

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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- Break
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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
```

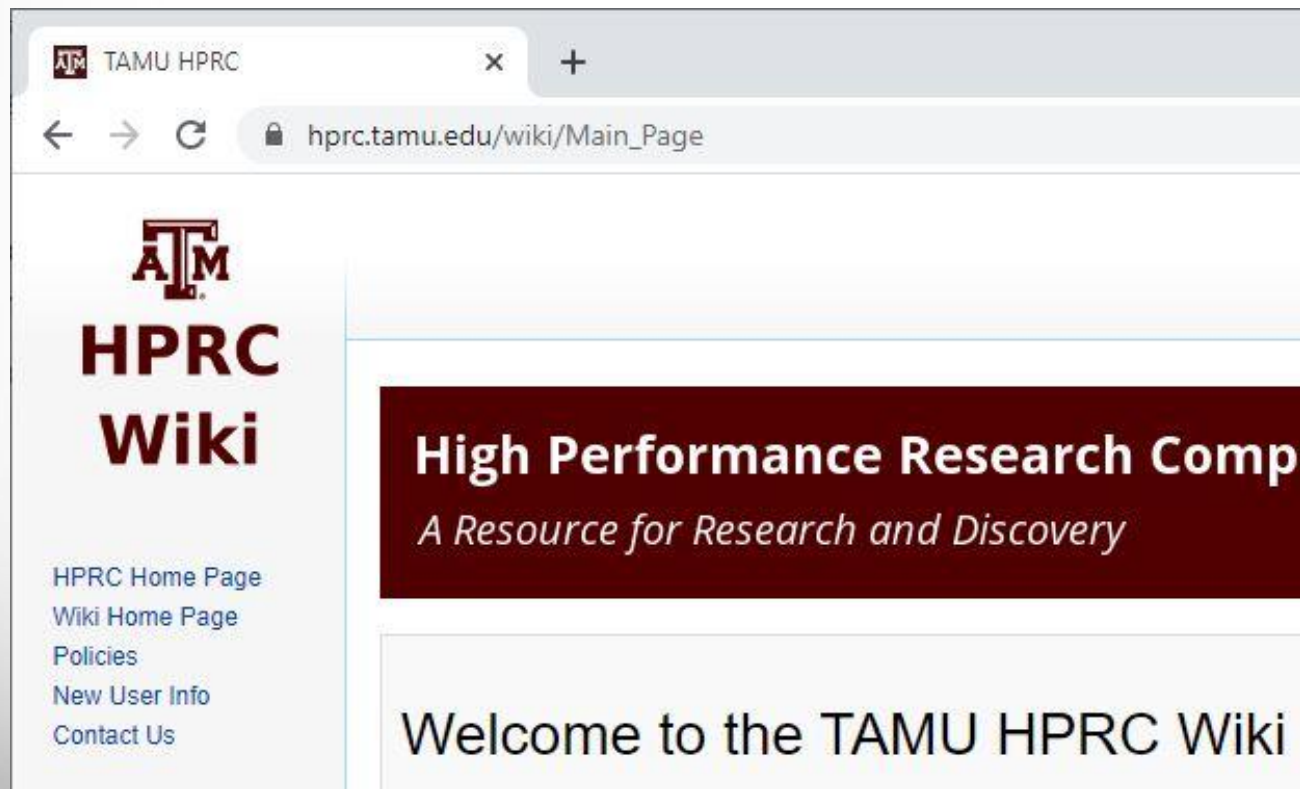
Content from our short courses are covered in the relevant Introduction and Primer videos on our Youtube Channel

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

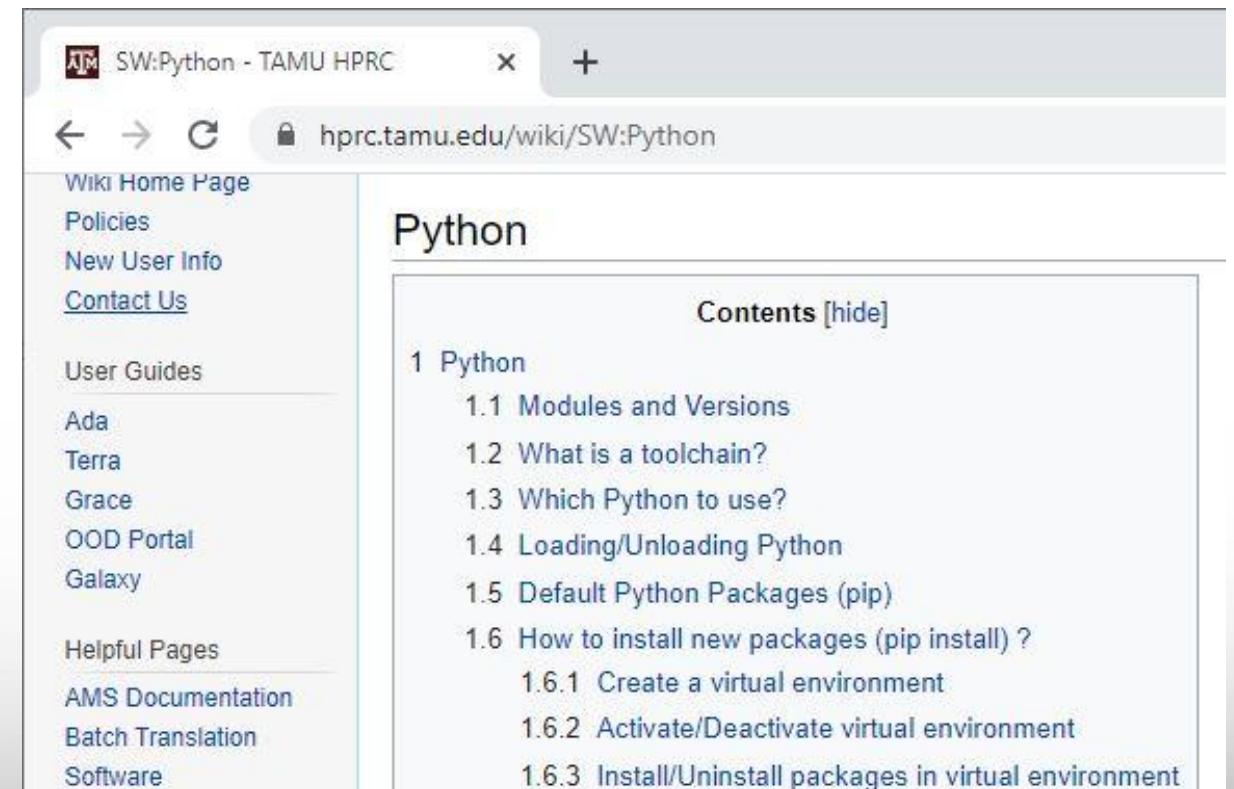
HPRC Wiki - Python

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>

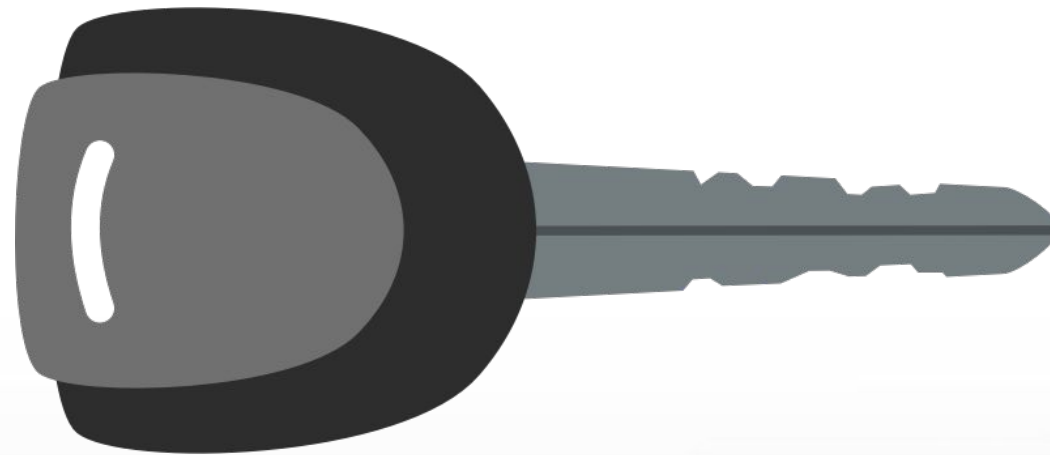


The screenshot shows the main page of the TAMU HPRC Wiki. The browser address bar displays 'hprc.tamu.edu/wiki/Main_Page'. The page features the TAMU HPRC Wiki logo on the left and a central banner with the text 'High Performance Research Computing' and 'A Resource for Research and Discovery'. Below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



The screenshot shows the 'SW:Python' page on the TAMU HPRC Wiki. The browser address bar displays 'hprc.tamu.edu/wiki/SW:Python'. The page has a sidebar on the left with navigation links: '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 includes 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 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'.

