

Interactive High-Performance Computing on Expanse

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EXPANSE
COMPUTING WITHOUT BOUNDARIES

EXPANSE

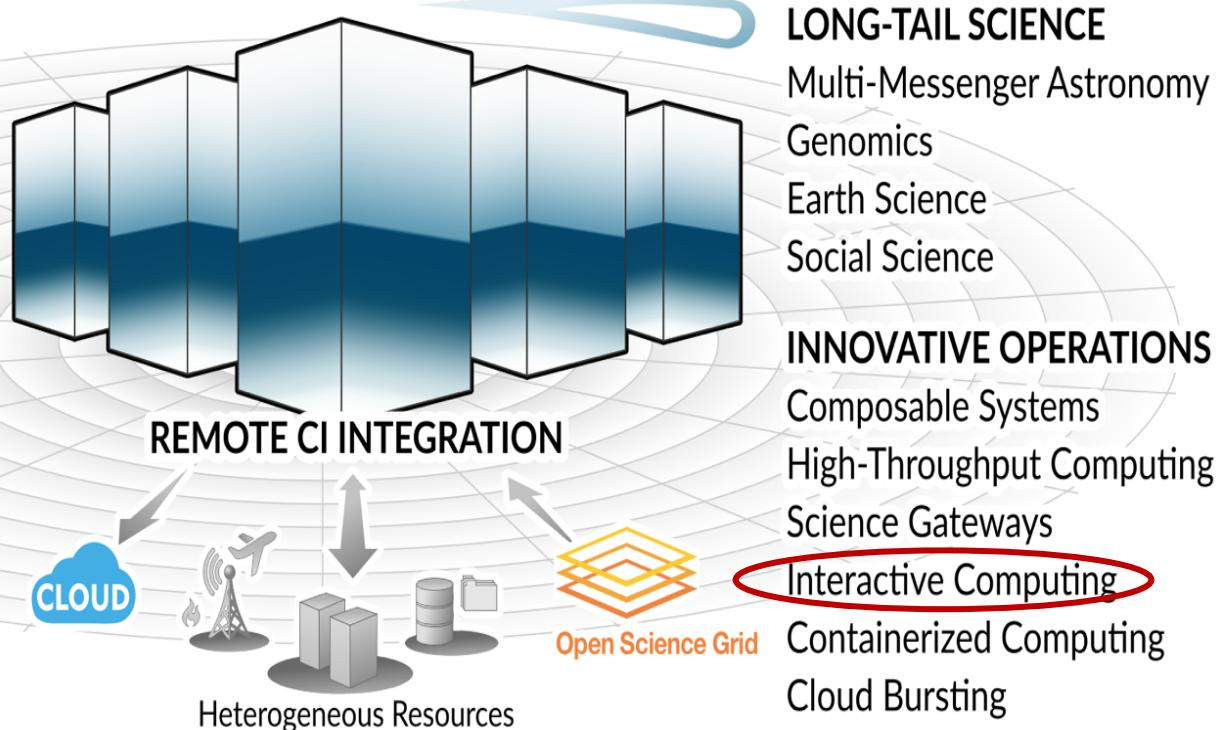
COMPUTING WITHOUT BOUNDARIES
5 PETAFLOP/S HPC and DATA RESOURCE

HPC RESOURCE

13 Scalable Compute Units
728 Standard Compute Nodes
52 GPU Nodes: 208 GPUs
4 Large Memory Nodes

DATA CENTRIC ARCHITECTURE

12PB Perf. Storage: 140GB/s, 200k IOPS
Fast I/O Node-Local NVMe Storage
7PB Ceph Object Storage
High-Performance R&E Networking



LONG-TAIL SCIENCE

Multi-Messenger Astronomy
Genomics
Earth Science
Social Science

INNOVATIVE OPERATIONS

Composable Systems
High-Throughput Computing
Science Gateways
Interactive Computing
Containerized Computing
Cloud Bursting

For more details see the Expanse user guide @ https://www.sdsc.edu/support/user_guides/expanse.html
and the "Introduction to Expanse" webinar @ https://www.sdsc.edu/event_items/202006_Introduction_to_Expanse.html

Outline

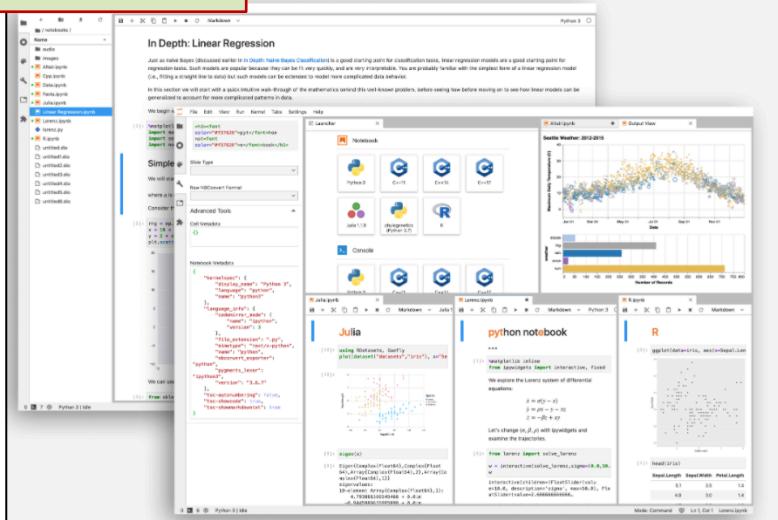
- What is Interactive High-Performance Computing?
- Types of Interactive Computing
- How to Access an Interactive Compute Node
- How to Run Applications
- How to Run Jupyter Notebooks

What is Interactive HPC-Computing

- In **computer science**, **interactive computing** refers to software which accepts input from the user as it runs.
 - **Interactive** software includes commonly used programs, such as word processors or spreadsheet applications.
- **Interactive HPC computing** involves *real-time* user inputs to perform tasks on a set of compute node(s) including:
 - Code development, real-time data exploration, and visualizations.
 - Used when applications have large data sets or are too large to download to local device, software is difficult install, etc.
 - User inputs come via command line interface or application GUI (Jupyter Notebooks, Matlab, R-studio).
 - Actions performed on remote compute nodes as a result of user input or program out.

