Things to Do While You are Waiting

- Open your web browser and visit hprc.tamu.edu
- Log into TAMU VPN (if you're off campus) and reconnect to Zoom
- If you don't have an HPRC account, please ask*

*speak up in chat or email help@hprc.tamu.edu

Introduction to Scientific Python

with exercises using HPRC Portal

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Outline

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- Getting Started
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- Break
- Python Exercises
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Usage Policies
(Be a good compute citizen)

- It is illegal to share computer passwords and accounts by state law and university regulation
- It is prohibited to use HPRC clusters in any manner that violates the United States export control laws and regulations, EAR & ITAR
- Abide by the expressed or implied restrictions in using commercial software

hprc.tamu.edu/policies

Follow Along

Short course material can be found on the short course page.

https://hprc.tamu.edu/training/intro_scientific_python.html

And on disk on Grace

```
/scratch/training/Scipy
```

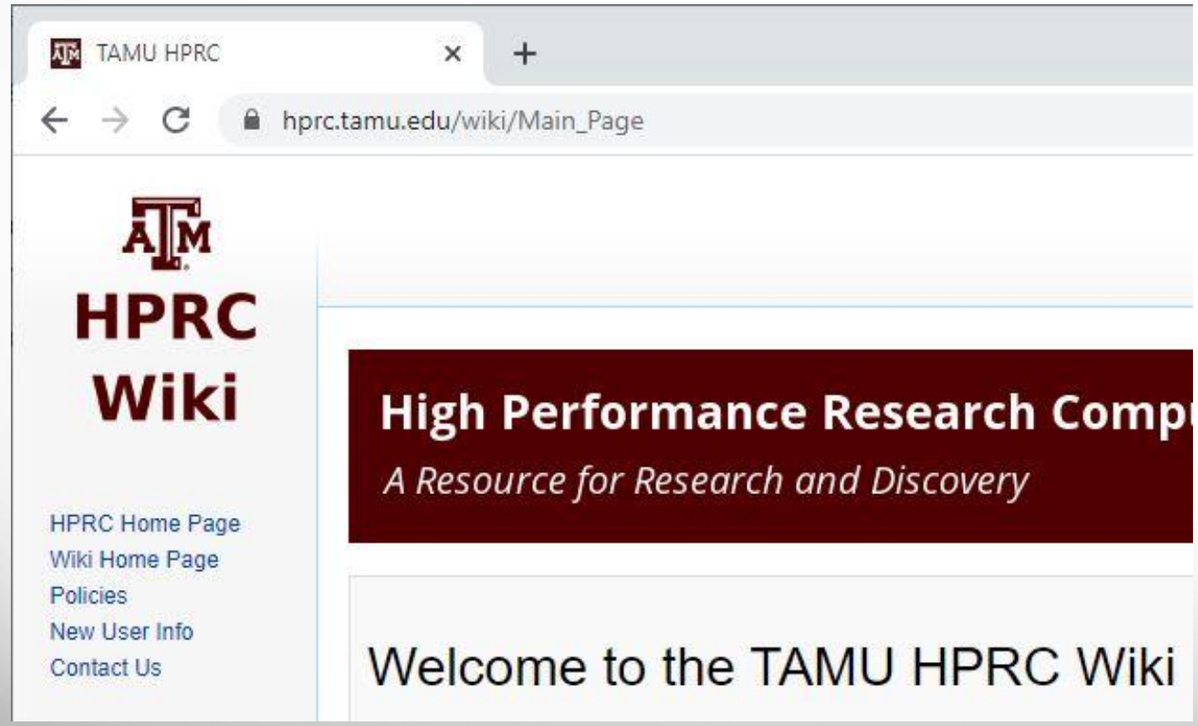
Content from our short courses are covered in the relevant Introduction and Primer videos on our Youtube Channel

