LINCC Science Platform

Release 0.1

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An initiative of the LSST Corporation aiming to help the LSST user community prepare for LSST science.

Key Goals:

- 1. Open the discovery space to a larger and more inclusive community (LINCC Frameworks/Infrastructure
- 2. Foster the creation and sharing of analysis tools and data for key LSST science goals (LINCC Frameworks)
- 3. Train and mentor future science leaders (LINCC Hubs, Catalyst Fellowships)

LINCC Hub Collaborators: Carnegie-Mellon University, Northwestern University (CIERA), University of Arizona, University of Washington (DiRAC Institute)

Note: This documentation site is under active development

ONE

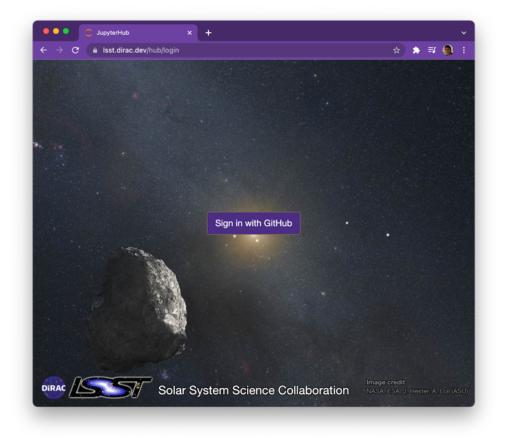
ACCESSING LINCC JUPYTERHUB

• To log in, you will need:

- 1. A GitHub account (https://github.com).
- 2. Membership in the lincc-hub GitHub organization (https://github.com/lincc-hub)
- To get an invitation to join the lincc-hub organization:
 - Join the **#lincc-hub** channel on LSSTC Slack
 - Post your github username, and one of our admins will send you an invitation in the next few minutes.
 - * Example message: "Hi, I'd like to get access to LINCC JupyterHub. My github ID is mjuric. Thanks!"

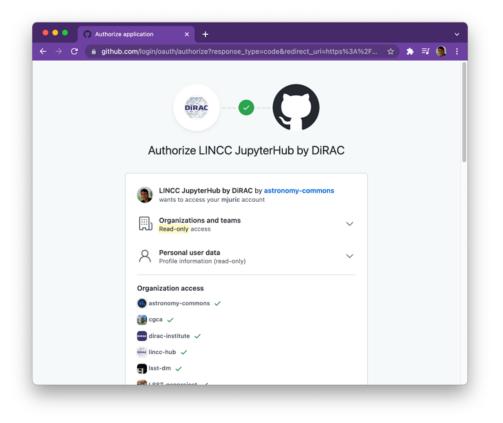
1.1 Logging In

- 1. Make sure to accept an invitation to join lincc-hub on github!
- 2. Go to https://lsst.dirac.dev

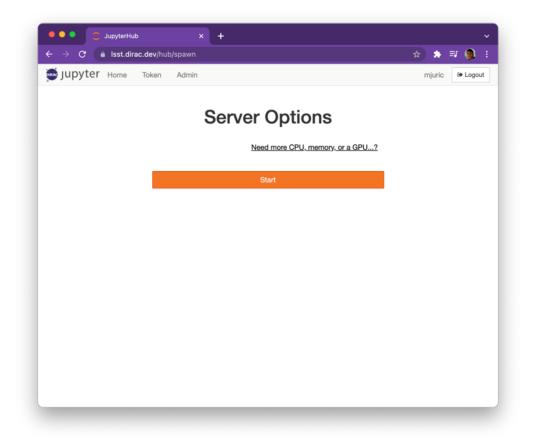


3. The first time you log in, GitHub will ask you to allow $access^{*0}$.

⁰ Grant access to organizations you wish to collaborate with within the hub



4. Upon clicking on the green button (left figure), you will be redirected and logged into the Hub



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INTRODUCTION TO JUPYTER

Your "Home in the Clouds"

• When you logged in and clicked "Start" (big orange button), Jupyter asked Amazon Web Services to allocate a dedicated machine* for your use.

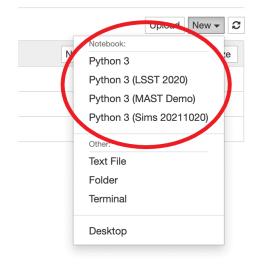
• • • JupyterHub × +	
> C 🔒 Isst.dirac.dev/hub/spawn	🔷 🖈 🗊 🚳 i
JUPyter Home Token Admin	mjuric 🕞 Logout
Server Options	
Need more CPU, memory, or a GPU?	
Start	

- While this machine is just yours to use, it has access to the shared directory with software and files. This is not unlike how office computers in many institutions see the same filesystem.
- This machine can only be accessed through Jupyter (Notebook, Lab, Terminal). Note: direct SSH access is in the works.

