

Introduction to Scientific Python

Course Material

Course files are available on the Texas A&M HPRC website:

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

Jupyter Notebook

We will be using the Grace portal to run **Jupyter Notebook** to view class material and run examples.

Requirements

To access the **Jupyter Notebook** application on the Grace portal, you must have an HPRC account. You will need to be on campus or connected via VPN. If you do not have an HPRC account or VPN, you can still view the notebook through google colab (instructions below).

Setup

- (1) Go to <https://portal.hprc.tamu.edu/> and click on **Grace OnDemand Portal** .
- (2) You may be asked to login to the Central Authentication Service (CAS) with your NetID and password.
- (3) On the top menu bar, click **Clusters** and then **>_grace Shell Access** .
- (4) Login using your NetID password and Duo authentication.
- (5) Enter the following commands which will create the directory

```
cd $SCRATCH cp -r
/scratch/training/Scipy/ .
cd Scipy
ls
```

or

```
cd $SCRATCH
git clone https://github.com/happidence1/Scipy.git
cd Scipy
ls
```

- (6) Return to the previous browser tab for the Grace Portal with the title “Dashboard”.
- (7) On the top menu, choose **Interactive Apps** and the scroll all the way down to **Jupyter Notebook**.

- (8) This opens a dialog page. Choose the **Type of environment** and **Module selected** as shown in the Figure below.

Type of environment

Module load + Python virtualenv ▼

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

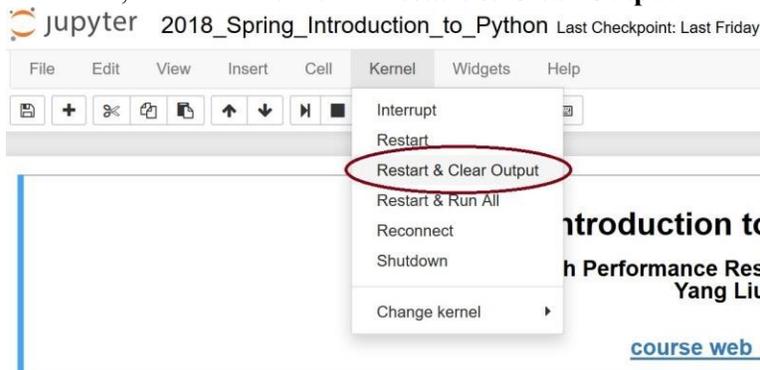
Module selected

SciPy_tamu/2021.10-Python-3.8.6 ▼

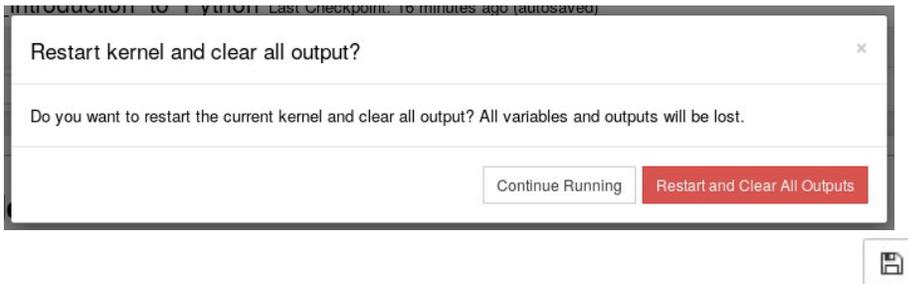
- (9) Scroll down to **Number of hours** and change the value to **3** to give you three hours to run Jupyter Notebook. Be aware that at the end of this time, your session will end, so remember to save your work before the time expires. Scroll to the bottom of the page and click **Launch**.
- (10) Once Jupyter Notebook launches, it will show you a listing of your scratch directory. Click on **Scipy** to navigate to the directory you just created with the git command above. Click on the **Scientific_Python.ipynb** file to open this notebook.

(11) You may want to restart your kernel and clear all outputs.

To do this, click on “**Kernel -> Restart & Clear Output**”



A warning message will pop up, click “**Restart and Clear All Outputs**”



Finally, click the **save icon** on the top left-hand side to save the changes:

(8) Once your changes have been saved, you are ready to begin the class.

IMPORTANT

The Jupyter notebook will only run for as long as the time you specified in the setup dialog. If you would like to save any changes you make to the file, please do so before the time expires or before logging out. You may also save the file to your local computer. This can be done by clicking on “**File -> Download As**” and choosing a file format.