Interactive HPC Scenarios

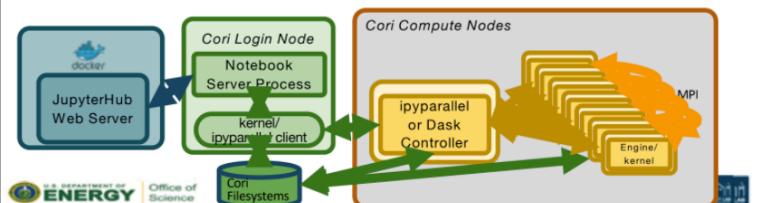
<https://jupyter.org/>



Interactive Distributed Computing with Jupyter (NERSC)

Jupyter architecture

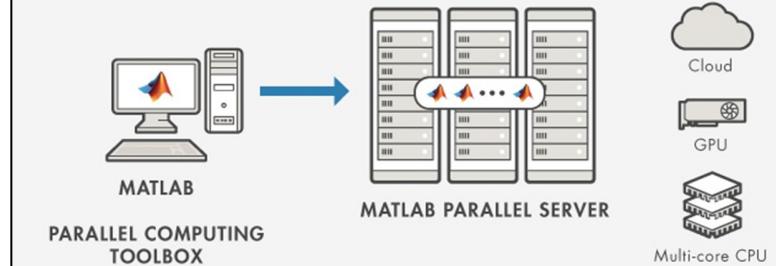
- Allocate nodes on Cori interactive queue and start ipyparallel or Dask cluster
 - Developed %ipcluster magic to setup within notebook
- Compute nodes traditionally do not have external address
 - Required network configuration / policy decisions
- Distributed training communication is via MPI Horovod or Cray ML Plugin



<https://drive.google.com/file/d/1-OFjrk1q3L1d3uakr2xkozrPn2c2VZpZ/view>

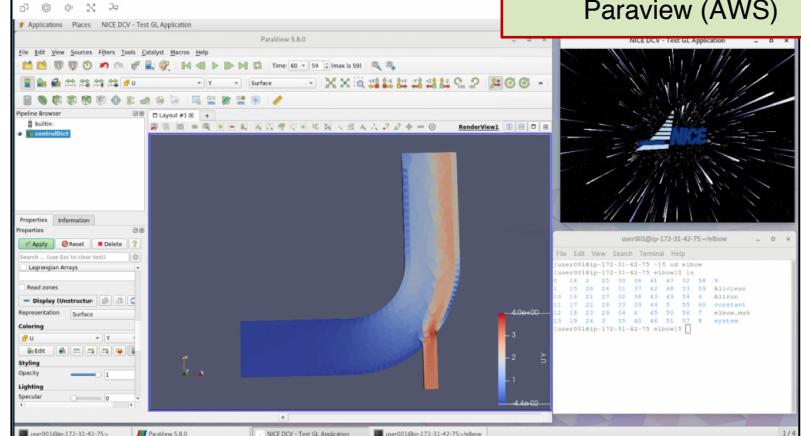
Parallel Matlab (AWS)

```
>> parpool(parcluster('HPC1'),100);
>> parfor i=1:3000
>> c(i,:) = eig(rand(1000));
>> end
```



<https://azuremarketplace.microsoft.com/en-us/marketplace/apps/mathworks-inc.matlab-parallel-server-listing?tab=Overview>

Paraview (AWS)



<https://aws.amazon.com/blogs/compute/how-to-run-3d-interactive-applications-with-nice-dcv-in-aws-batch/>

Accessing Interactive Compute Nodes on Expanse

- Use the *srun* command to obtain nodes for ‘live,’ command line interactive access:
- Notes:
 - account info is required
 - Start your testing using shared or debug partitions

CPU	<pre>srun --partition=shared --pty --nodes=1 --ntasks-per-node=16 --mem=248 -t 00:30:00 --wait=0 --export=ALL --account=abc123 /bin/bash</pre>
GPU	<pre>srun --partition=gpu-shared --pty -- nodes=1 --ntasks-per-node=16 -- mem=374 --gpus=1 -t 00:30:00 --wait=0 -- export=ALL --account=abc123 /bin/bash</pre>

Running Jupyter Services on HPC Systems at SDSC

- What is Jupyter?

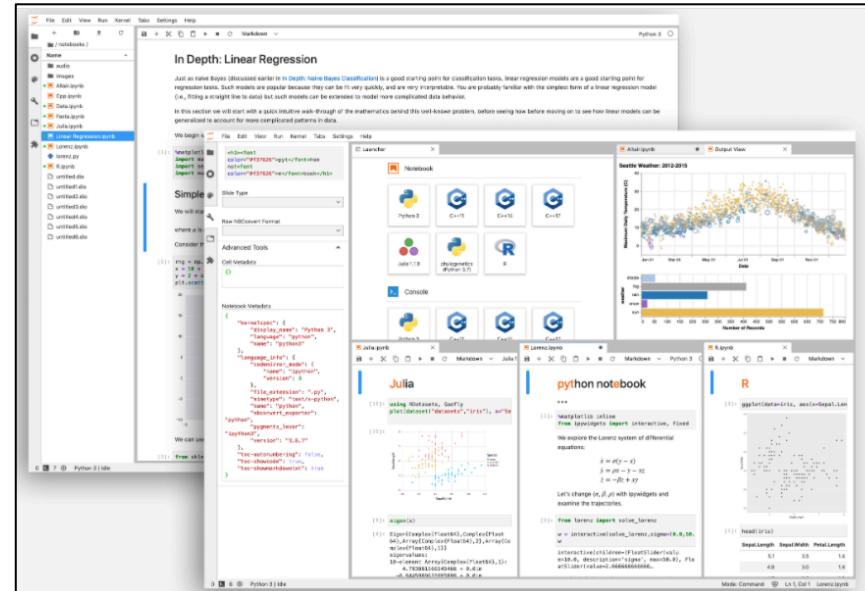
*Jupyter is a free, open-source, **interactive** web tool known as a computational notebook, which researchers can use to combine software code, computational output, explanatory text and multimedia resources in a single document. (J. Perkel, <https://www.nature.com/articles/d41586-018-07196-1>)*