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:

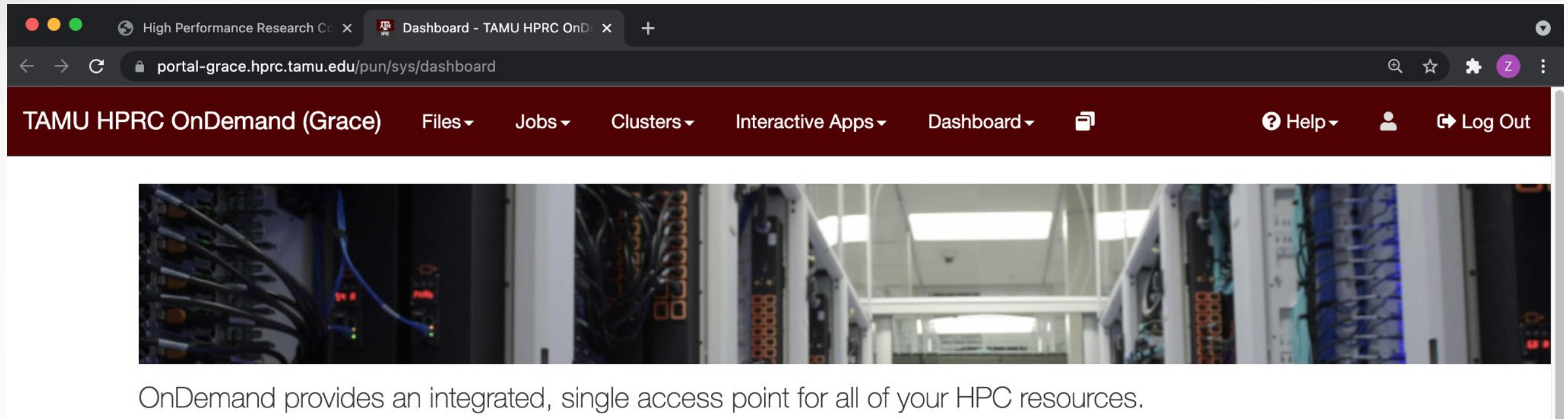
Activate TAMU VPN

Go to:

portal.hprc.tamu.edu

Once you have logged in, respond to a poll

portal.hprc.tamu.edu



TAMU HPRC OnDemand (Grace) Files Jobs Clusters Interactive Apps Dashboard Help Log Out

OnDemand provides an integrated, single access point for all of your HPC resources.

