Open OnDemand
  - Web interface for compute cluster
- ACCESS  
(Advanced Cyberinfrastructure  
Coordination Ecosystem:  
Services & Support)



# What is JupyterHub?

- Platform to host Jupyter Notebooks for multiple users on a shared resource.
- What is a Jupyter Notebook?
  - Interactive, web based "notebook" that allows users to create/edit documents with inline Python code and text.

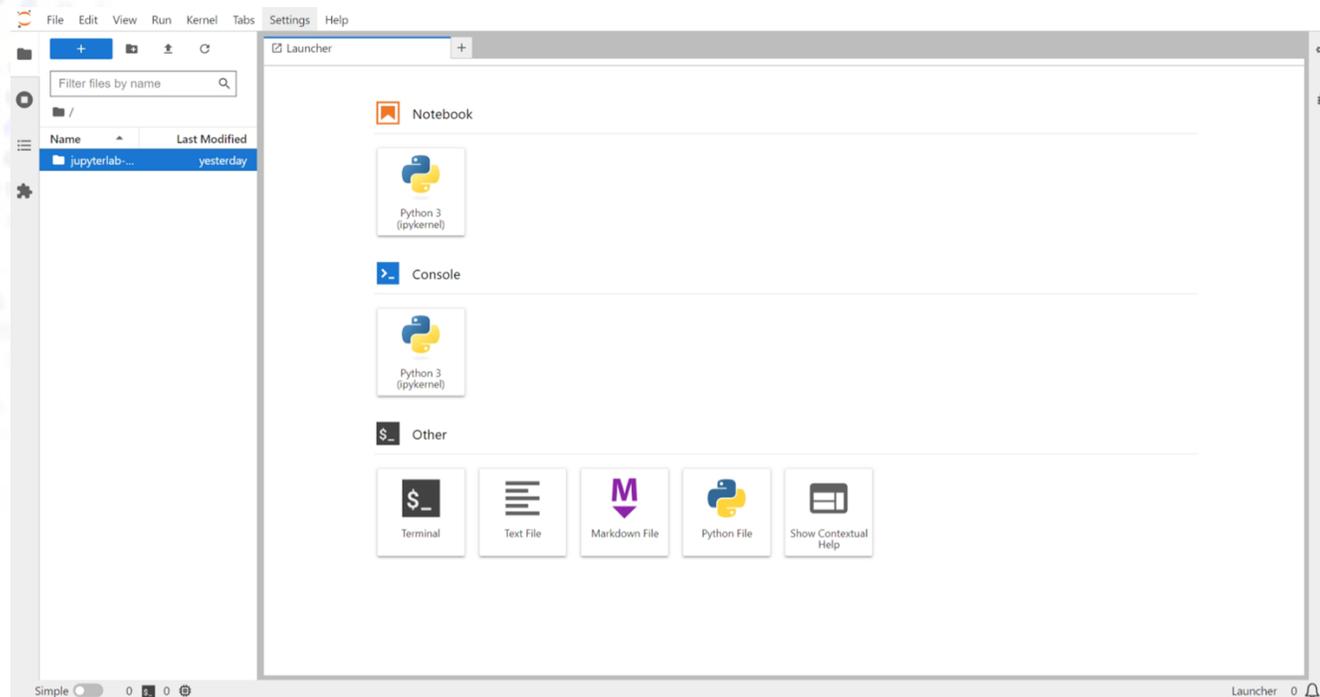
# How do I access JupyterHub?

- Hosted on an OpenStack virtual machine on UKY network
  - 8 vCPUs, 16 GB RAM, 128 GB HD  
(Can be scaled to fit demand)
  - Meant for small data analysis tasks, class/workshops, etc...
- <https://jupyterhub.ccs.uky.edu>

# How do I use JupyterHub?

<https://jupyterhub.ccs.uky.edu>

Log in with CILogon (uses linkblue account)

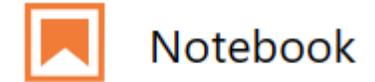


*Note: first time users will see a "Spawning Server" screen which may take a few minutes.*