Important: If you don't use it for more than an hour (close the browser with Jupyter), it will be shut down to conserve resources. Disk data will be preserved, but all running Jupyter notebooks will be shut down.

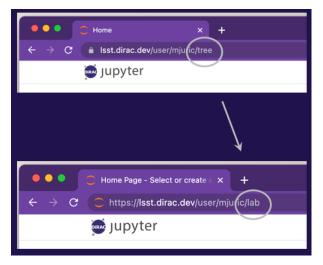
2.1 Jupyter Notebooks

You can access a notebook from the Jupyter homepage by clicking the "New" button and selecting a virtual environment for your notebook.



2.1.1 Accessing JupyterLab

If you prefer the JupyterLab interface, replace the 'tree' in your URL with 'lab'.



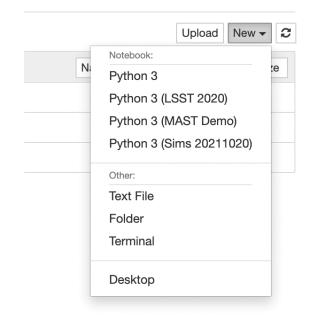
2.2 Terminal

To access the Terminal, click the "New" button and select the "Terminal" option. This will open a new terminal instance for your server.

	Upload New - 2								
	Notebook:								
Nam	Python 3								
	Python 3 (LSST 2020)								
	Python 3 (MAST Demo)								
	Python 3 (Sims 2021)								
	Other:								
	Text File								
	Folder								
	Terminal								
	Desktop								

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(100c) mjul	total	used		ree	shar	ed bu	ff/cache	available					
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Swap:		0											
(lsst) mjur													
top - 06:26													
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MiB Swap:	0.0 to		0.0 free,		0.0 use		031.9 ava						
PID USER	PR N		RES	SHR S		%MEM		COMMAND					
1 root		0 2508	604	532 S	0.0	0.0	0:00.03						
11 root 376 root		0 8764 0 0	4300	3860 S 0 Z	0.0	0.1	0:00.02	sudo start-singleuse					
408 root		0 7160		1692 S	0.0	0.0		start-singleuse					
431 mjuri		0 444764		2080 S		1.5	0:07.35						
	20	0 7508		3344 S	0.0	0.1	0:00.66	bash					
1699 mjuri		0 7508		3404 S		0.1	0:00.59						
5437 mjuri	20	0 8900		3792 S		0.1	0:00.00						
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You can use this to manage your directories, edit files, install and run codes, etc.



2.3 Available Software

- Python 3: Python 3 with the current LSST Stack Release.
- Python 3 (Sims NNNNN): Python 3 with a recent install of the rubin_sims tools (https://github.com/lsst/rubin_sim)
- Python 3 (xxx): Older LSST Stack releases and custom environments prepared for events.

THREE

CUSTOMIZING YOUR HUB

3.1 Adding software: Conda Environments

You can create any number of personal conda environments where you have complete control over the software available. To create and activate a new conda environment, run the following in a terminal:

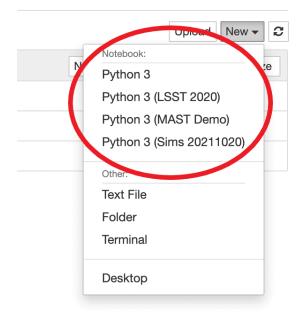
```
$ conda create -n my_environment python=3
$ conda activate my_environment
```

Feel free to change "my_environment" to any environment name you desire. After activating the environment, you can use conda and pip commands to install any software you desire.

It may be helpful to install the mamba software, a faster version of conda:

\$ conda install mamba

If the ipykernel package is installed in the environment, it will automatically show up in your list of kernels and be available for use in a Jupyter notebook.



To install ipykernel use this command,

\$ conda install ipykernel

or

\$ mamba install ipykernel

Important: These environments are only accessible to you (they're personal).

FOUR

COLLABORATING USING OUR PLATFORM

4.1 Collaboration Facilities

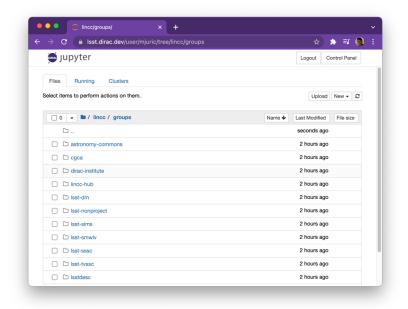
Every user has a 'lincc' folder in their home directory, with three subdirectories:

- data: shared, centrally managed, data.
- groups: group-owned, group-managed, files.
- shared: a folder anyone can write to, and readable by everyone on LINCC JupyterHub.

