Running Jupyter Notebooks on the Open On Demand Portal

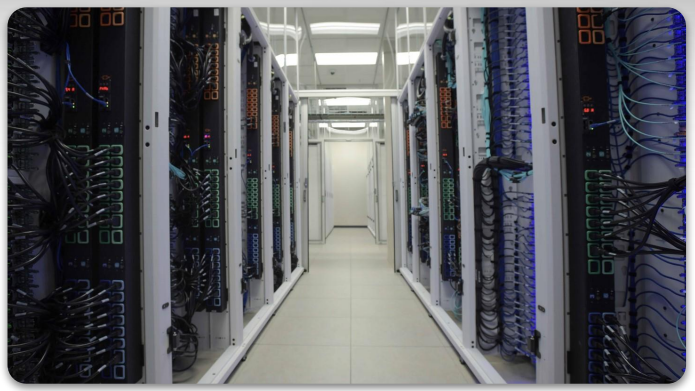
Abhinand Nasari

01/28/22

DIVISION OF RESEARCH
TEXAS A&M UNIVERSITY

HPRC's Newest Cluster

Grace is a 925-node Intel cluster from Dell with an InfiniBand HDR-100 interconnect, A100 GPUs, RTX 6000 GPUs and T4 GPUs. There are 925 nodes based on the Intel Cascade Lake processor.



Grace Status: Testing and Early user onboarding

Grace
3TB Large Memory-80 cores/nodes
Other Login Nodes-48 cores/node

Login Nodes	5
384GB memory general compute nodes	800
GPU - A100 nodes with 384GB memory	100
GPU - RTX 6000 nodes with 384GB memory	9
GPU - T4 nodes with 384GB memory	8
3TB Large Memory	8

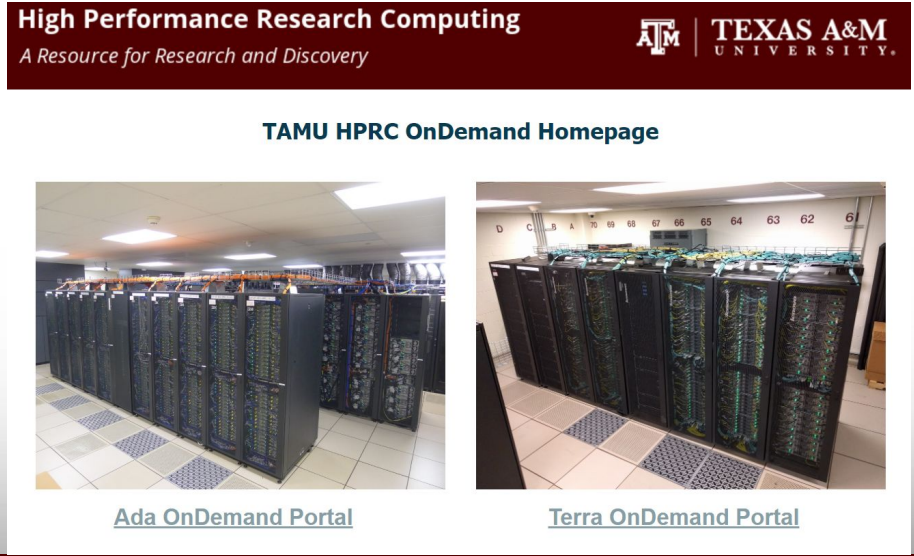
Available late Spring 2021

For more information:
https://hprc.tamu.edu/wiki/Grace:Intro

HPRC Portal

- HPRC Portal is an open source web platform through which users can access HPC clusters and services with a web browser
- Both ada and terra portal can be accessed through the landing page: https://portal.hprc.tamu.edu/

- Key services provided:
  - Job submission and monitoring
  - File transfer and management
  - File editing
  - Shell access
  - Interactive applications



Accessing the HPRC Portal

Access

- On campus: https://portal.hprc.tamu.edu/
  - Off campus:
    - Set up and start VPN (Virtual Private Network): u.tamu.edu/VPnetwork
    - Then access the link: https://portal.hprc.tamu.edu/
    - *Two-Factor Authentication* enabled