# How do I use JupyterHub?

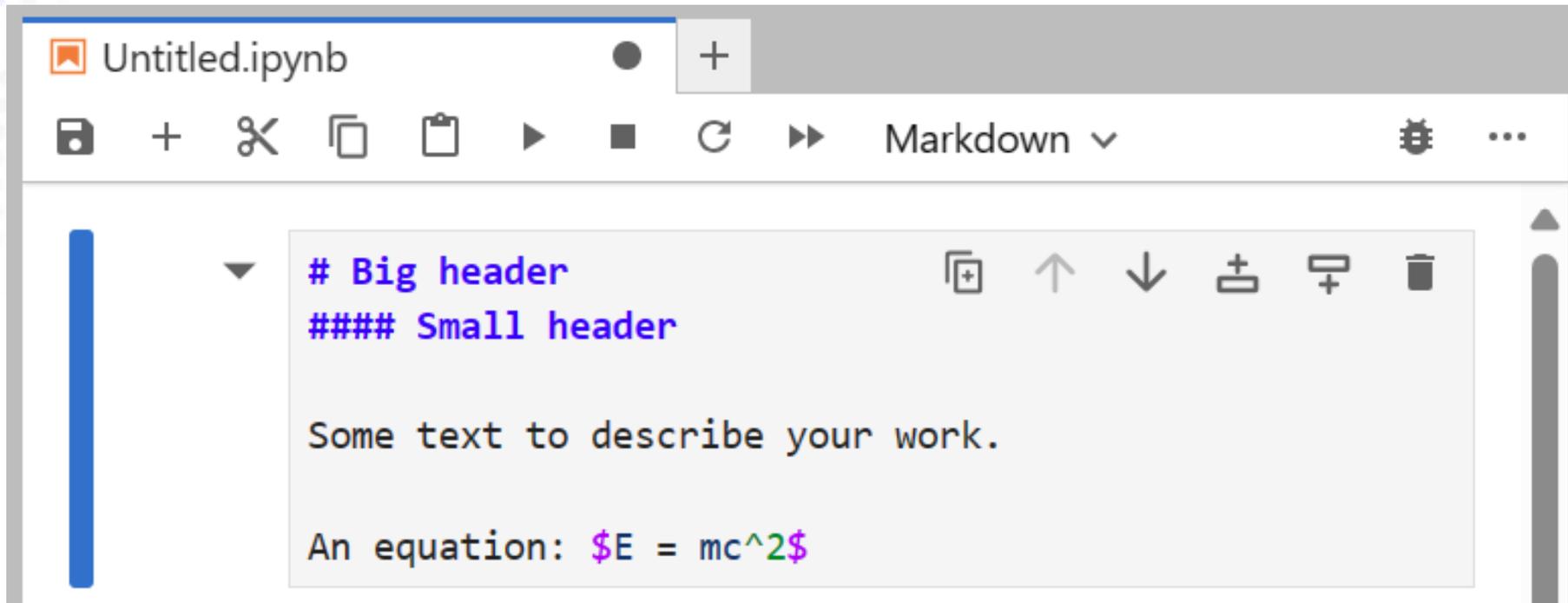
## Create a new Notebook

- Click icon for "Python 3 (ipykernel)" under Notebook heading
- A new notebook will be initialized in your home directory.



# How do I use JupyterHub?

## Markdown Cell



The screenshot shows a Jupyter Notebook interface with a single cell selected. The cell is a Markdown cell, as indicated by the 'Markdown' label in the toolbar. The content of the cell is as follows:

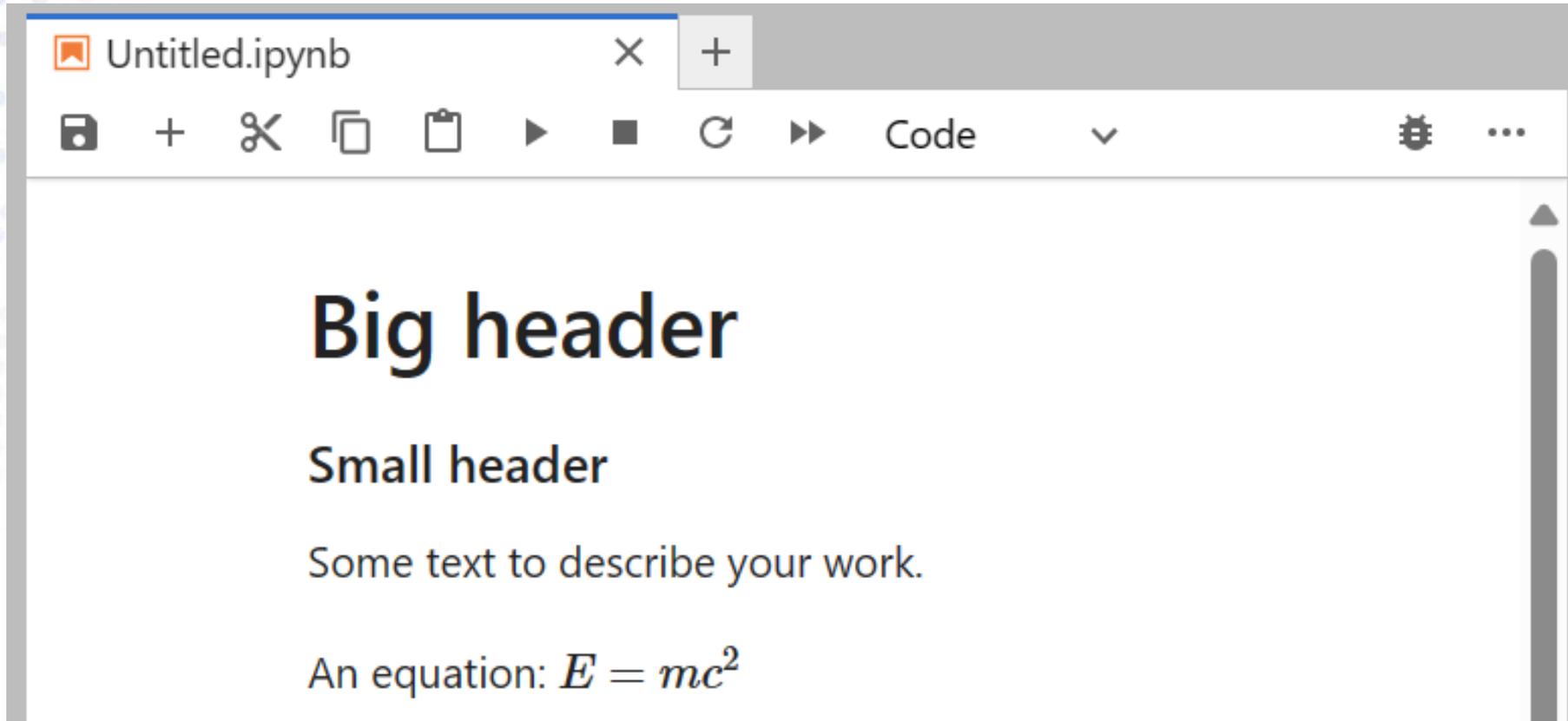
```
# Big header
#### Small header

Some text to describe your work.

An equation:  $E = mc^2$ 
```

The interface includes a toolbar with various icons for file operations (save, copy, paste, delete), cell actions (run, stop, refresh), and a dropdown menu currently set to 'Markdown'. The cell content is displayed in a monospaced font with syntax highlighting for headers and mathematical notation.

