

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

- Usage Policies
- References
- Getting Started
- Break
- Python Exercises
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- Python Exercises
- Need Help?

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 Terra

```
/scratch/training/SciPy
```

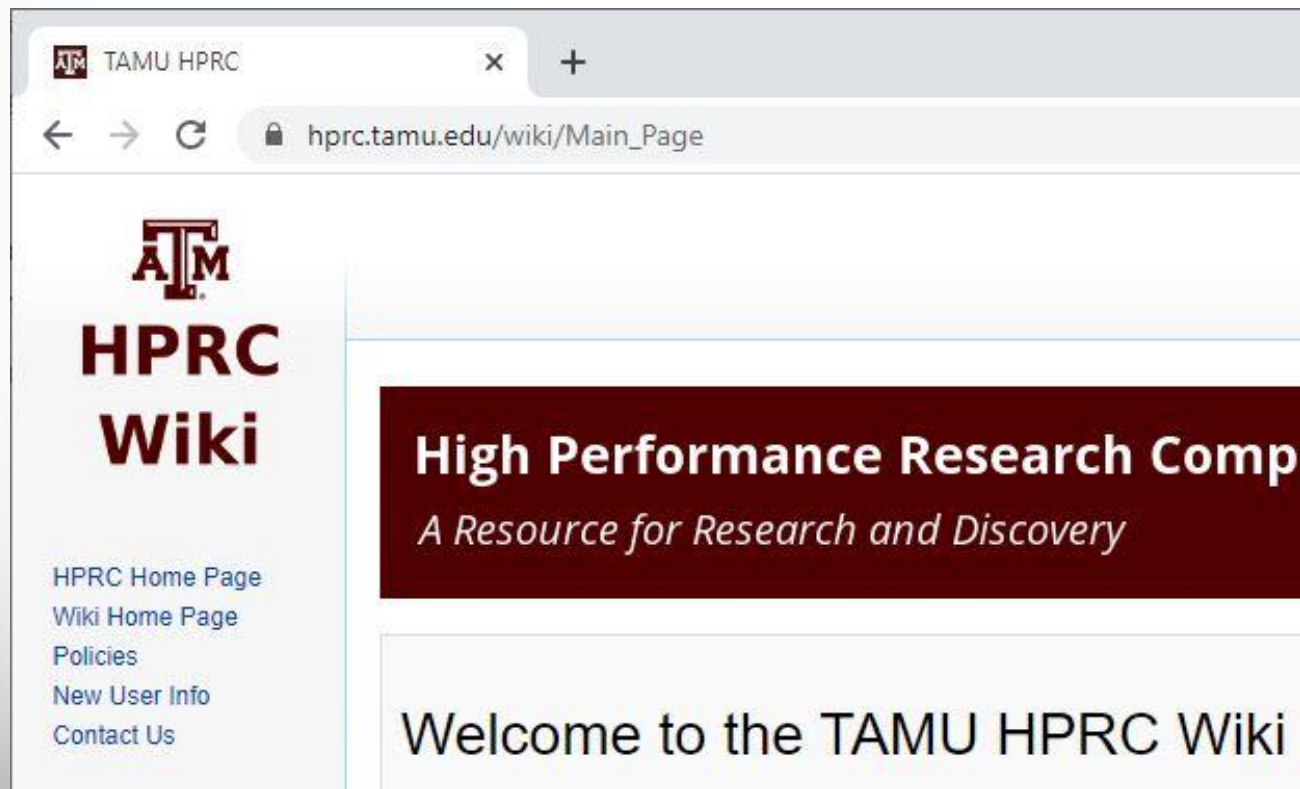
Content from our shortcourses are covered in the relevant Introduction and Primer videos on our Youtube Channel

[youtube.com channel "Texas A&M HPRC"](https://www.youtube.com/channel/UC...)