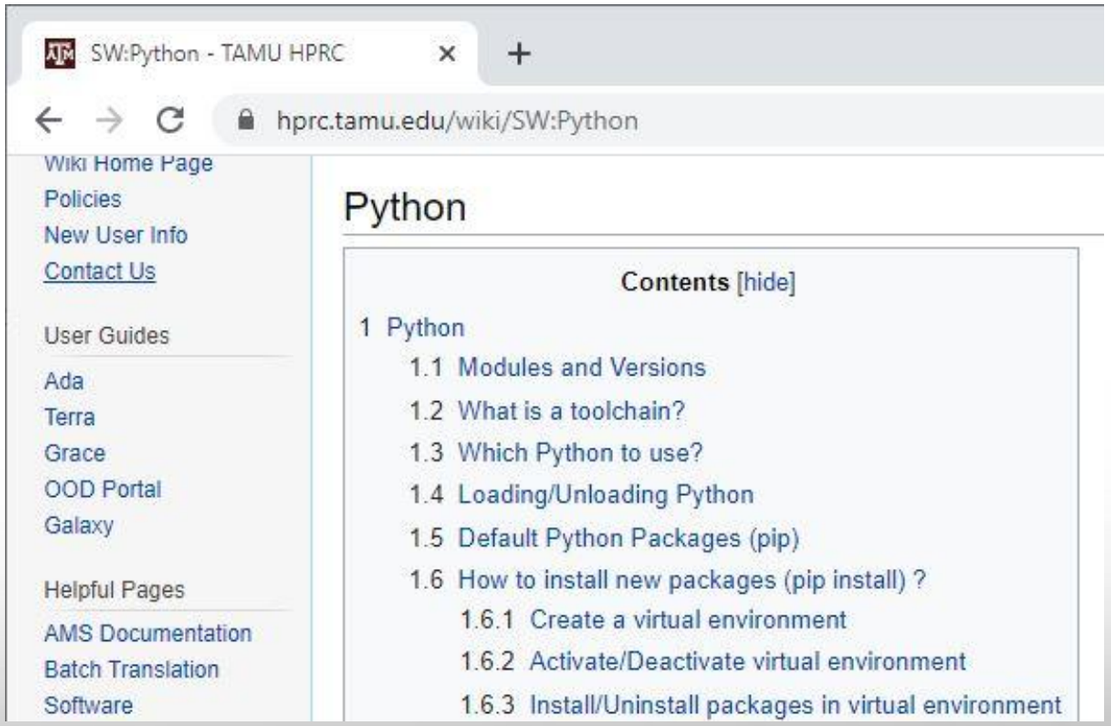
Texas A&M HPRC YouTube Channel

HPRC Wiki - Python

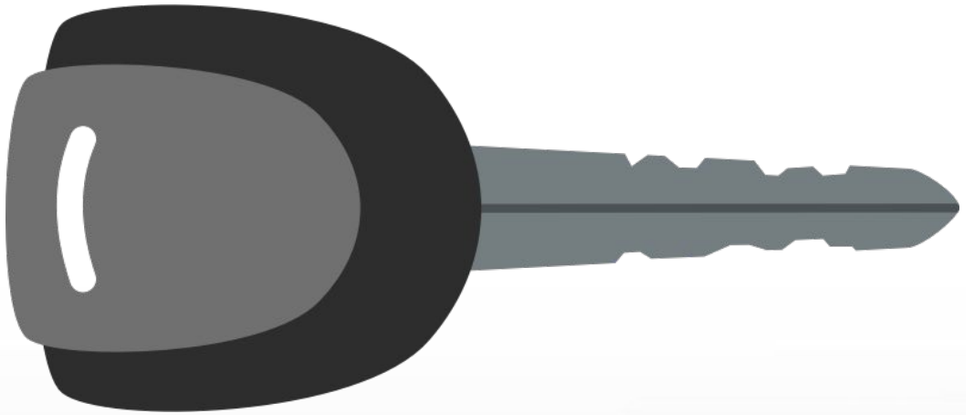
Visit our wiki for frequently asked questions https://hprc.tamu.edu/wiki/Main_Page

For example, information about using Python https://hprc.tamu.edu/wiki/SW:Python





Getting Started



Authentication and Access

Three steps to access HPRC resources.