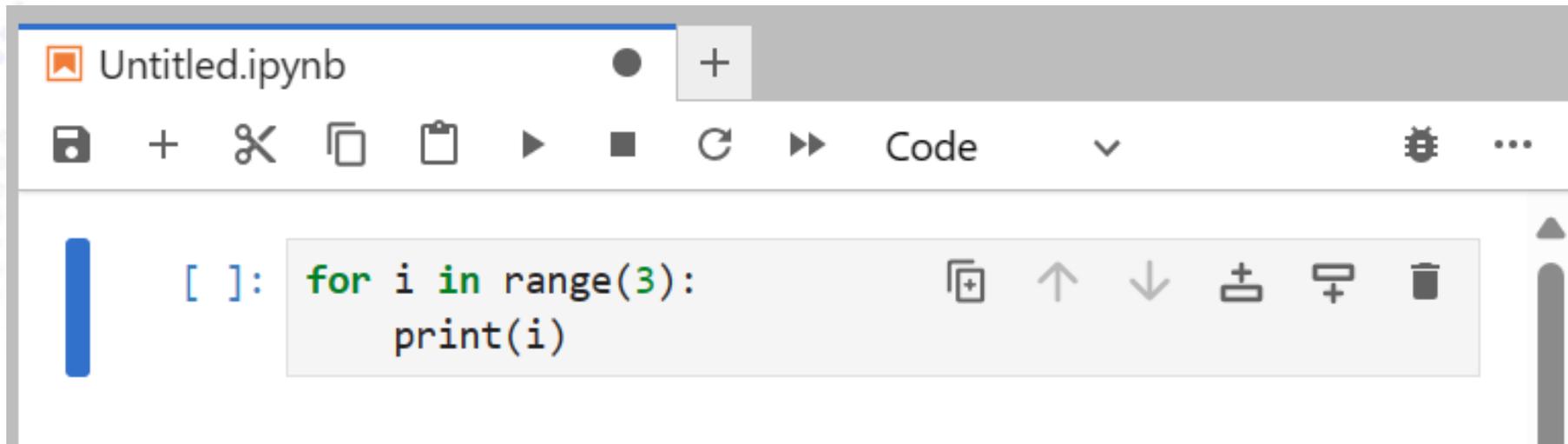
# How do I use JupyterHub?



See more at: <https://www.markdownguide.org/cheat-sheet/>

# How do I use JupyterHub?

## Code Cell

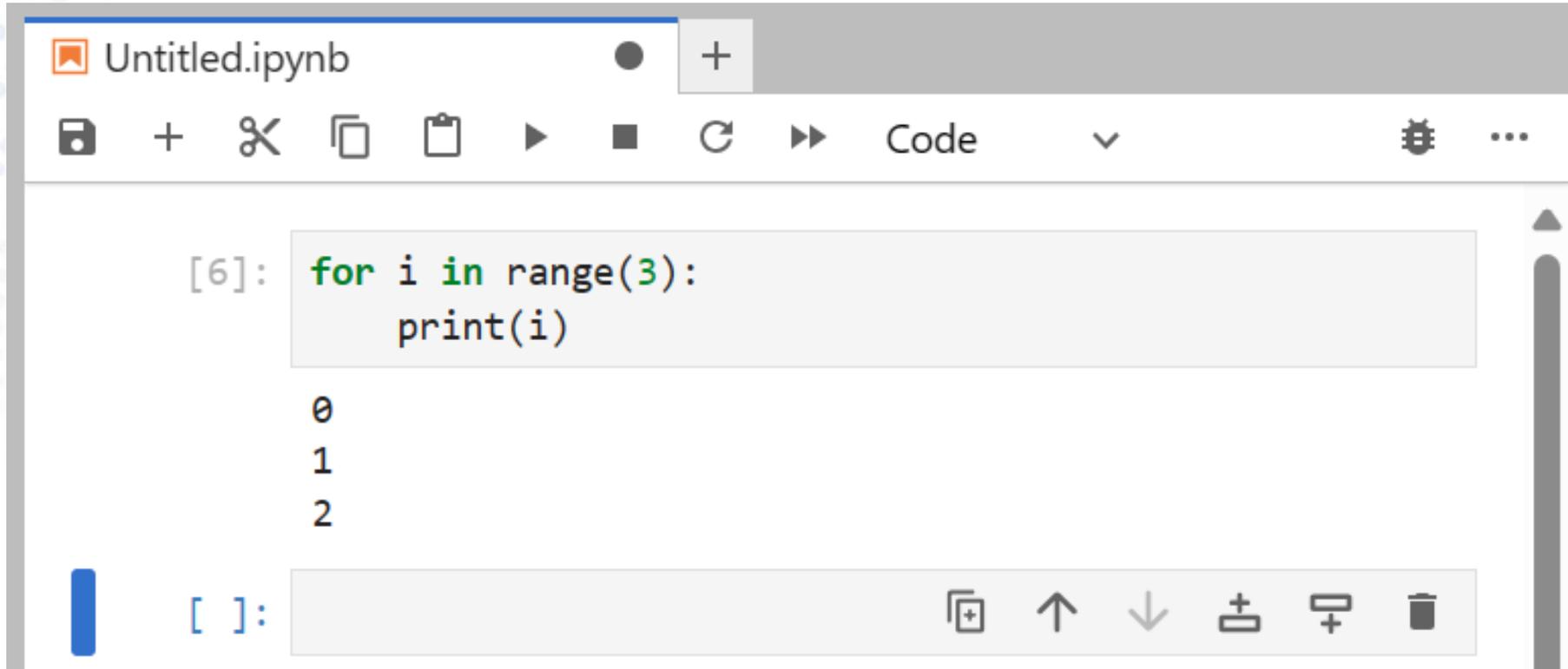


The screenshot shows a Jupyter Notebook interface. At the top, there is a tab labeled 'Untitled.ipynb'. Below the tab is a toolbar with various icons for file operations (save, new, copy, paste), execution (run, stop), and other functions (refresh, expand, Code dropdown, bug report, and a menu). The main area contains a code cell with the following Python code:

```
[ ]: for i in range(3):  
      print(i)
```

On the right side of the code cell, there are icons for adding a new cell, moving up/down, adding a new cell below, and deleting the cell.

# How do I use JupyterHub?



The screenshot shows a Jupyter Notebook window titled "Untitled.ipynb". The interface includes a toolbar with icons for saving, adding, deleting, copying, pasting, running, and refreshing. The code cell contains the following Python code:

```
[6]: for i in range(3):  
      print(i)
```

The output of the code cell is:

```
0  
1  
2
```

Below the code cell is an empty code cell with a toolbar containing icons for adding, moving up, moving down, adding a new cell, and deleting.