- Common Jupyter Services:

- Jupyter Notebooks (single user)
- JupyterLab: advanced version of notebook
- JupyterHub: multiuser Jupyter service

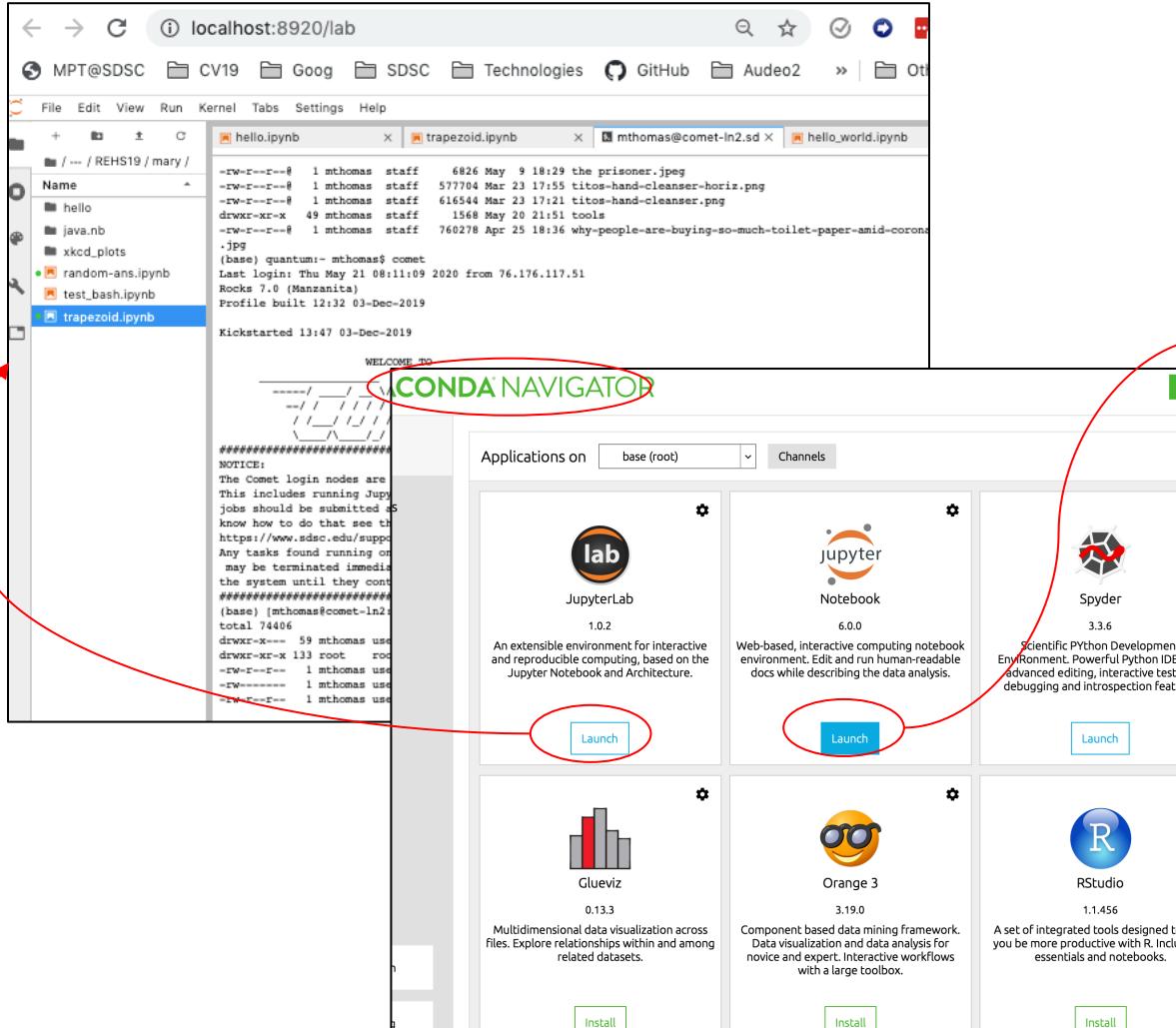
- To run Juptyer services:

- Laptop/local host, use Anaconda:
 - <https://docs.anaconda.com/anaconda/install/>
- HPC systems: use miniconda:
 - <https://docs.conda.io/en/latest/miniconda.html>



Related Tutorial: <https://hpc-training.sdsc.edu/notebooks-101/notebook-101.html>

Using Anaconda on Local Host or Laptop



The screenshot shows a Jupyter notebook interface at `localhost:8807/tree/dev/sdsc....`. The top navigation bar includes 'jupyter', 'Files', 'Running', and 'IPython Clusters'. The left sidebar shows a file tree with several Jupyter notebooks and Python files. The bottom panel contains a terminal window displaying command-line logs related to Jupyter and Python execution. A red arrow points from the 'Launch' button in the first screenshot to the 'Launch' button in the Jupyter interface here.

```
mthomas — jupyter_mac.command — python -bash — 82x43
! May 20 23:47:17 on ttys003
!jupyter_mac.command : exit:
~ mthomas$ /anaconda3/bin/jupyter_mac.command : exit:
; NotebookApp: The port 8888 is already in use, trying another port.
; NotebookApp: The port 8890 is already in use, trying another port.
; NotebookApp: The port 8891 is already in use, trying another port.
? NotebookApp: The port 8892 is already in use, trying another port.
! NotebookApp: Loading IPython parallel extension
! NotebookApp: JupyterLab extension loaded from /anaconda3/lib/python
iges/jupyterlab
! NotebookApp: JupyterLab application directory is /anaconda3/share/
;
NotebookApp: Serving notebooks from local directory: /Users/mthoma
;
NotebookApp: The Jupyter Notebook is running at:
; NotebookApp: http://localhost:8798/?token=681f898da657418d5cce6909
;100fdcccf
; NotebookApp: or http://127.0.0.1:8798/?token=681f898da657418d5cce
;1313c100fdcccf
; NotebookApp: Use Control-C to stop this server and shut down all k
;o skip confirmation.
; NotebookApp:
;
the notebook, open this file in a browser:
;/Users/mthomas/Library/Jupyter/runtime/nbserver-55091-open.html
; I paste one of these URLs:
;/localhost:8798/?token=681f898da657418d5cce69096829b6064b3313c100fdcc
;
! NotebookApp: Could not open static file '':
; NotebookApp: 404 GET /static/components/react/react-dom.production
; min.js (:::1) 1 @0ms referer=http://localhost:8798/tree?token=681f898da657418d5cce
; 69096829b6064b3313c100fdcccf
```