- [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

>_ Open in Terminal

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

(...or your favorite copy method)

Launch Interactive Apps

Navigate

- Interactive Apps > Jupyter Notebook (TESTING)

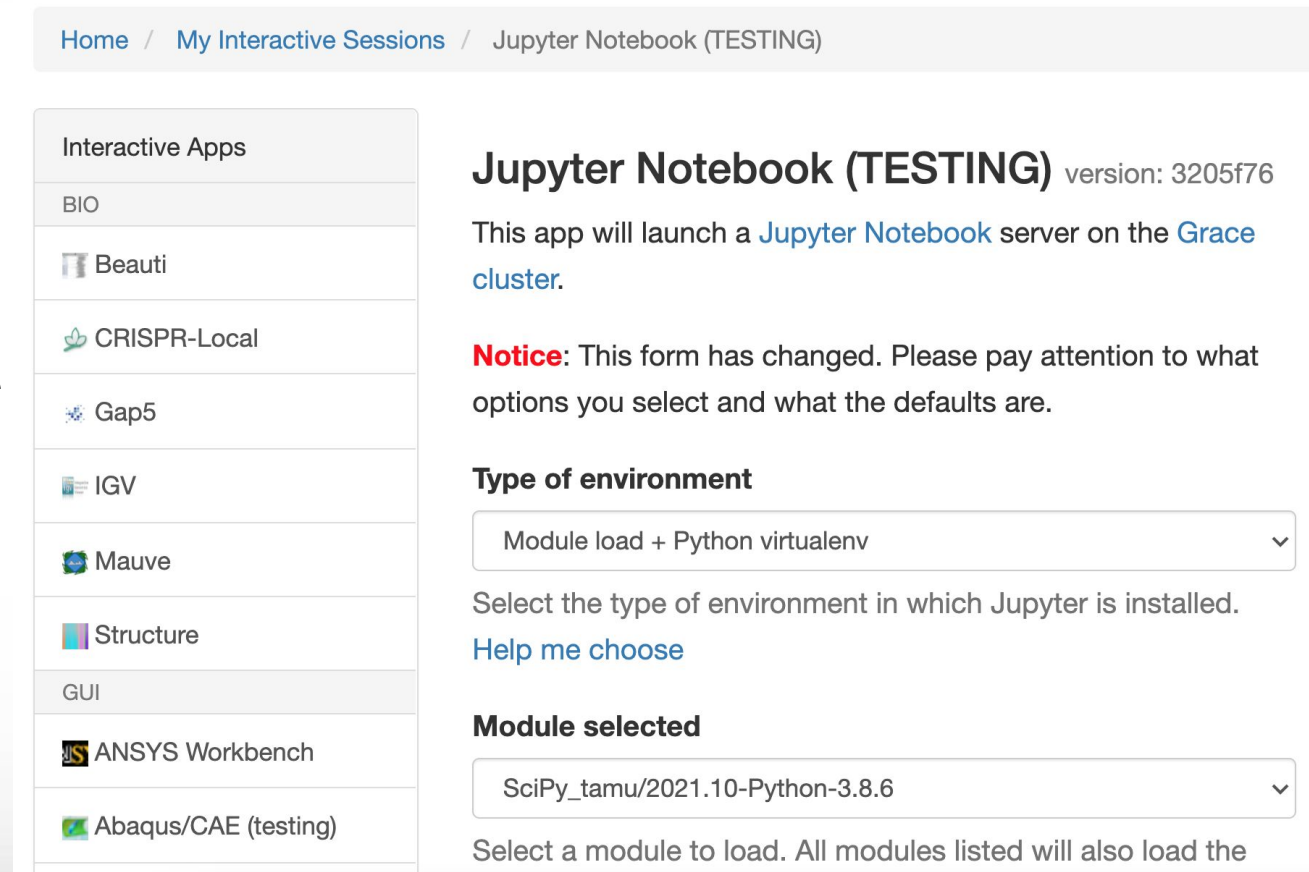
Choose a Type of environment

- Module load + Python virtualenv

Choose a module

- SciPy_tamu/2021...

Launch



Home / My Interactive Sessions / Jupyter Notebook (TESTING)

Interactive Apps

- BIO
- Beauti
- CRISPR-Local
- Gap5
- IGV
- Mauve
- Structure

GUI

- ANSYS Workbench
- Abaqus/CAE (testing)

Jupyter Notebook (TESTING) version: 3205f76

This app will launch a [Jupyter Notebook](#) server on the [Grace cluster](#).

Notice: This form has changed. Please pay attention to what options you select and what the defaults are.

Type of environment

Module load + Python virtualenv

Select the type of environment in which Jupyter is installed.