# Data Analysis Example

- Collaborator has posted new code on Github
- You have a small dataset you would like to analyze using this code
- Clone repository from Github to JupyterHub server:  
`Start a new terminal.`  
`git clone https://github.com/bwfarm2/ExtraFastDataAnalyzer.git`
- Install dependencies from "environment.yml" file  
`cd ExtraFastDataAnalyzer`  
`conda env update -f environment.yml --prune`  
**OR** `conda install XXXX for all entries in environment.yml file`
- Upload your test data
- Run cell (shift+enter)

# Addendum - Anaconda

- Anaconda is a package manager for Python.
- Allows for easy installation of packages and corresponding dependencies.
- Default environment has numpy, pandas, matplotlib, etc...
- Can install packages using following command:  

```
!conda install ... from within a notebook
```
- Can export environment:  

```
!conda env export > environment.yml
```
- Additional documentation to create a custom Anaconda environment & kernel available at:

<https://docs.ccs.uky.edu> > Other Services > JupyterHub

# MCC/LCC Demo

 jupyterhub Home Token

bwfarm2 [Logout](#)

Start My Server

# MCC/LCC Demo

## Server Options

Customize your JupyterHub compute resources.

Account:

e.g. col\_vgazu2\_uksr

Queue:

SKY32M192\_L (LCC)

Time:

e.g. 4:00:00

Number of cores:

e.g. 4

Memory (GBs):

e.g. 16

Number of GPUs:

e.g. 1

Public key for LCC/MCC:

```
ssh-rsa
AAAAB3NzaC1yc2EAAAABJQAAAQEA4j/NNFtWFcl8okQcn5hHQuZjbJW3Au+KuQNJIfrl+SrGeMN2rQikxaywFD
4ym1ShWIKjdP1H0WrSelSxjo9eCTlLsH9lklZdlfulFs6ESnkjYFqOfzVXbllkBaG5e/gnH9MaVhtvKhZeO+FgNC98Z9
a88XY3B/6Qlp0RNtg92udWlajwhlEZ4BaXcMHmwsh93jslU8Hflon+SRBje4OzmK/ajObbTg4Ckhkux5dotf4UGY9
JJNzUaElfHMoeB5E+3P5IQNUFFUX6HCk3z/KixbMyHkIRhVXL3OCnmWHnZcsCCER3X3g+JawD6bumo2u4uH
Ahu9GmydRBP6ASopP+w==
```

# MCC/LCC Demo

## Server Options

Customize your JupyterHub compute resources.

Account:

### Queue:

SKY32M192\_L (LCC)

SKY32M192\_L (LCC)

CAL48M192\_L (LCC)

normal (MCC)

jumbo (MCC)

P4V16\_HAS16M128\_L (P100-16GB LCC)

P4V12\_SKY32M192\_L (P100-12GB LCC)

V4V16\_SKY32M192\_L (V100-16GB LCC)

V4V32\_SKY32M192\_L (V100-32GB LCC)

V4V32\_CAS40M192\_L (V100-32GB LCC)

### Memory (GBs):

```
a88X Y 3B/6QipukNtg9ZudvviawhIEZ4BaXcmHmwsn93jsiU8HfL0n+SrBje4UzmK/ajUdb I g4CknKUX500tI4UGY9  
JJNzUaElfHMoeB5E+3P5IQNUFFUX6Hck3z/KixbMyHkIRhVXL3OCnmWHnZcsCCER3X3g+JawD6bumo2u4uH  
Ahu9GmydRBp6ASopP+w==
```

# MCC/LCC Demo

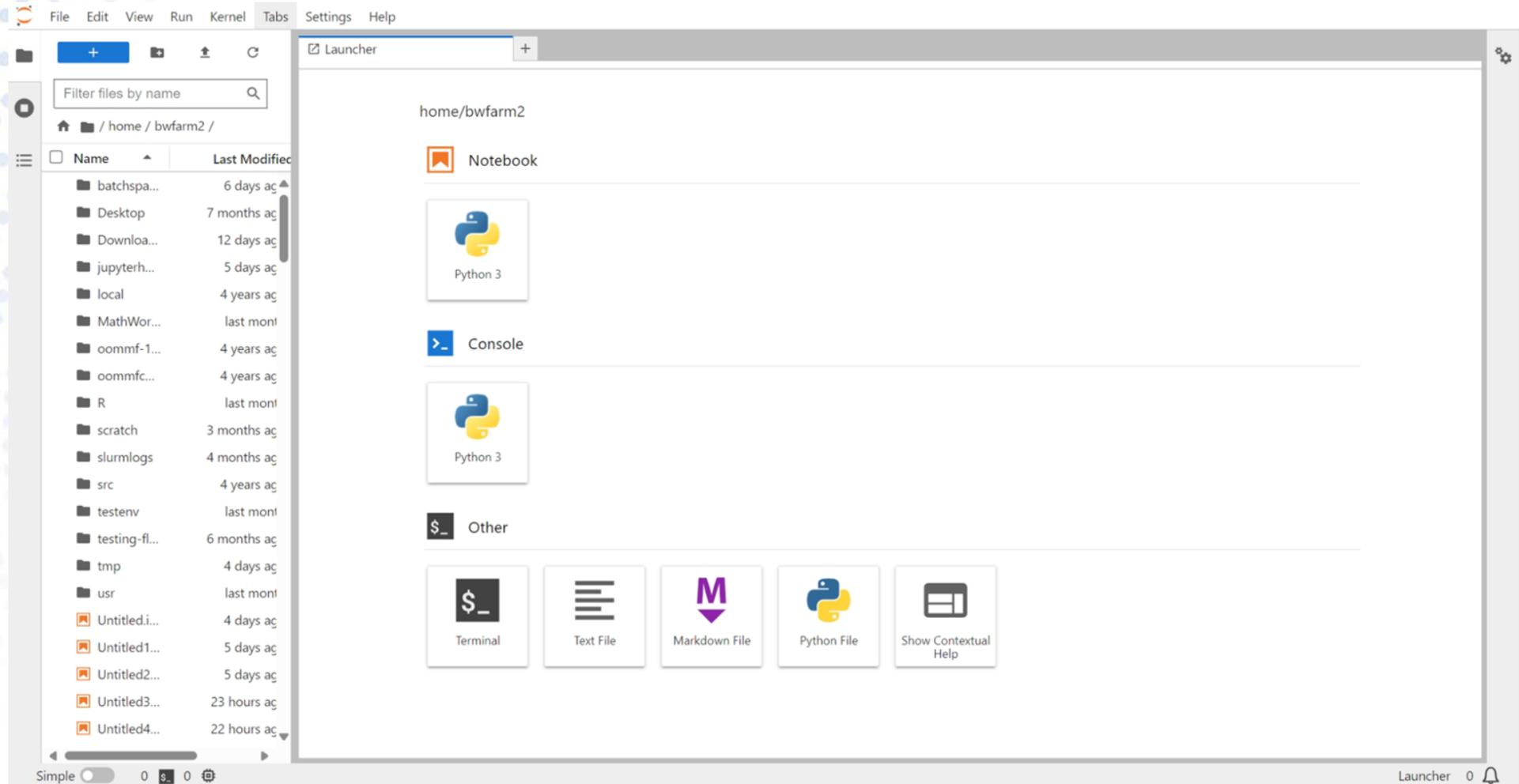
Your server is starting up.