HPC Systems: Use Conda

- Conda: open-source package and environment management system:
 - Runs on Windows, macOS, and Linux.
 - Less overhead than Anaconda
- Created for Python programs:
 - Can package and distribute software for any language.
- Download: <https://docs.conda.io/projects/conda/en/latest/>
- To Install Conda on Expanse, see Notebooks tutorial:
 - <https://hpc-training.sdsc.edu/notebooks-101/notebook-101.html#software-prerequisites>
 - Note: do not put the conda activation code into the .bashrc or .bash_profile files
 - This ends up making the login process extremely long,
- When you are ready to use notebooks, run these commands

```
[user@login01 ~] . /home/user/miniconda3/etc/profile.d/conda.sh  
[user@login01 ~]conda activate  
(base) [user@login01 ~]
```
- Conda Cheat Sheet:
 - https://kapeli.com/cheat_sheets/Conda.docset/Contents/Resources/Documents/index

Conda Environments

(<https://docs.conda.io/projects/conda/en/latest/user-guide/concepts/environments.html>)

- You can load the conda environment in 2 ways: at login (from your .bash_profile) or via command line (when you are ready to use conda, run Juptyer)
 - On installation of miniconda, the code will install the activation commands in your .bashrc file automatically. This takes time which delays your login process.
 - SDSC recommends that you remove those lines and save in a text file.
- The example below shows how to do this:

```
Last login: Thu Mar  4 06:42:34 2021 from 76.176.117.51
[user@login01 ~]$ cat conda-activate.txt
### Commands to activate Conda environment
. /home/user/miniconda3/etc/profile.d/conda.sh
conda activate
[user@login01 ~]$ . /home/user/miniconda3/etc/profile.d/conda.sh
[user@login01 ~]$ conda activate
(base) [user@login01 ~]$
```

- The **(base)** prefix to the command line prompt shows that we are running in the base conda environment. Note that (base) was not present until the conda activation commands were run.

Custom Conda Virtual Environments

- Use conda to create a virtual environment
 - \$ conda create --name example_env
- To see which virtual environments you've created:
`[user@login01 ~]conda env list`
- To use a particular virtual environment (e.g., one named ‘example_env’), run:
`$ source activate example_env`
(Note: don’t use ‘conda activate’)

Conda Enviromnet Example

```
(base) [user@login01 ~]$ conda list
# packages in environment at /home/user/miniconda3:
#
# Name           Version        Build  Channel
_libgcc_mutex    0.1            main
argon2-cffi      20.1.0       py38h7b6447c_1
[SNIP 20-30 lines]
zlib             1.2.11        h7b6447c_3
(base) [user@login01 ~]$ conda create --name demo_env
Collecting package metadata (current_repodata.json): done
Solving environment: done
## Package Plan ##
environment location:
/home/user/miniconda3/envs/demo_env
Proceed ([y]/n)? y
Preparing transaction: done
Verifying transaction: done
Executing transaction: done
#
# To activate this environment, use
#
# $ conda activate demo_env
#
# To deactivate an active environment, use
#
# $ conda deactivate
```

```
(base) [user@login01 ~]$ conda activate demo_env
(base) [user@login01 ~]$ conda list
# packages in environment at /home/ user
/miniconda3/envs/demo_env:
#
# Name           Version        Build  Channel
(demo_env) [user@login01 ~]$ conda install numpy
Collecting package metadata (current_repodata.json): done
Solving environment: done
[SNIP][several mins later]
(demo_env) [user @login01 ~]$ conda list
# packages in environment at /home/ user
/miniconda3/envs/demo_env:
#
# Name           Version        Build  Channel
_libgcc_mutex    0.1            main
blas             1.0            mkl
[SNIP]
xz               5.2.5          h7b6447c_0
zlib             1.2.11         h7b6447c_3
(demo_env) [user @login01 ~]$
(demo_env) [user @login01 ~]$conda deactivate
(base) [user @login01 ~]$ conda deactivate
[user@login01 ~]$
```

