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

Stuti Trivedi

Spring 2021
Outline

- Usage Policies
- References
- Getting Started
- Break
- Python Exercises
- 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_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"
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/)

<table>
<thead>
<tr>
<th>Course</th>
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<tbody>
<tr>
<td>Introduction to Quantum Chemistry Simulations with ORCA</td>
<td>Friday, March 12</td>
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<tr>
<td>Drug Docking with Schrodinger</td>
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<td>Scientific Machine Learning</td>
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<tr>
<td>Technology Lab: AI techniques usage - Jupyter Notebook</td>
<td>Friday, April 2 10:00 am</td>
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<tr>
<td>Introduction to Julia</td>
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<td>Introduction to Pytorch</td>
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<tr>
<td>Introduction to Deep Learning with TensorFlow</td>
<td>Friday, April 16 1:30 pm</td>
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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

OnDemand provides an integrated, single access point for all of your HPC resources.
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](hprc.tamu.edu/wiki/HPRC:CommonProblems)
  - Also try the Terra User Guide [hprc.tamu.edu/wiki/Terra](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?