You will be redirected automatically when it's ready for you.

Cluster job running... waiting to connect

Event log

# MCC/LCC Demo



# MCC/LCC Demo

The screenshot shows a Jupyter Notebook environment with a file explorer on the left and a terminal window on the right. The file explorer shows a directory structure with files like 'slurmlogs', 'src', 'testenv', etc. The terminal window displays the output of the command '!nvidia-smi'.

```
[1]: !hostname
gpdnode001

[2]: !nvidia-smi
Tue Apr 30 09:27:22 2024
+-----+
| NVIDIA-SMI 550.54.14              Driver Version: 550.54.14      CUDA Version: 12.4     |
+-----+-----+
| GPU   Name           Persistence-M   Bus-Id        Disp.A    Volatile Uncorr. ECC  |
| Fan  Temp  Perf    Pwr:Usage/Cap     Memory-Usage  GPU-Util  Compute M. |
|-----+-----+-----+-----+-----+-----+-----+
| 0   Tesla P100-SXM2-16GB     Off          00000000:04:00:0 Off      |    0%      0
| N/A   27C    P0              30W / 300W           0MiB / 16384MiB      |              Default |
|-----+-----+-----+-----+-----+-----+
+-----+

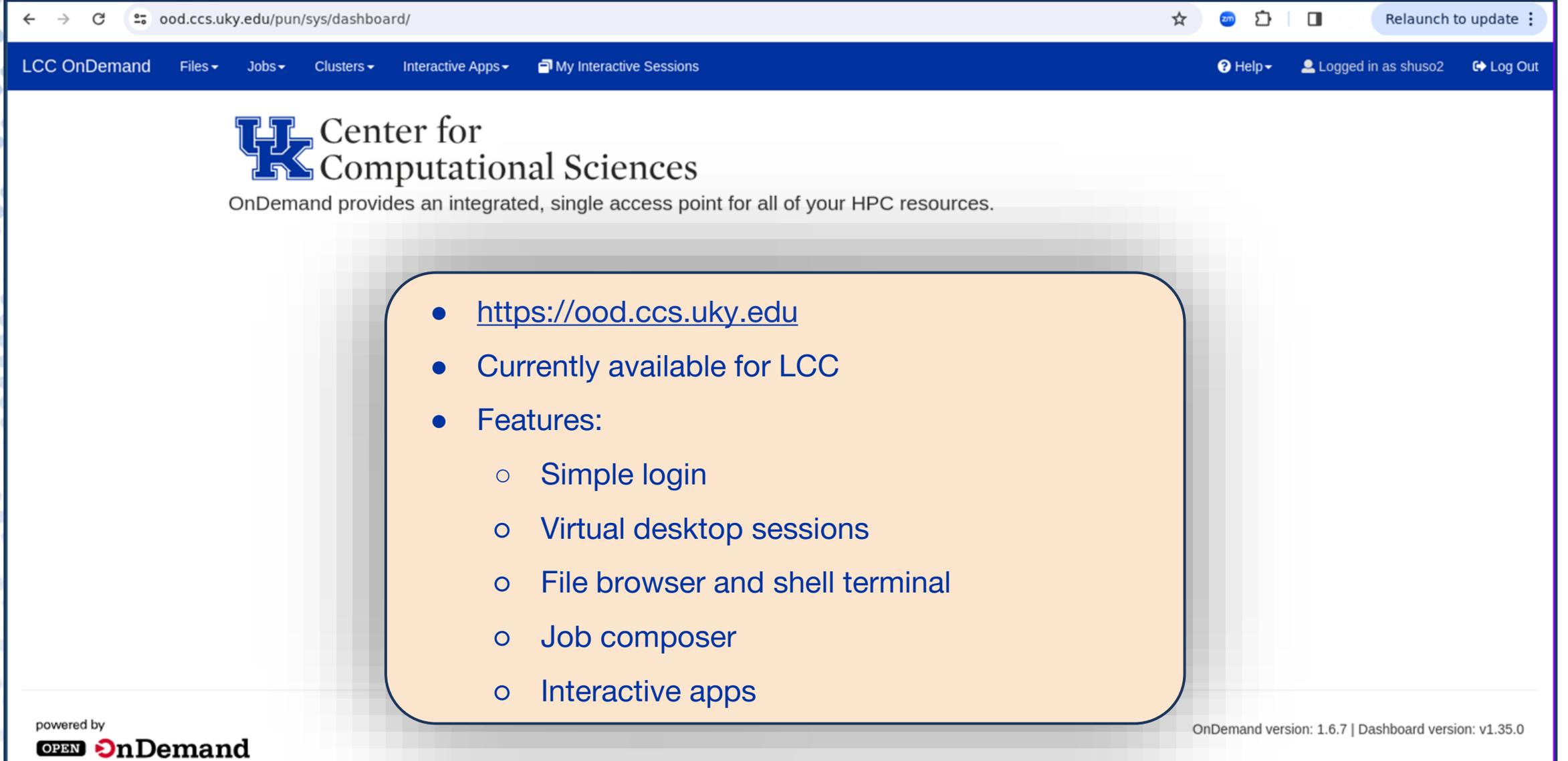
+-----+
| Processes:
| GPU   GI   CI        PID   Type   Process name                        GPU Memory |
|-----+-----+-----+-----+-----+-----+-----+
|              ID   ID                 |              Usage              |
+-----+-----+-----+-----+-----+-----+
| No running processes found
+-----+

[ ]:
```

# MCC/LCC Demo - Future Plans

- Allow to spawn into containers developed for specific workflows:
  - Machine Learning
  - R / Bioinformatics
  - Customized by research group?
- Install containers with AI models (e.g. llama3) for easy exploration
- Need to test security
- Expected rollout in a few months...