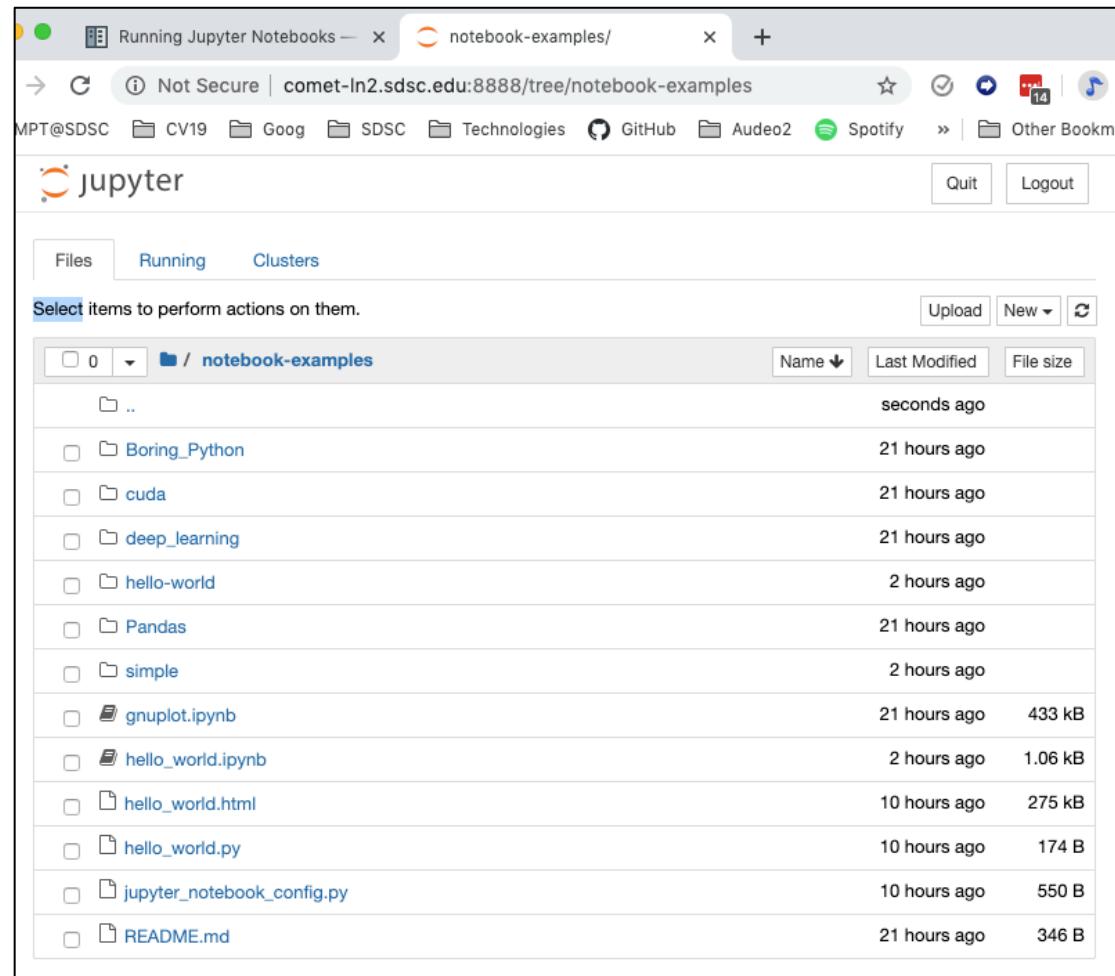
Installing Jupyter Servers

- To run Jupyter servers (notebooks, jupyterlab), you need to install them using *conda*.
- To Install Jupyter Notebooks, see:
 - <https://comet-notebooks-101.readthedocs.io/en/master/prerequisites.html#install-jupyter-notebook>
- To Install JupyterLab, see:
 - <https://comet-notebooks-101.readthedocs.io/en/master/prerequisites.html#install-jupyterlab>
- Note: installing conda, and Jupyter can take a very long time (5-10 minutes)

Jupyter Has a Key Vulnerability: Jupyter Servers Provide Access to HPC File Systems

SDSC Jupyter Services Policy:

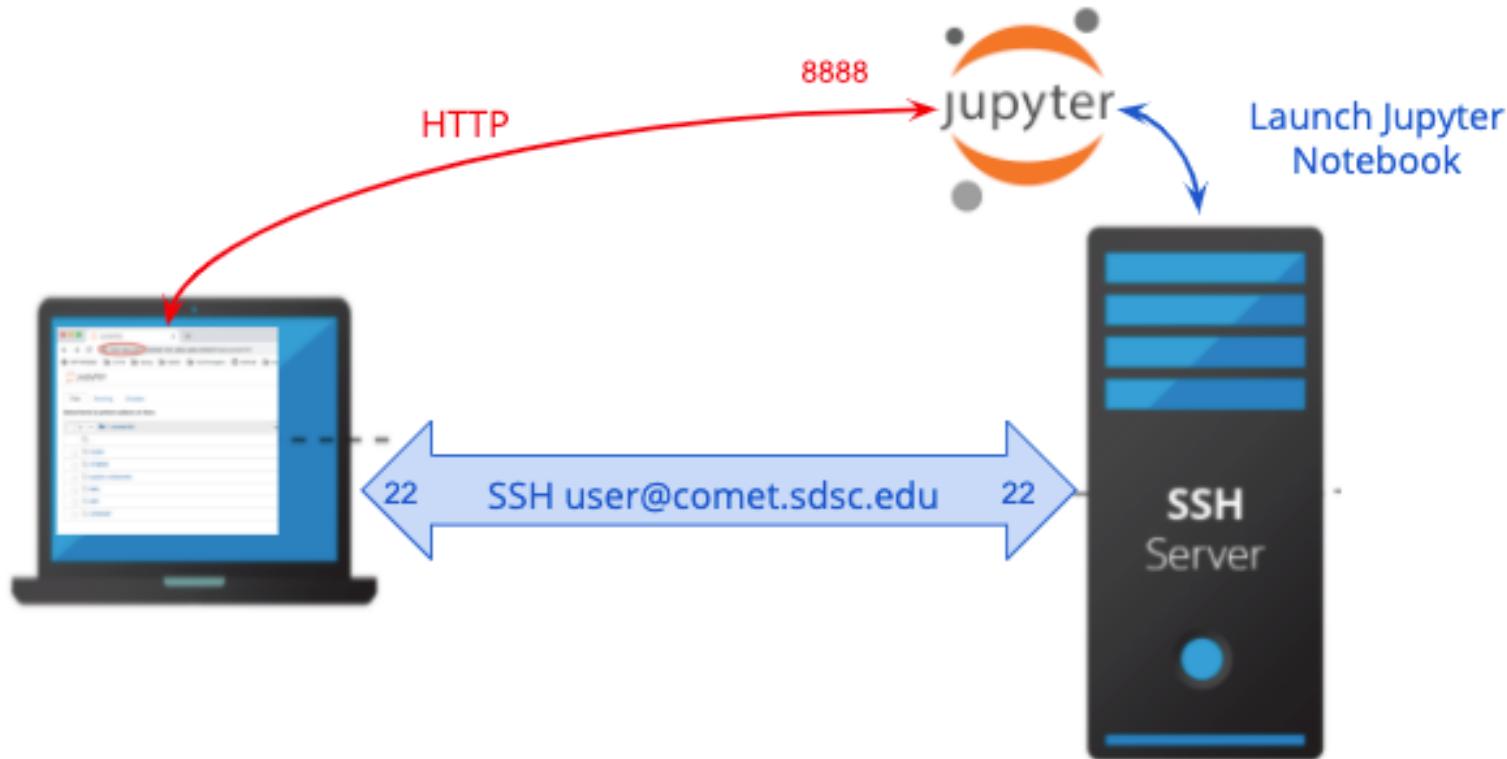
- Portals, JupyterHub, and other services cannot be mounted directly to disk (must be on VM or external)
 - Many use root in vulnerable ways
 - If a user launches Jupyter Lab or Notebooks, the jobs will be killed.
- No applications can run on login nodes
- **SDSC recommendation:**
 - use secure connections: when you choose unsecure connections your account is vulnerable to hacking