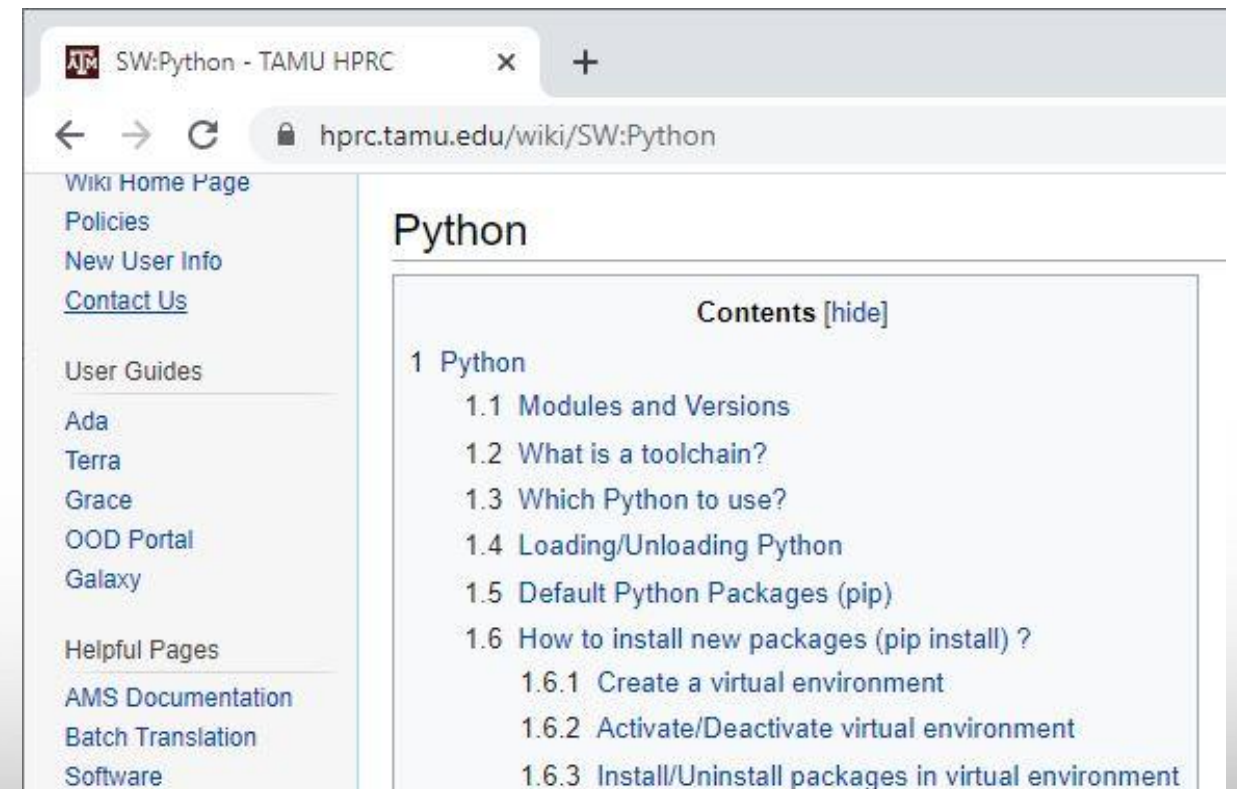
HPRC Wiki - Python

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>



The screenshot shows the main page of the TAMU HPRC Wiki. The browser address bar displays 'hprc.tamu.edu/wiki/Main_Page'. On the left, there is a navigation menu with links to 'HPRC Home Page', 'Wiki Home Page', 'Policies', 'New User Info', and 'Contact Us'. The main content area features the TAMU HPRC Wiki logo and a dark red banner with the text 'High Performance Research Computing' and 'A Resource for Research and Discovery'. Below the banner, it says 'Welcome to the TAMU HPRC Wiki'.