# Open OnDemand: Web interface for Supercomputing Clusters



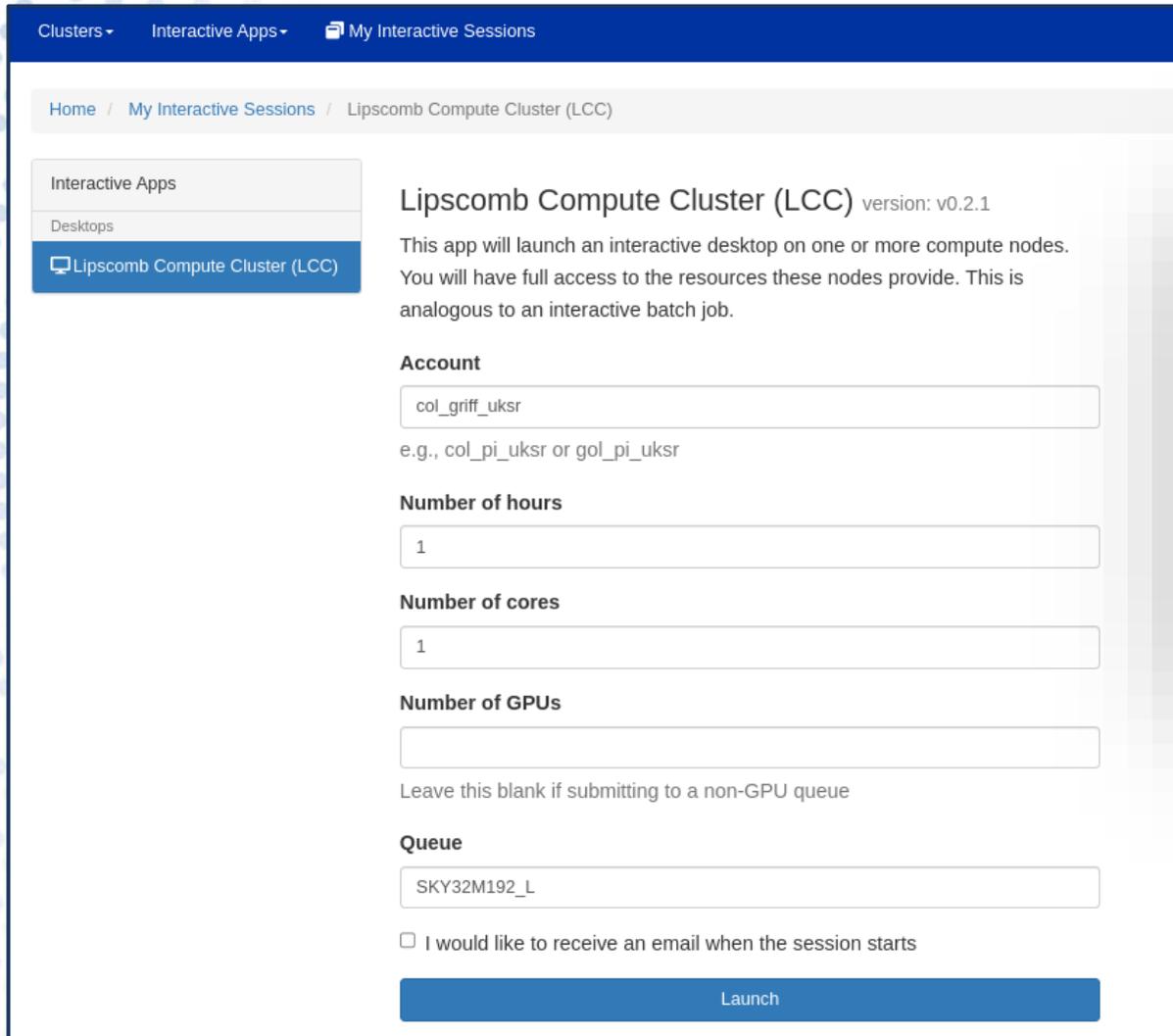
The screenshot shows a web browser window with the URL `ood.ccs.uky.edu/pun/sys/dashboard/`. The page header includes navigation links for "LCC OnDemand", "Files", "Jobs", "Clusters", "Interactive Apps", and "My Interactive Sessions". It also shows a user logged in as "shuso2" and a "Log Out" button. The main content area features the University of Kentucky logo and the text "Center for Computational Sciences" and "OnDemand provides an integrated, single access point for all of your HPC resources." A central orange box contains a bulleted list of features and the URL. The footer includes the "powered by OPEN OnDemand" logo and version information: "OnDemand version: 1.6.7 | Dashboard version: v1.35.0".

powered by  
**OPEN** OnDemand

- <https://ood.ccs.uky.edu>
- Currently available for LCC
- Features:
  - Simple login
  - Virtual desktop sessions
  - File browser and shell terminal
  - Job composer
  - Interactive apps

OnDemand version: 1.6.7 | Dashboard version: v1.35.0

# Open OnDemand Virtual Desktop Session



The screenshot shows the OnDemand web interface for launching a virtual desktop session. The top navigation bar includes 'Clusters', 'Interactive Apps', and 'My Interactive Sessions'. The breadcrumb trail is 'Home / My Interactive Sessions / Lipscomb Compute Cluster (LCC)'. A sidebar on the left lists 'Interactive Apps', 'Desktops', and 'Lipscomb Compute Cluster (LCC)'. The main content area is titled 'Lipscomb Compute Cluster (LCC) version: v0.2.1' and includes a description: 'This app will launch an interactive desktop on one or more compute nodes. You will have full access to the resources these nodes provide. This is analogous to an interactive batch job.' Below this are several form fields: 'Account' (with value 'col\_griff\_ukrs' and examples 'col\_pi\_ukrs' or 'gol\_pi\_ukrs'), 'Number of hours' (with value '1'), 'Number of cores' (with value '1'), 'Number of GPUs' (empty), and 'Queue' (with value 'SKY32M192\_L'). There is also a checkbox for 'I would like to receive an email when the session starts' and a 'Launch' button at the bottom.