Methods for Running Notebooks on Comet/Expanse

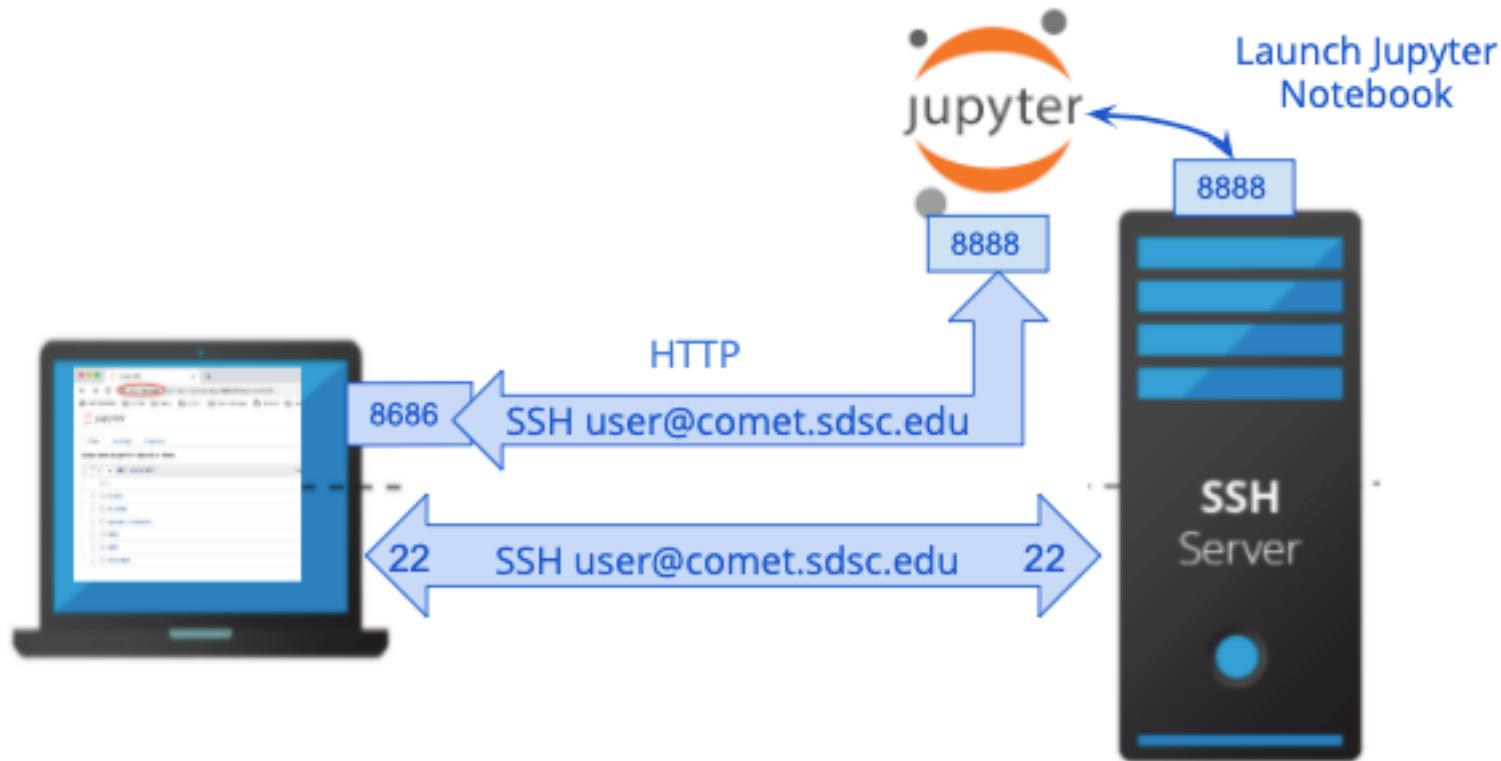
- Connection scenarios:
 - Connection to Notebook over HTTP (insecure)
 - Connection to Notebook over SSH tunneling (secure, but inconvenient)
 - Connection to Notebook over HTTPS using the [Reverse Proxy Service](#) (very secure) [Beta testing]
 - Coming Soon: Galileo remote notebook launcher
- SDSC allows Jupyter Services to be run on the following nodes:
 - Interactive node
 - Compute node
 - GPU node

Connection over HTTP (unsecure)