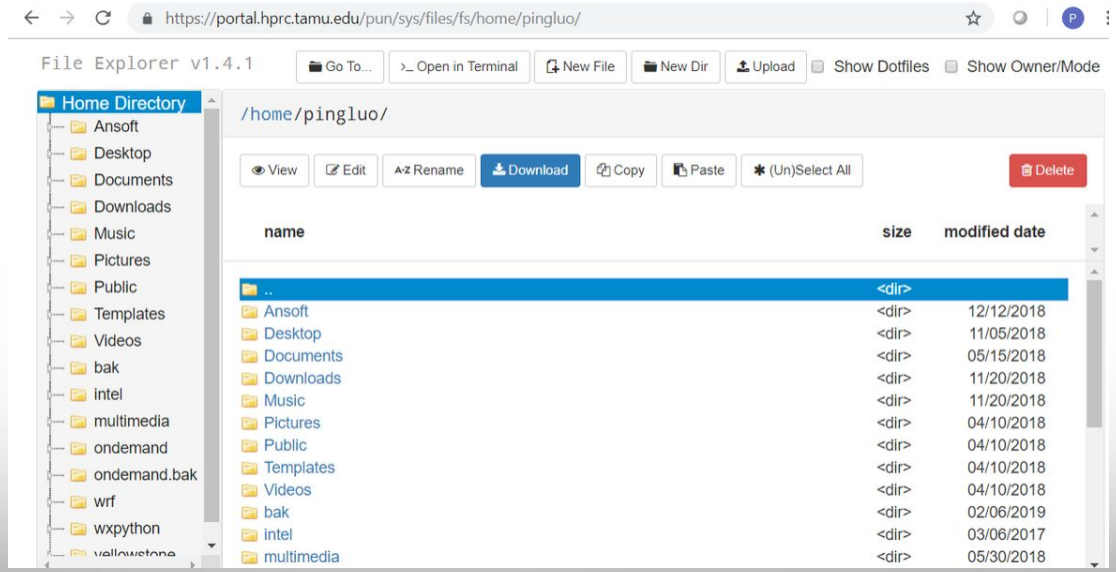
- OnDemand user guide helps to navigate the easy-to-use interface and access the interactive applications:
  https://hprc.tamu.edu/wiki/SW:Portal

hprc.tamu.edu/wiki/HPRC:Access

Navigating through the Portal

File Explorer

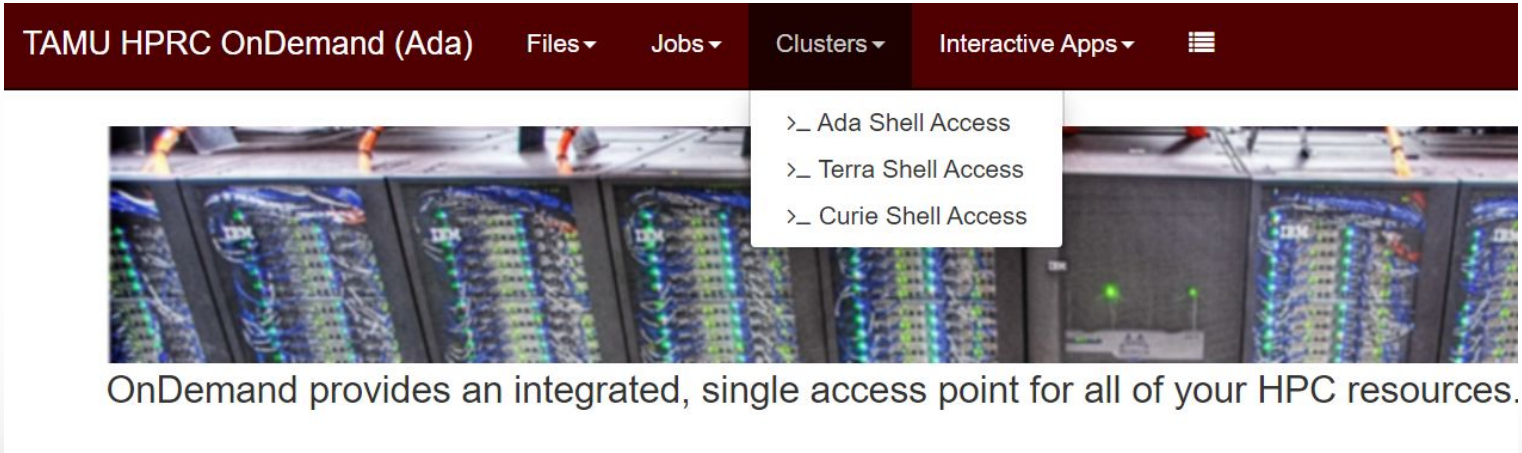
- Using the Files visual interface, a user can view a file explorer at either their home directory or scratch directory
- Files on portal can be used for viewing, editing and creating new files as well as directories on clusters