[Help me choose](#)

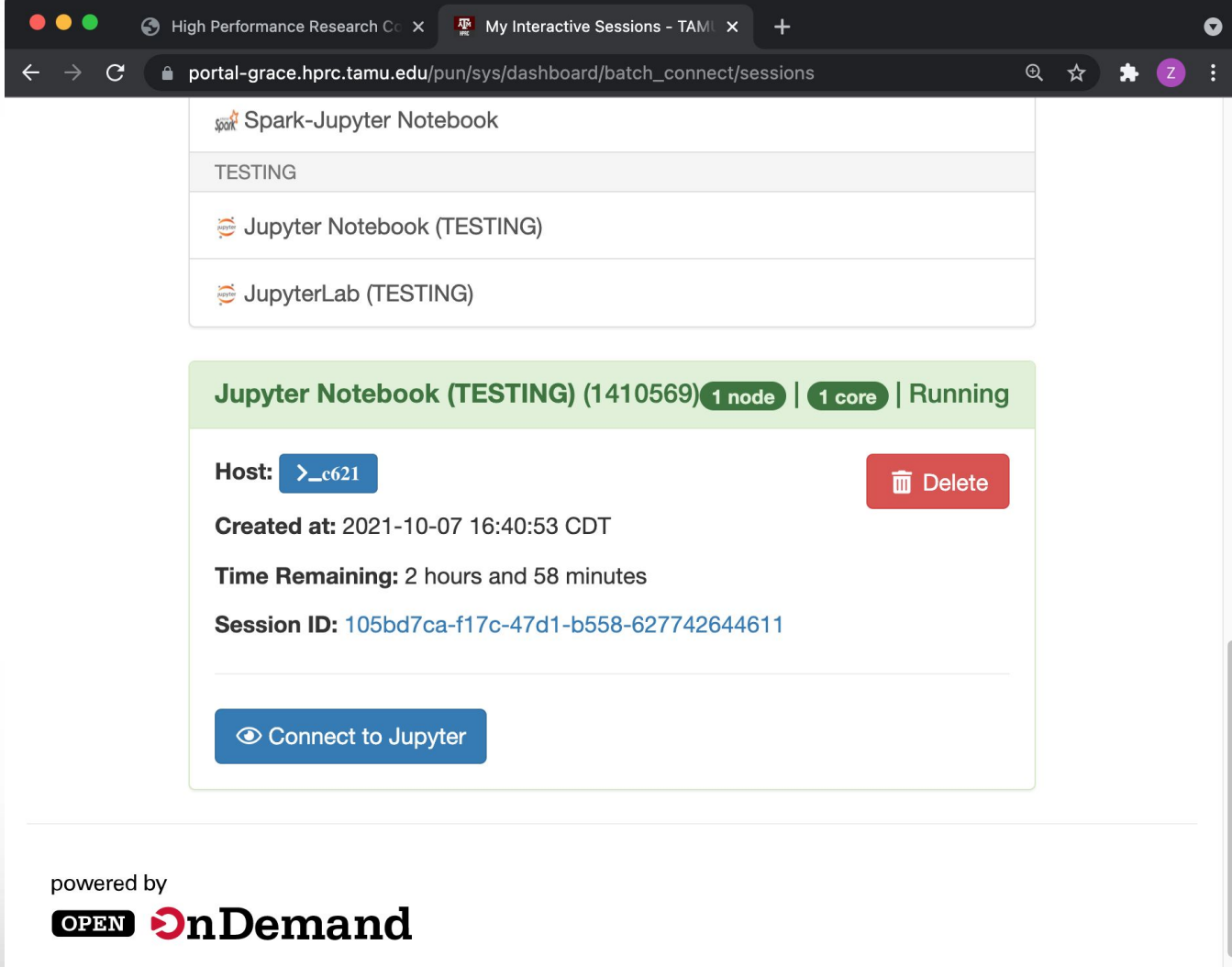
Module selected

SciPy_tamu/2021.10-Python-3.8.6

Select a module to load. All modules listed will also load the

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.