- Virtual session is submitted like a typical compute job
- Increase # of cores as needed for the computation
- Use debug partition to test out setup

# Open OnDemand Virtual Desktop

LCC OnDemand Files Jobs Clusters Interactive Apps My Interactive Sessions Help Log

Home / My Interactive Sessions

Interactive Apps  
Desktops  
Lipscomb Compute Cluster (LCC)

**Lipscomb Compute Cluster (LCC) (2331988)** 1 node | 1 core | Running

Host: >\_skylake009 Delete

Created at: 2024-03-28 16:00:18 EDT

Time Remaining: 46 minutes

Session ID: 5b98de6e-513c-4d10-84e4-c28ebfcf6b4c

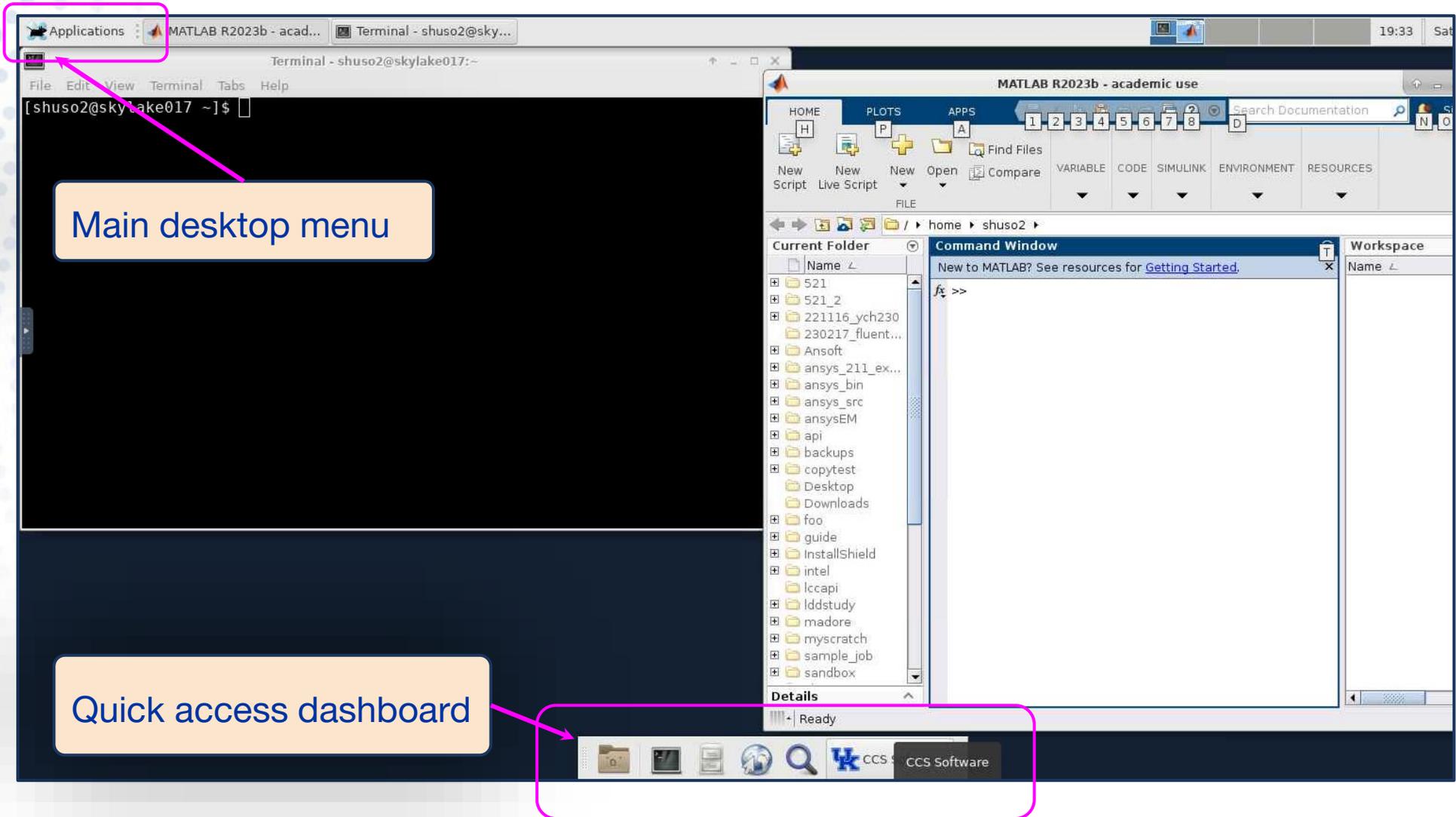
Compression 0 (low) to 9 (high)

Image Quality 0 (low) to 9 (high)

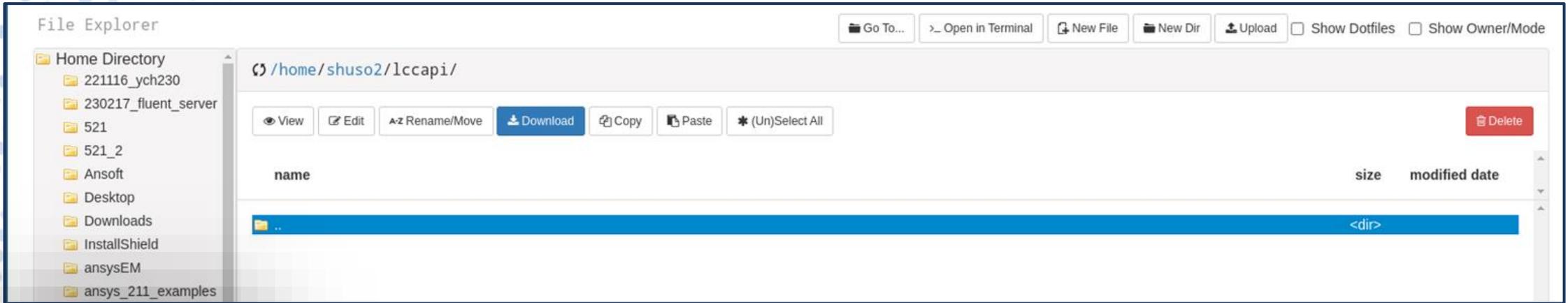
Launch Lipscomb Compute Cluster (LCC) View Only (Share-able Link)