1. Get a HPRC account
2. VPN to TAMU campus
3. Web login (**Portal**, Globus) through CAS
   or
   SSH/SFTP to HPRC clusters

- Duo NetID two-factor authentication used to enhance security (it.tamu.edu/duo/)
- (Faculty and staff) Use Duo Keys - u.tamu.edu/get_duo_keys
- Instructions in two-factor wiki page (hprc.tamu.edu/wiki/Two_Factor)

Example: SSH login with Duo

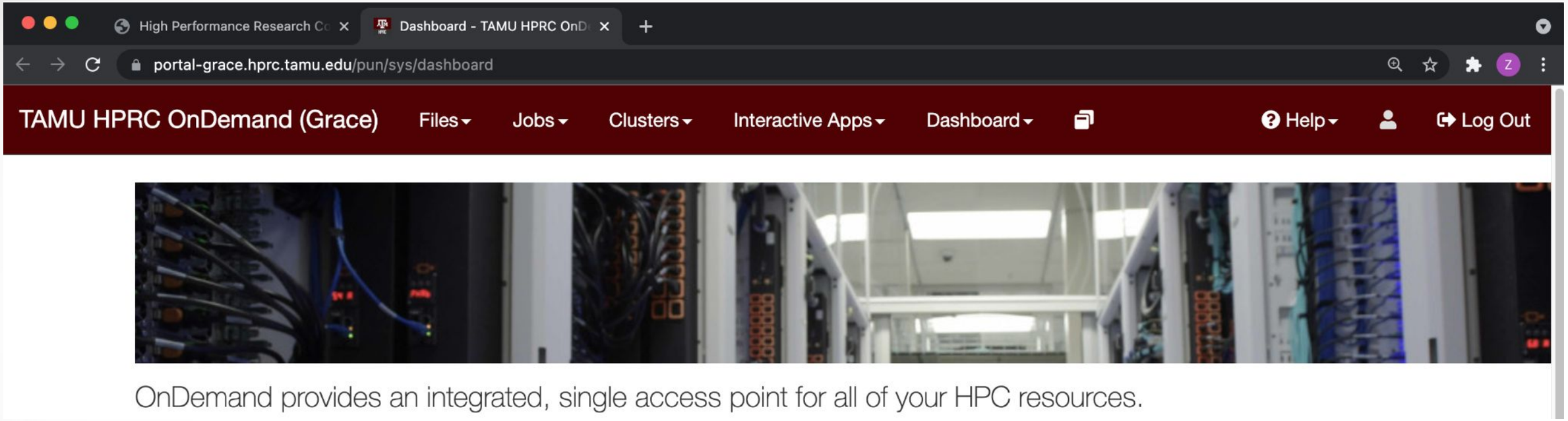
```
$ ssh NetID@grace.hprc.tamu.edu
**************************************************************
…. warning message (snipped) …….
**************************************************************

Password:
Duo two-factor login for UserNetID

Enter a passcode or select one of the following options:

 1. Duo Push to XXX-XXX-1234
 2. Phone call to XXX-XXX-1234
 3. SMS passcodes to XXX-XXX-1234 (next code starts with: 9)

Passcode or option (1-3): 1
Success. Logging you in...
```

Hands-on exercises:

Activate TAMU VPN
Go to:
portal.hprc.tamu.edu

Once you have logged in, respond to a poll

portal.hprc.tamu.edu



- Files > copy and edit files on the cluster's filesystems
- Jobs > submit and monitor cluster jobs
- Clusters > open a shell terminal (command line) on a login node
- Interactive Apps > start graphical software on a compute node and connect to it
- Dashboard > view file quotas and computing account allocations

Hands-on exercise:

Copy files to your scratch directory

Files > /scratch/user/<netid>

Click 

Execute

```
$ cp -r /scratch/training/Scipy .
```

(...or your favorite copy method)