→ C	☆ 🗯 🗐 🥘
💀 Jupyter	Logout Control Panel
Files Running Clusters	
Select items to perform actions on them.	Upload New - 2
0 - Iincc	Name Last Modified File size
۵	seconds ago
🗋 🗀 data	2 hours ago
groups	2 hours ago
□ □ shared	2 hours ago

4.2 Group file spaces

- When you log in, any organization that you're a member of on github (and to which you've granted LINCC JupyterHub access; see slide #7), is given:
 - a UNIX group on LINCC JupyterHub
 - a directory in lincc/groups, readable and writable only by members of that group.



- You can place shared notebooks, datafiles, software here...
- Works for any github organization, and is fully automatic.
- Enables seamless collaboration!

4.3 Group-controlled environments and software

- A frequent use for shared directories is to install and maintain common software environments.
- It's good to protect such environments from accidental corruption or deletion.
 - E.g., it's too easy to accidentally run 'pip install some_package' and ruin a carefully curated conda environment.
 - Especially true for large groups (e.g. science collaborations).
- To defend against this, each group has an admin account, designed to own its software and important files.

Here is an example of how to use an admin account in the terminal:

```
# login as admin for dirac-institute
$sudo -u dirac-institute -s
$cd
```

install a new environment

(continues on next page)

(continued from previous page)

```
$conda create -n solarsystem openorb
exit
# check that we have access to the env
$conda env list
$conda activate solarsystem
$oorb
# make it accessible in Jupyter
$sudo -u dirac-institute -s
$cd
$conda activate solarsystem
$mamba install ipykernel
```

Note: Only GitHub organization owners have access to the admin account.

Tip:

- Your home directory is visible only by you. Keep any private files there.
- A group directory is visible only to eponymous GitHub organization's members. Keep common files there.
- The **shared directory** is visible (readable and writable) to anyone. Place files there that you want to share with the entire hub (that are public).

FIVE

AVAILABLE RESOURCES

5.1 Disk space

1TB of space shared by everyone. We can add more if (when) needed.

5.2 Computational resources

- Machines are available with different combinations of CPU, RAM, and GPU.
- Please use the smallest machine that can fit your workload (to help us conserve \$\$).
- Also, larger machines may take more time to start up (up to ~5 minutes).

You can access different server options by clicking *Need more CPU, memory, or a GPU...*? on the Server Options page.

images/picture11.png

SSH

A SSH "jump host" is deployed with this chart to allow users to use *scp* and *sftp* to copy files to the NFS. Each notebook server starts its own SSH service, allowing users to access their notebook servers using *ssh* via the jump host.

If a user wants to utilize this, they should perform the following steps:

- 1. Launch their notebook server.
- 2. Start a terminal and open the file ~/.ssh/authorized_keys with a text editor.
- 3. On their local machine, the user should generate a new or reuse an old SSH public key. Existing public/private key pairs may be named ~/.ssh/id_rsa.and ~/.ssh/id_rsa.pub. New public/private key pairs can be generated by running ssh-keygen. The user should copy their public key from their local machine and add it as a new line in the file from (2) on the remote machine.
- 4. The user should edit the file ~/.ssh/config on their local machine to include the following, replacing <username> with their username on the JupyterHub:

```
Host lsst-hub-ssh
User <username>
Hostname ssh.lsst.dirac.dev
Host lsst-hub
User <username>
Hostname lincc-<username>.notebooks
```

- - -

For example:

```
Host lsst-hub-ssh
User stevenstetzler
Hostname ssh.lsst.dirac.dev
```

ProxyJump lsst-hub-ssh

```
Host lsst-hub
User stevenstetzler
Hostname lincc-stevenstetzler.notebooks
ProxyJump lsst-hub-ssh
```

5. On their local machine, the user can ssh to their running notebook server using:

```
$ ssh lsst-hub
```

Alternatively, they can specify the jump host explicitly:

\$ ssh -J <username>@ssh.lsst.dirac.dev <username>@lincc-<username>.notebooks

SEVEN

SUPPORT AND DEVELOPMENT

#lincc-hub on LSSTC Slack is the main communication channel. Join and give us comments, questions, or feature requests there!

Support team on Slack:

• @Aditi Chauhan, @Aidan Berres, @Paulo Andres Stevens Barrera

Developers and researchers:

- @Steven Stetzler @mjuric @colin
- A larger software development team coming in 2022 (follow us on https://dirac.us/linkedin to be notified of job openings)

Warning: LINCC JupyterHub is a new system, still under heavy development. We apologize for the occasional glitch!

EIGHT

INDICES AND TABLES

- genindex
- modindex
- search