This page updates the current status of the requested desktop session

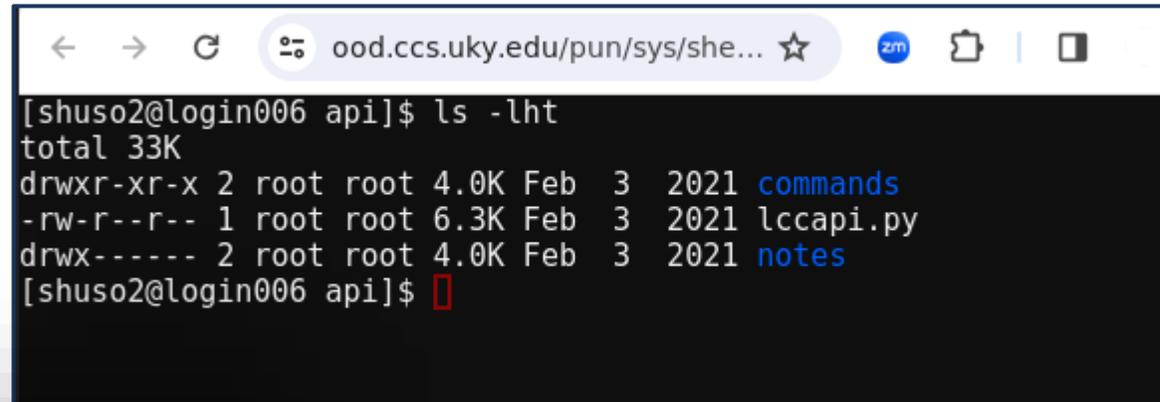
# Open OnDemand Virtual Desktop



# Open OnDemand File Browser & Terminal



File browser



Terminal

# Open OnDemand Job Composer

LCC OnDemand / Job Composer Jobs Templates

## Jobs

[+ New Job](#) [★ Create Template](#)

[Edit Files](#) [Job Options](#) [Open Terminal](#) [Submit](#) [Stop](#) [Delete](#)

Show  entries Search:

Created	Name	ID	Cluster	Status
March 21, 2024 7:57am	(default) Simple container Job		Lipscomb Compute Cluster (LCC)	Not Submitted
March 21, 2024 7:50am	(default) Simple Sequential Job		Lipscomb Compute Cluster (LCC)	Not Submitted

Showing 1 to 2 of 2 entries [Previous](#) [1](#) [Next](#)

### Job Details

Job Name:  
**(default) Simple container Job**

Submit to:  
Lipscomb Compute Cluster (LCC)

Account:  
Not specified

Script location:  
/scratch/shuso2/ondemand/projects/default/2

Script name:  
main\_job.sh

Folder Contents:  
[/main\\_job.sh](#)

# Open OnDemand SLURM Job Submission

LCC OnDemand / Active Jobs

Your Jobs ▾ All Clusters ▾

## Active Jobs

Show  entries Filter:

ID	Name	User	Account	Time Used	Queue	Status	Cluster
> 2331988	sys/dashboard/sys/bc_desktop/lcc	shuso2	col_griff_uksr	00:12:35	SKY32M192_L	Running	Lipscomb Com...

Showing 1 to 1 of 1 entries Previous **1** Next

# ACCESS-CI

- **What is ACCESS-CI?**

- Advanced Cyberinfrastructure Coordination Ecosystem: Services & Support (<https://access-ci.org/>)
- Connects researchers to computational resources in the U.S.

- **Key Features:**

- Diverse computing resources, Data and storage services, Scientific applications, workflow management and science gateways.
- Comprehensive user support, resources for your class, training, and workshops, as well as connecting with communities that share your interests and learn from one another (affinity groups).

# Engaging with ACCESS-CI

## Using ACCESS-CI:

–Requesting project credits(allocations).

- **EXPLORE** —For resource evaluation, graduate student projects, small classes and training events, benchmarking, code development and porting, and similar small-scale uses.(400,000 credits), only an overview is needed.
- **DISCOVER** — Designed for research grants with modest resource needs, large classes and training events, NSF graduate fellowships, benchmarking and code testing at scale (1,500,000 credits), 1-page proposal.
- **ACCELERATE** — Best for experienced users with mid-scale resource needs, consolidating multi-grant programs, collaborative projects, preparing for Maximize ACCESS requests, and gateways with growing communities(3,000,000 credits), 3-page proposal.
- **MAXIMIZE** — The choice for large-scale research activities that need more resources than the limit for Accelerate ACCESS projects, a 10-page proposal.

## Benefits for Researchers:

–Access to computational tools.

Enhanced research efficiency and collaboration.

# Pegasus Workflow Management System

## Overview of Pegasus:

- Automates large-scale scientific computations.
- Scalable, fault-tolerant, and efficient data management.

## Benefits:

- Describe complex workflows in a simple way
- Access distributed, heterogeneous data and resource
- Easy to deal with resources/software that change over time
- Ease of use. Ability to debug and monitor large workflows
- Streamlines data analysis.
- Supports reproducible research.

For more Pegasus details see <https://pegasus.isi.edu/>

# Pegasus in Action

Workflow examples : <https://support.access-ci.org/tools/pegasus>

- Astrophysics: Data from the Large Hadron Collider.
- Genomics: DNA sequence analysis.

Impact:

- Efficient resource use.
- Advances in scientific discoveries.

# Science Gateways: Bridging Research and Resources

## What are Science Gateways?

- Online platforms for shared scientific resources, a community space for sharing knowledge of methods, code, data, results, and training materials.
- Support research and education across disciplines.

## Features:

- Customizable interfaces.
- Easy access to computational tools.

# Science Gateway Resources

Examples of some gateways: (<https://support.access-ci.org/tools/science-gateways>)

- Climate research and environmental modeling.
- Advances in bioinformatics and genetic disease understanding.

## Achievements:

- Contributions to scientific research and education.
- Enhanced accessibility for diverse research needs.

# Questions ?

For all your support needs

<https://ukyrcd.atlassian.net/servicedesk/customer/portals>