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 Python

with exercises using HPRC Portal

Richard Lawrence
Outline

- Usage Policies
- References
- About Python
- Getting Started
- Break
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- Break
- 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_python.html

And on disk on Terra

/scratch/training/Intro-python

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

youtube.com channel "Texas A&M HPRC"
HPRC Wiki - Python

Visit our wiki for frequently asked questions [https://hprc.tamu.edu/wiki/Main_Page](https://hprc.tamu.edu/wiki/Main_Page)

For example, information about using Python [https://hprc.tamu.edu/wiki/SW:Python](https://hprc.tamu.edu/wiki/SW:Python)
Further Learning

For further learning on other topics, attend one of our upcoming short courses: [https://hprc.tamu.edu/training/](https://hprc.tamu.edu/training/)

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<td>Introduction to Scientific Python</td>
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About Python
What is Python?

Python is a High-level language, which means:

- Syntax is similar to human language syntax
- Supports abstract concepts
- Takes care of mundane hardware tasks for you

Python is designed to simplify the development process so you can focus on what matters.
Is Python right for me?

No programming language is perfect for every task.

Python is best for research and rapid development.

Pros
- Easy to use
- Modules are readily available
- Portable

Cons
- Not the fastest
- Not the best starting language
- Source code style is mandatory
Where does Python come from?

Python is an Open Source project administered by the Python Software Foundation. As such, it is both freely available and distributed by multiple package managers.

- Windows offers Python in the app store, with Visual Studio integration.
- Mac and Linux often come with Python pre-installed, but it is most likely the older Python 2. Update to Python 3 strongly recommended. It is available through your OS’s repository manager.
- The HPRC maintains up-to-date Python installations, accessible through your web browser.
Python is an interpreted language, which means Python code is executed by Python’s interpreter at run-time.

Broadly speaking, there are three ways to use the Python interpreter.

1. Interactive: Launch the interpreter, and type in Python commands. Each command is executed as soon as it’s entered.

2. Script: Save your code in a file, and tell the interpreter to read it.

3. Integrated Development Environment (IDE): combines the above two strategies: edit your files and execute them in the same window.
Python Usage Examples

Method 1. Interactive

```bash
$ python
>>> print("hello world")
>>> exit()
```

Method 2. Script

File ‘hello.py’ contains:
```python
print("hello world")
```

```bash
$ python hello.py
```

Method 3. IDE (Jupyter notebook)

```python
In [ ]: print("hello world")
```
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/](http://it.tamu.edu/duo/))
- (Faculty and staff) Use Duo Keys - ([u.tamu.edu/get_duo_keys](http://u.tamu.edu/get_duo_keys))
- Instructions in two-factor wiki page ([hprc.tamu.edu/wiki/Two_Factor](http://hprc.tamu.edu/wiki/Two_Factor))

**Example: SSH login with Duo**

```bash
$ 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

Execute

$ cp -r /scratch/training/Intro-python .

(...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

Leave other fields blank

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 **Intro-python** directory you copied to your scratch space.

Click the file name **Introduction_to_Python.ipynb** to open the Notebook.
Hands-on exercises:
Launch a Jupyter Notebook

Once you have the notebook open, respond to a poll
Python Basics

(continued in Python Notebook)
Need Help?

● Try these:
  − First check the FAQ [hprc.tamu.edu/wiki/HPRC:CommonProblems](http://hprc.tamu.edu/wiki/HPRC:CommonProblems)
  − Also try the Terra User Guide [hprc.tamu.edu/wiki/Terra](http://hprc.tamu.edu/wiki/Terra)
  − Email your questions to [help@hprc.tamu.edu](mailto: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?