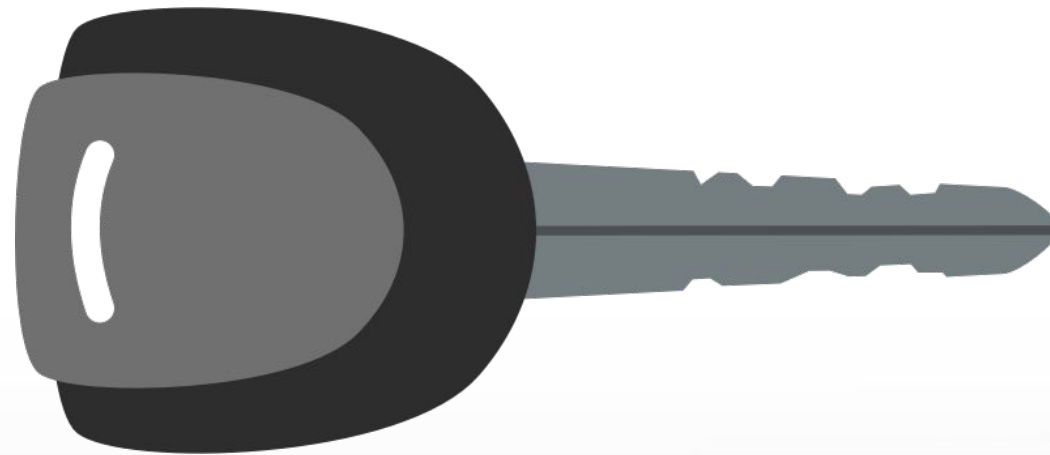
The screenshot shows the 'SW:Python' page on the TAMU HPRC Wiki. The browser address bar displays 'hprc.tamu.edu/wiki/SW:Python'. On the left, there is a navigation menu with links to 'Wiki Home Page', 'Policies', 'New User Info', 'Contact Us', 'User Guides', 'Ada', 'Terra', 'Grace', 'OOD Portal', 'Galaxy', 'Helpful Pages', 'AMS Documentation', 'Batch Translation', and 'Software'. The main content area is titled 'Python' and contains a 'Contents [hide]' section with a list of links: '1 Python', '1.1 Modules and Versions', '1.2 What is a toolchain?', '1.3 Which Python to use?', '1.4 Loading/Unloading Python', '1.5 Default Python Packages (pip)', and '1.6 How to install new packages (pip install) ?'. Under '1.6', there are three sub-links: '1.6.1 Create a virtual environment', '1.6.2 Activate/Deactivate virtual environment', and '1.6.3 Install/Uninstall packages in virtual environment'.

Further Learning

For further learning on other topics, attend one of our upcoming short courses: <https://hprc.tamu.edu/training/>

Introduction to Quantum Chemistry Simulations with ORCA	Friday, March 12
Drug Docking with Schrodinger	Friday, March 26
Scientific Machine Learning	Friday, March 26
Technology Lab: AI techniques usage - Jupyter Notebook	Friday, April 2 10:00 am
Introduction to Julia	Friday, April 2 1:30 pm
Introduction to Pytorch	Friday, April 16 10:00 am
Introduction to Deep Learning with TensorFlow	Friday, April 16 1:30 pm

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 terra.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:

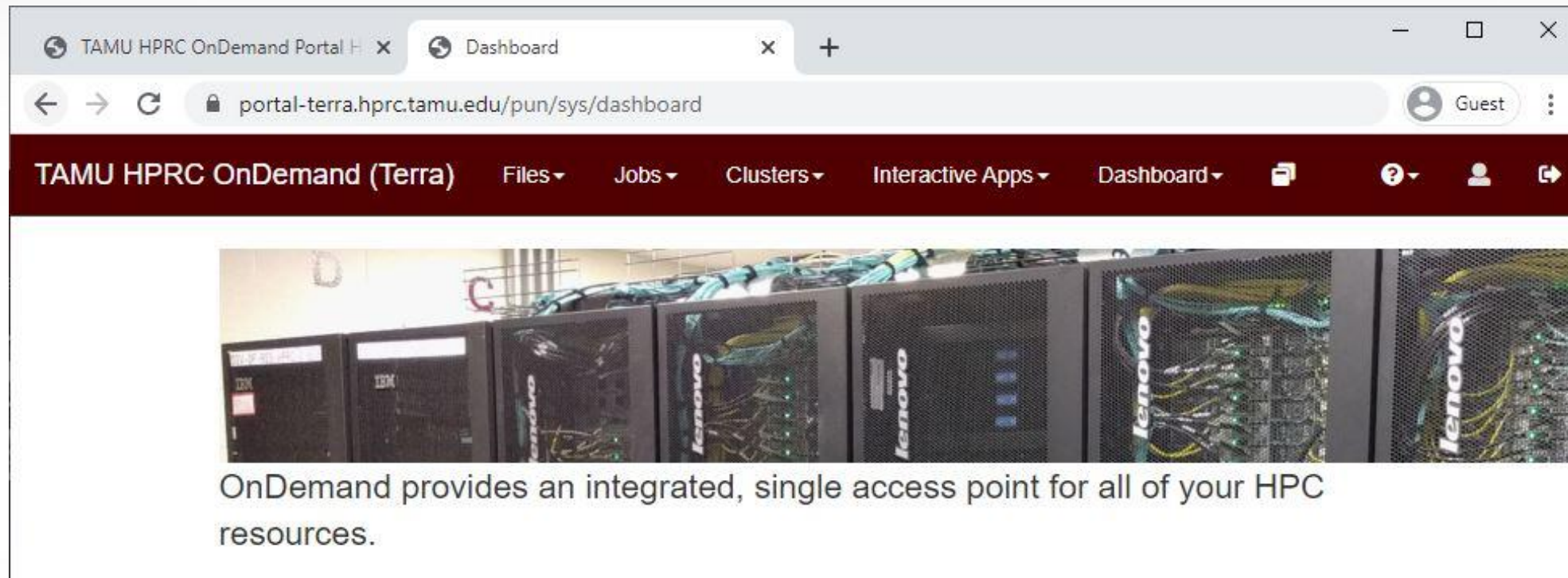
Activate TAMU VPN

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

Menu > Files > /scratch/user/<netid>

Click

>_ Open in Terminal

Execute `$ cp -r /scratch/training/SciPy .`

(...or your favorite copy method)