Launch Interactive Apps

Navigate

- Interactive Apps > Jupyter Notebook

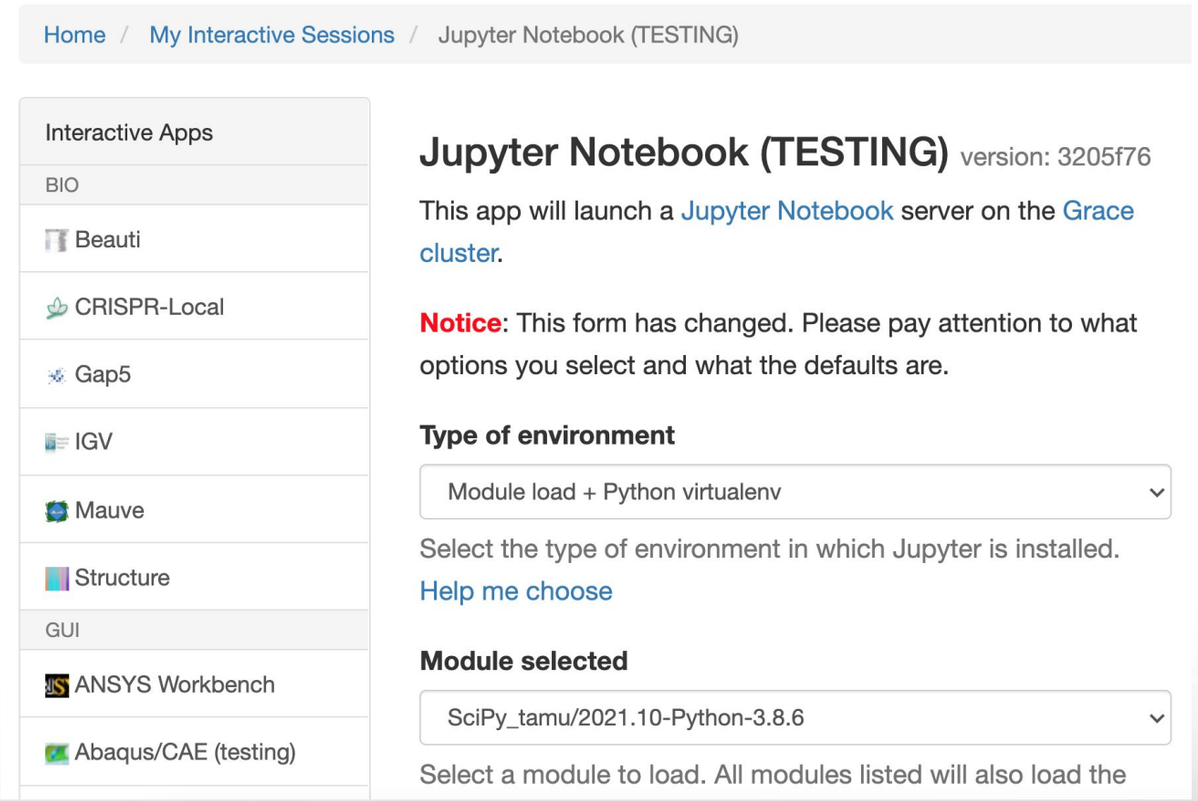
Choose a Type of environment

- `Module load + Python virtualenv`

Choose a module

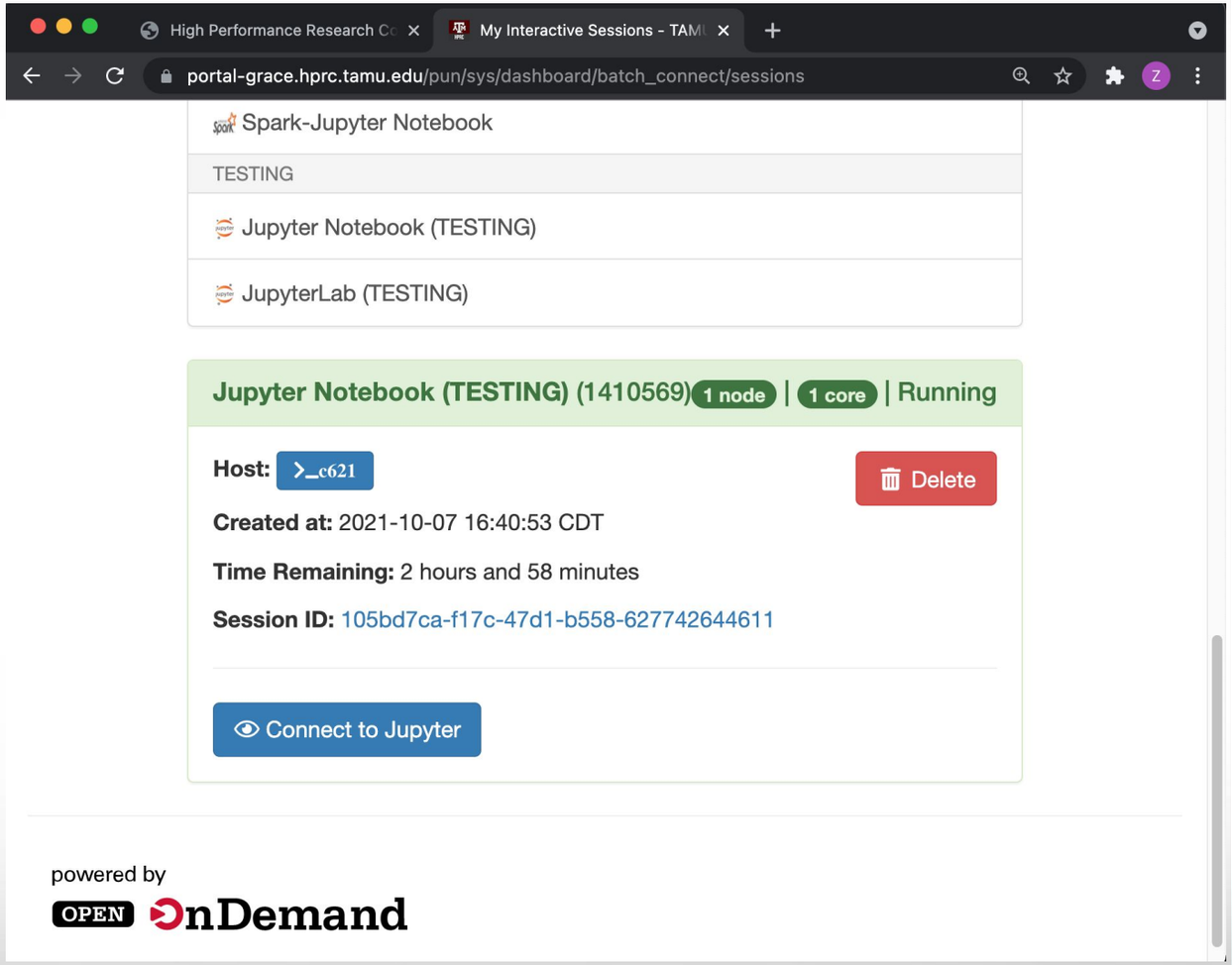
- `SciPy_tamu/2021...`

Launch



Connect to Interactive Apps

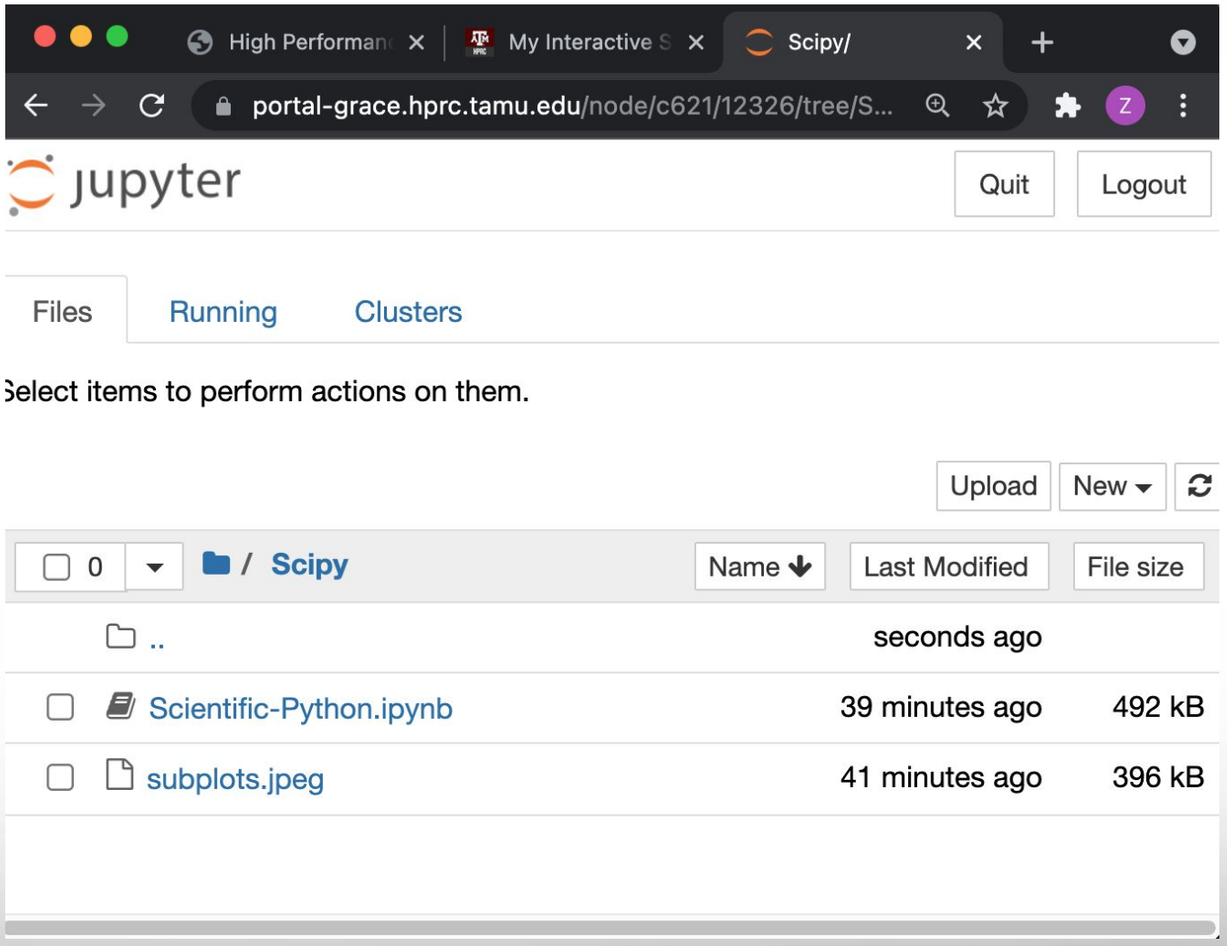
- Portal submits a job to the cluster, which runs on a compute node.
- Wait (about minute), Refresh page, Connect to Jupyter.



Interactive Apps

Jupyter starts in a File Browser. Navigate to the `Scipy` directory you copied to your scratch space.

Click the file name Scientific_Python.ipynb to open the Notebook.



Hands-on exercises:
Launch a Jupyter Notebook

Once you have the notebook open,
respond to a poll

Scientific Python

(continued in Python Notebook)

Need Help?

- Try these:
  - First check the FAQ hprc.tamu.edu/wiki/HPRC:CommonProblems
  - Also try the Terra User Guide hprc.tamu.edu/wiki/Terra
  - Email your questions to **help@hprc.tamu.edu**. (Managed by a ticketing system)
- Help us, help you -- we need more info
  - Which Cluster
  - UserID/NetID (*UIN is not needed!*)
  - Job id(s) if any
  - Location of your jobfile, input/output files
  - Application used if any
  - Module(s) loaded if any
  - Error messages
  - Steps you have taken, so we can reproduce the problem
- Or visit us @ 114A Henderson Hall (Making an appointment is recommended.)

Thank you.

Please fill out the post-course Survey.

Questions?