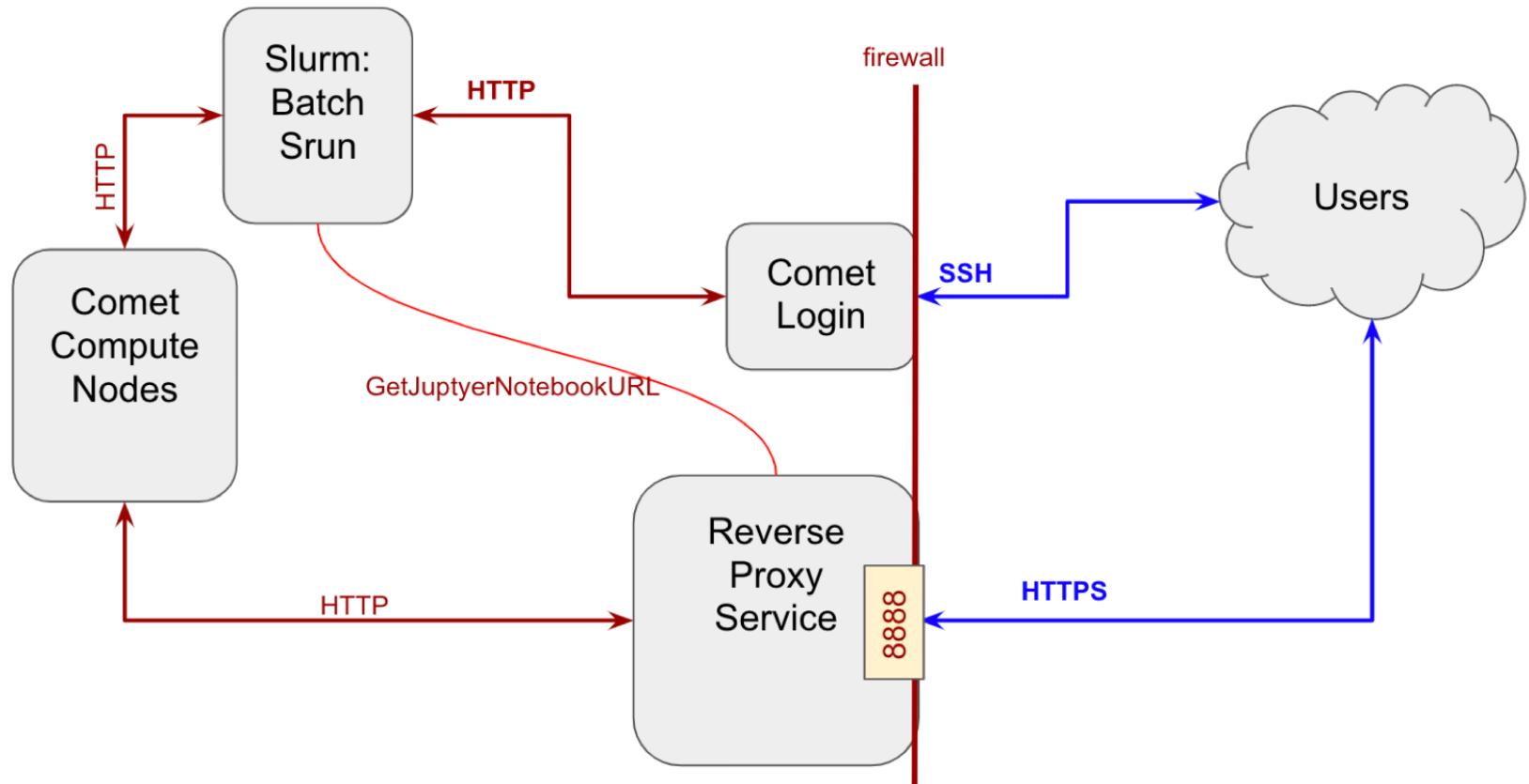
Secure Connection over SSH Tunneling

(secure but inconvenient and unstable)



For instructions on how to set up SSH Tunneling, see:
<https://comet-notebooks-101.readthedocs.io/en/master/methods/tunneling.html>

SDSC Reverse Proxy Service (RPS) (secure, convenient and stable)



Documentation: <https://hpc-training.sdsc.edu/notebooks-101/>

GitHub Repo: <https://github.com/sdsc-hpc-training-org/reverse-proxy>

SDSC Reverse Proxy Service Usage

- Using RPS is very simple and requires no tunneling and is secure (produces HTTPS URLs).
- To use JRPS:
 - SSH to an Expanse login node: `login.expanse.sdsc.edu`
 - Clone the Repo:
`git clone https://github.com/sdsc-hpc-training-org/reverse-proxy.git`
 - Check your software environment on the login node: conda, Jupyter (notebooks, lab), and other Python packages needed for you application.
- See installation instructions:
 - <https://hpc-training.sdsc.edu/notebooks-101/notebook-101.html#software-prerequisites>

Install Reverse Proxy Scripts

```
[user@login01 ~]$ git clone https://github.com/sdsc-hpc-training-org/reverse-proxy.git
Cloning into 'reverse-proxy'...
remote: Enumerating objects: 265, done.
remote: Counting objects: 63% (167/265)
remote: Counting objects: 100% (265/265), done.
remote: Compressing objects: 100% (167/167), done.
remote: Total 969 (delta 163), reused 192 (delta 97), pack-reused 704
Receiving objects: 100% (969/969), 7.60 MiB | 16.28 MiB/s, done.
Resolving deltas: 100% (553/553), done.
[user@login01 ~]$ Cloning into 'reverse-proxy'...
-bash: Cloning: command not found
[user@login01 ~]$
[user@login01 ~]$ cd reverse-proxy/
[user@login01 reverse-proxy]$ ls -al
total 118
drwxr-xr-x  9 user abc123  14 Mar  4 06:47 .
drwxr-x--- 28 user abc123  48 Mar  4 06:47 ..
drwxr-xr-x  2 user abc123   4 Mar  4 06:47 batch
-rw-r--r--  1 user abc123  588 Mar  4 06:47 .config
-rw-r--r--  1 user abc123 6148 Mar  4 06:47 .DS_Store
drwxr-xr-x  2 user abc123   5 Mar  4 06:47 .examples_images
drwxr-xr-x  8 user abc123  13 Mar  4 06:47 .git
-rw-r--r--  1 user abc123  12 Mar  4 06:47 .gitignore
drwxr-xr-x  2 user abc123   9 Mar  4 06:47 lib
-rw-r--r--  1 user abc123 5981 Mar  4 06:47 README.md
drwxr-xr-x  2 user abc123   5 Mar  4 06:47 slurm
drwxr-xr-x  2 user abc123   4 Mar  4 06:47 slurm_expanse
-rwxr-xr-x  1 user abc123 9555 Mar  4 06:47 start-jupyter
drwxr-xr-x  2 user abc123   4 Mar  4 06:47 torque
```

Usage

The `start-jupyter` script performs the following tasks:

- Sends request to the reverse proxy server (RPS) to get a one-time token and a port number
- Launches the `jupyter service` command using the token and port number.
- Prints a secure URL (`https`) containing the token to the terminal, so that the user can copy/paste the URL into a local browser.

```
./start-jupyter [-p <string>] [-d <string>] [-A <string>] [-b <string>] [-t time] [-i]
```

- -p: the partition to wait for (debug or compute). Default Partition is "compute"
- -d: the top-level directory of your Jupyter notebook. Default Dir is /home/\$USER
- -A: the project allocation to be used for this notebook. Default Allocation is your sbatch system default allocation (also called project or group)
- -b: the batch script you want to submit with your notebook. Only those in the `batch` folder are supported. Default batch script is ./batch/batch_notebook.sh
- -t: the time to run the notebook. Your account will be charged for the time you put here so be careful. Default time is 30 minutes.
- -i: Get extra information about the job you submitted using the script.