Launch Interactive Apps

Navigate

- **Menu > Interactive Apps > Servers: Jupyter Notebook**

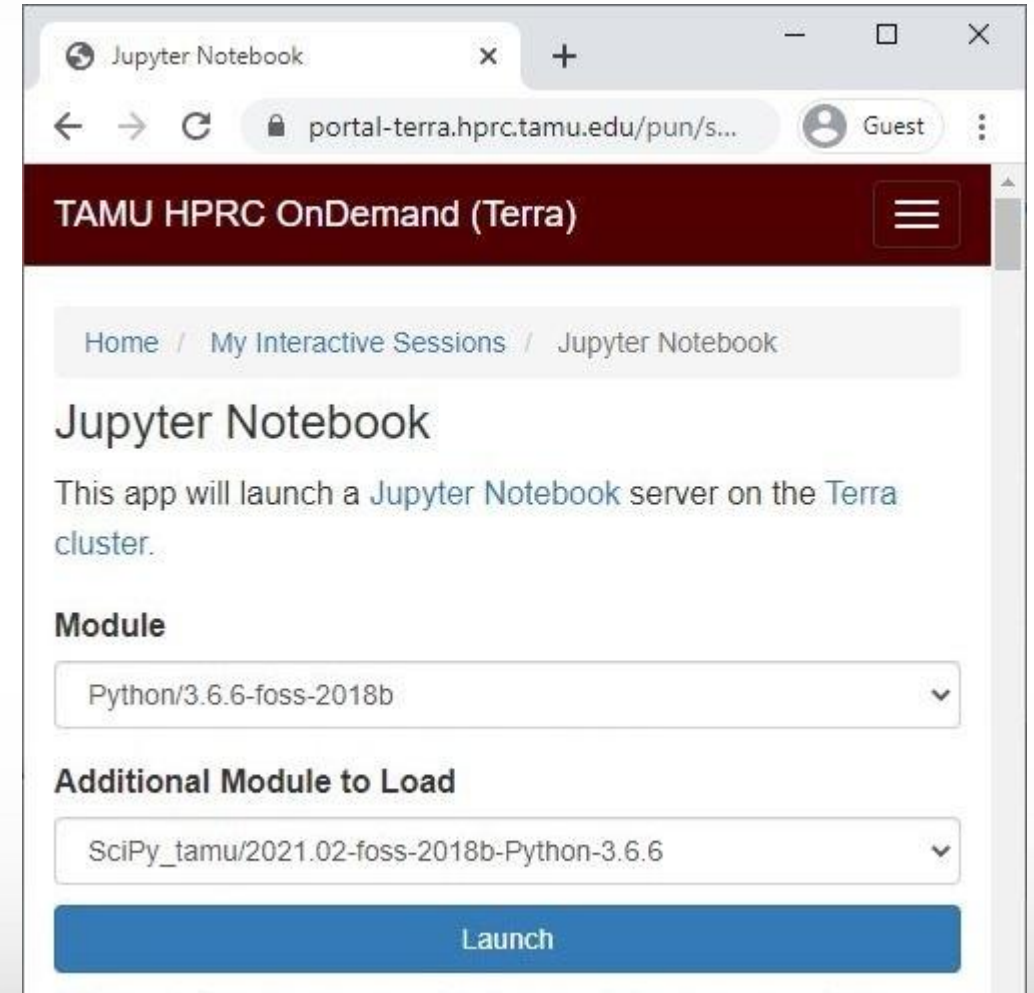
Choose a Python module

- `Python/3.6.6-foss-2018b`

Choose an additional module

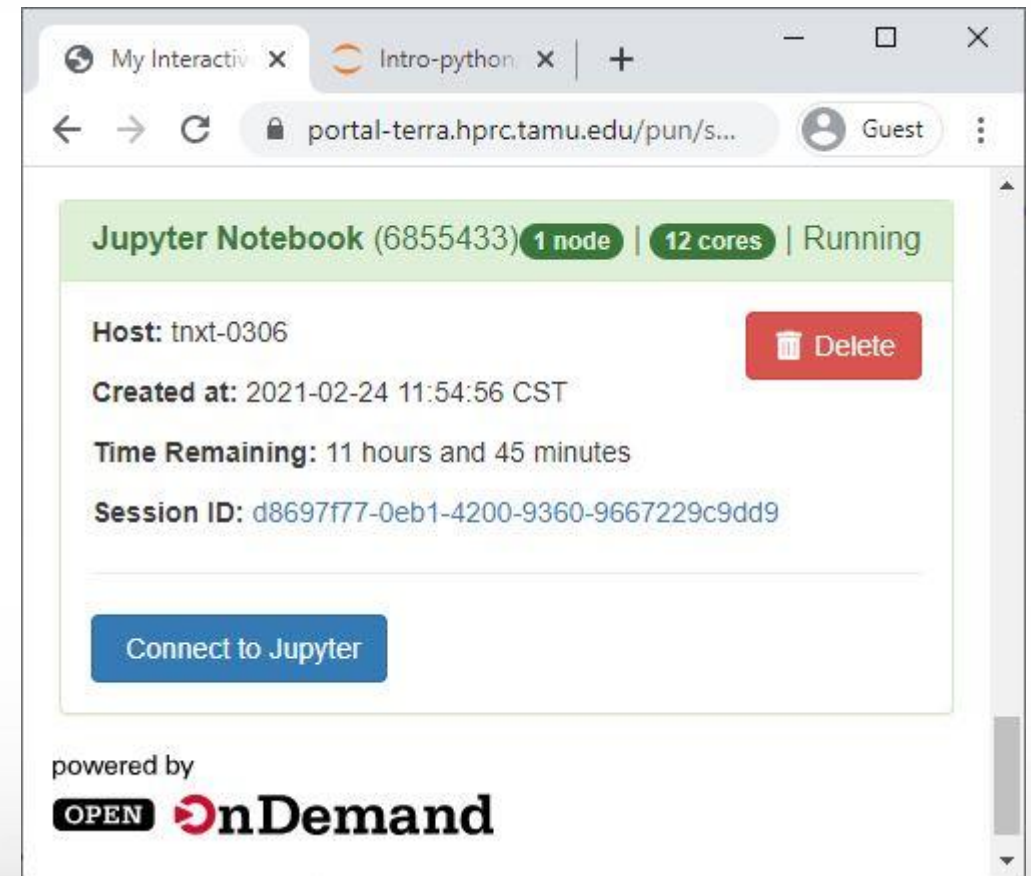
- `SciPy_tamu/2021...`

Launch



Connect to Interactive Apps

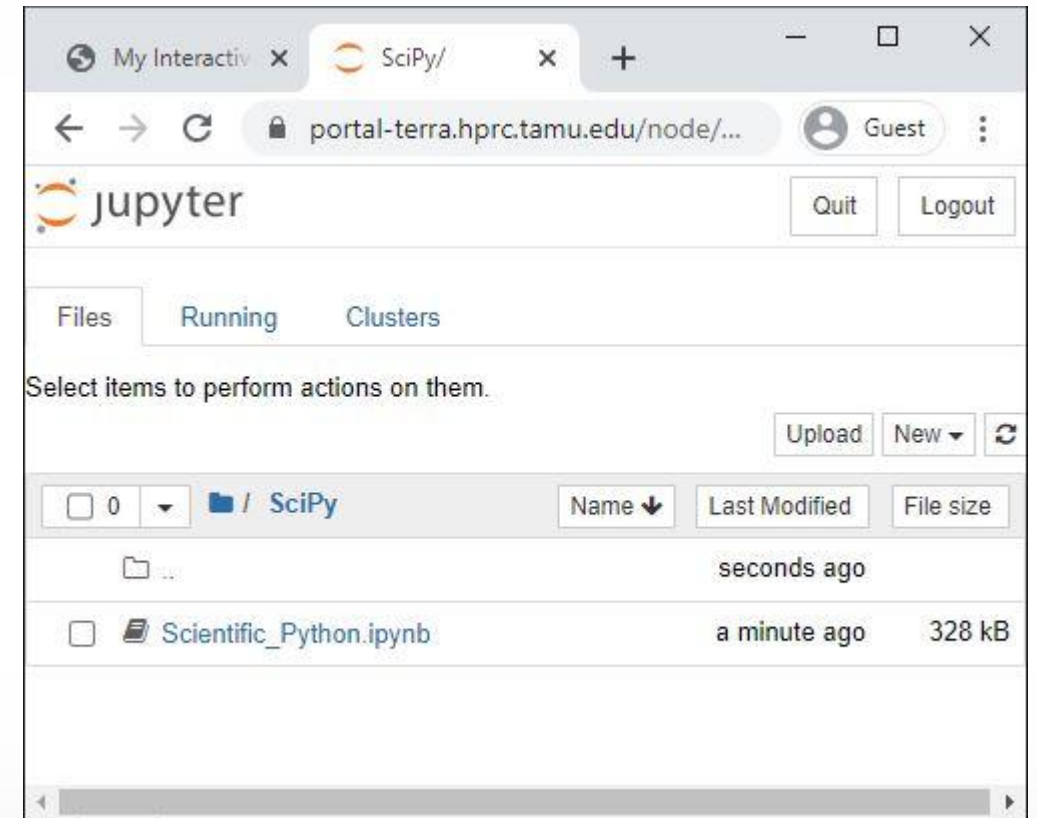
- Portal submits a job to the cluster, which runs on a compute node.
- The job is a Jupyter server. Portal maintains a tunnel.
- Wait (about minute), Refresh page, Connect to Jupyter.



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.)



**HIGH PERFORMANCE
RESEARCH COMPUTING**
TEXAS A&M UNIVERSITY

Thank you.

Please fill out the post-course Survey.

Questions?