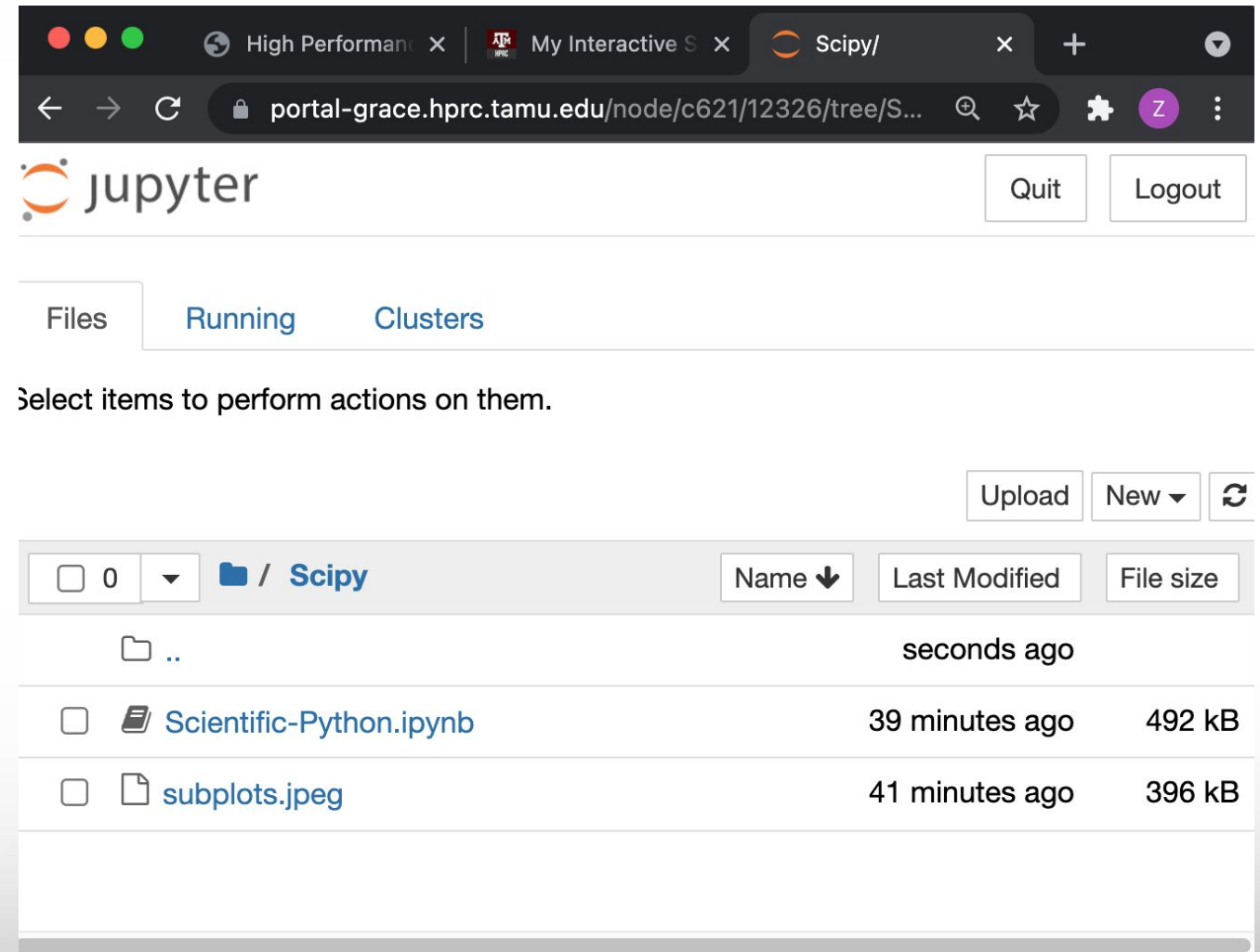


The screenshot shows a web browser window with the URL `portal-grace.hprc.tamu.edu/pun/sys/dashboard/batch_connect/sessions`. The page displays a list of interactive sessions. The first session is a Spark-Jupyter Notebook in a TESTING state. Below it, a detailed view for a Jupyter Notebook (TESTING) session (ID: 1410569) is shown. This session is running on 1 node with 1 core. The host is `>_c621`. It was created on 2021-10-07 at 16:40:53 CDT and has 2 hours and 58 minutes remaining. A 'Delete' button is visible next to the host information. A 'Connect to Jupyter' button is located at the bottom of the session details. The page is powered by OPEN and nDemand.

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.



The screenshot shows a web browser window with the URL `portal-grace.hprc.tamu.edu/node/c621/12326/tree/S...`. The page displays the Jupyter interface with tabs for 'Files', 'Running', and 'Clusters'. Below the tabs, there is a message: 'Select items to perform actions on them.' To the right of this message are buttons for 'Upload', 'New', and a refresh icon. Below this is a table listing files in the current directory:

<input type="checkbox"/>	0		Name ↓	Last Modified	File size
		📁	..	seconds ago	
<input type="checkbox"/>		📄	Scientific-Python.ipynb	39 minutes ago	492 kB
<input type="checkbox"/>		📄	subplots.jpeg	41 minutes ago	396 kB

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?