Using start-jupyter

base == active conda env

(1) Launch start-notebook process

```
(base) [user@comet-ln3 reverse-proxy]$ ./start-jupyter -b slurm/jupyterlab.sh
Your notebook is here:
https://headscarf-barber-unframed.comet-user-content.sdsc.edu?token=3b587a19a8c4ba79f3af754e9fa2a8f5
```

Using default partition: compute
No time given. Default is 30 mins

```
(base) [user@comet-ln3 reverse-proxy]$ cat slurm/jupyterlab.sh
#!/bin/bash
## =====
## This is an example batch script which can be submitted as part of a
## reverse proxy jupyter notebook. This batch script creates the jupyter
## notebook on a compute node, while the start notebook script is used to
## submit this batch script. You should never submit this batch script on
## its own, e.g. `sbatch batch_notebook.sh`. Don't do that :). You can
## specify this particular batch script by using the -b flag, e.g.
## start_notebook.sh -b batch/batch_notebook.sh
## =====
## You can add your own slurm directives here, but they will override
## anything you gave to the start_notebook script like the time_partition, etc.
## ATCH --nodes=1
## ATCH --ntasks-per-node=24
##### Define modules here. #####

```

(2) start-notebook builds batch script and submits job to Slurm queue; prints out the URL.

Comet Reverse Proxy Service

Phase 2 of 2: Mapped

Your job has started and checked in with the proxy. Please wait up to two minutes for the URL mapping to take effect.

Seconds to auto-reload: 4

Stop Reloading

(3) Grab URL, enter into browser. Monitor status window:
If the queue is busy this may take a long time

File Edit View Run Kernel Tabs Settings Help

hello_world.ipynb

remember to activate your Conda environment before running this notebook

```
(base) [mthomas@comet-12-66 reverse-proxy]$ ls
total 146
drwxr-xr-x 8 mthomas use300 18 Oct 29 13:17 .
drwxr-xr-x 3 mthomas use300 3 Oct 12 14:44 ..
drwxr-xr-x 2 mthomas use300 4 Oct 12 14:44 batch
-rw-r--r-- 1 mthomas use300 6148 Oct 12 14:44 .DS_Store
drwxr-xr-x 2 mthomas use300 5 Oct 12 14:44 examples_images
drwxr-xr-x 8 mthomas use300 15 Oct 29 03:11 .git
-rw-r--r-- 1 mthomas use300 12 Oct 12 14:44 .gitignore
drwxr-xr-x 2 mthomas use300 6 Oct 12 14:44 lib
-rw-r--r-- 1 mthomas use300 5049 Oct 12 14:44 README.md
drwxr-xr-x 2 mthomas use300 4 Oct 12 14:44 slurm
-rw-r--r-- 1 mthomas use300 1309 Oct 12 15:15 slurm-36369149.out
use300 1855 Oct 29 03:59 slurm-36708798.out
use300 1820 Oct 29 04:06 slurm-36708915.out
use300 1424 Oct 29 2020 slurm-36718821.out
use300 7076 Oct 12 14:44 start-jupyter
use300 7585 Oct 12 14:44 start_notebook
use300 4 Oct 12 14:44 torque
use300 200 Oct 12 14:44 .tmp

```

(4) When notebook is ready on compute node, Jupyter service will appear in your browser

II exit 1

token&port=\$PORT"

```
-12-66 reverse-proxy]$ host
-12-66 reverse-proxy]$ 
```

(5) When done, be sure to QUIT the Jupyter service – this will kill the job.

Security Note:

- The URL is like a password: DO NOT SHARE.
- The Jupyter service will run for as long as you requested. If you are done early, be sure to QUIT the notebook to save SU's

Using Reverse Proxy from Expanse Portal: Terminal Window

Comet Portal Files Jobs Clusters Interactive Apps

Home / My Interactive Sessions

Interactive Apps

GUIs

MATLAB

RSTUDIO

You have no active sessions.

(1) Log onto the Portal

Last login: Thu Oct 29 13:19:01 2020 from 76.176.117.51
Rocks 7.0 (Manzanita)
Profile built 13:03 03-Dec-2019
Kickstarted 14:18 03-Dec-2019

WELCOME TO

NOTICE:
The Comet login nodes are not to be used for running processing tasks.
This includes running Jupyter notebooks and the like. All processing
jobs should be submitted as jobs to the batch scheduler. If you don't
know how to do that see the Comet user guide
https://www.sdsc.edu/support/user_guides/comet.html#running.
Any tasks found running on the login nodes in violation of this policy
may be terminated immediately and the responsible user locked out of
the system until they contact user services.

(2) Launch a terminal window

jupyter

Select items to perform actions on them.

Name	Last Modified	File size
bigdatafiles	2 years ago	
comet-dev-old	9 months ago	
comet-examples	3 months ago	
comet-examples-OLD	6 months ago	
covabmc	2 months ago	
covABMClone	2 months ago	
cuda	a year ago	
dev	a month ago	
gnuplot	a month ago	
gpu-hackathon-notes	5 months ago	
hackathon	7 months ago	
hello-mpi		

(3) Copy the URL

(5) Access your Jupyter Service

Comet Reverse Proxy Service

Phase 1 of 2: Pending

Waiting for your job to start on a compute node...

Seconds to auto-reload: 4

Stop Reloading

(4) Monitor status window:
If the queue is busy this may take a long time

Thank You

Resources

- Expanse User Guide
 - https://www.sdsc.edu/support/user_guides/expanse.html
- GitHub Repo for this workshop:
 - <https://github.com/sdsc-hpc-training-org/comet-to-expanse-transition/tree/main/2021-Comet-to-Expanse-Transition-Tutorial>
- GitHub Repo for Expanse Notebooks:
 - <https://hpc-training.sdsc.edu/notebooks-101/>
- SDSC Training Resources
 - https://www.sdsc.edu/education_and_training/training
 - <https://github.com/sdsc-hpc-training/webinars>
- XSEDE Training Resources
 - <https://www.xsede.org/for-users/training>
 - <https://cvw.cac.cornell.edu/expanse/>