Navigating through the Portal

Cluster Shell

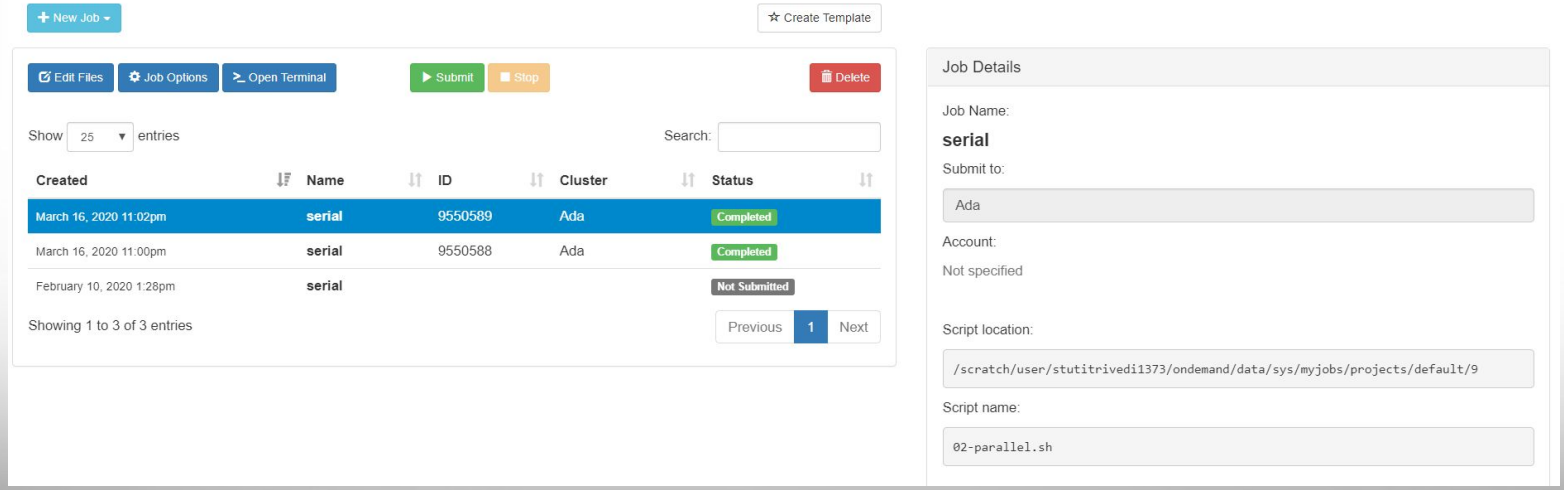
- Shell access to any of the three clusters is available from this drop down menu with one click
- Similar to ssh client such as Putty and MobaXterm using Netid and password



Navigating through the Portal

Jobs

- **Active Jobs**:Provides information regarding jobs running on the cluster, JobID, name, user, account, time used, queue, and status
- **Job Composure**:Provides template job scripts to create new jobs
  Refer the wiki link for more details on job submission:https://hprc.tamu.edu/wiki/Ada:Batch_Processing_LSF



Navigating through the Portal

Interactive Apps

- Most common GUI software like MATLAB, Abaqus etc. along with servers like Jupyter Notebooks, RStudio.can be directly launched by providing mentioned parameters.
- Required job parameters:
  - number of cores
  - wall time
  - memory
  - type of node
- If a software is not available, you can always run it within VNC

> *To load ABAQUS using VNC*:
>
> module load ABAQUS
> vglrun abaqus cae

- For more details on running VNC, refer: https://hprc.tamu.edu/wiki/Ada:Remote-Viz

Launch Jupyter Notebook on HPRC Portal

Jupyter

- Jupyter interactive app on portal will launch Jupyter Notebook server on clusters
- Jupyter Notebook environment can be created using Python or Anaconda(module version specified) on HPRC Portal
- Note: Run the command "**showquota**" to check if available file limit >10,000 as conda and pip creates thousands of files
- Jupyter Notebook session data will be saved in user's home directory by default. This can be modified by creating virtual environment under user's scratch directory
- To launch Jupyter Notebooks, go to **Interactive Apps-> Server->Jupyter Notebooks**

Launch Jupyter Notebook on HPRC Portal

Jupyter

- Choose **Module**(Python/Anaconda version)
- Provide **number of hours** for running notebooks on clusters
- Specify **number of cores** [1-28] allocated on node on clusters
- Requested **total memory** (2-112GB)

  If total mem from all cores is <=54G, the job will run on a 64G memory node

  If total mem from all cores is >54G, the job will run on a 128G memory node
- Provide **node type** (GPU/Any)
- Specify account details and email to receive a pop-up when session is ready to launch

Launch Jupyter Notebook on HPRC Portal

Optional Environment Activation-Python

- Existing virtual environments created on clusters can be used to launch Jupyter Notebooks. Alternately, Python or Anaconda module can be used to new create virtual environment
- For creating virtual environment using Python, create new directory under scratch

```
mkdir -p /scratch/user/mynetid/pip_envs
```

- Load Python module(select from the list of module available on portal). Create virtual environment named *my_notebook-python-3.6.6-foss-2018b*

```
module purge  virtualenv
/scratch/user/mynetid/pip_envs/my_notebook-python-3.6.6-foss-2018b
```

Launch Jupyter Notebook on HPRC Portal

Optional Environment Activation-Python

- Activate virtual environment

Install notebook and python packages

```
source /scratch/user/mynetid/pip_envs/my_notebook-python-3.6.6-foss-2018b/bin/activate
pip install notebook
pip install python_package_name
```

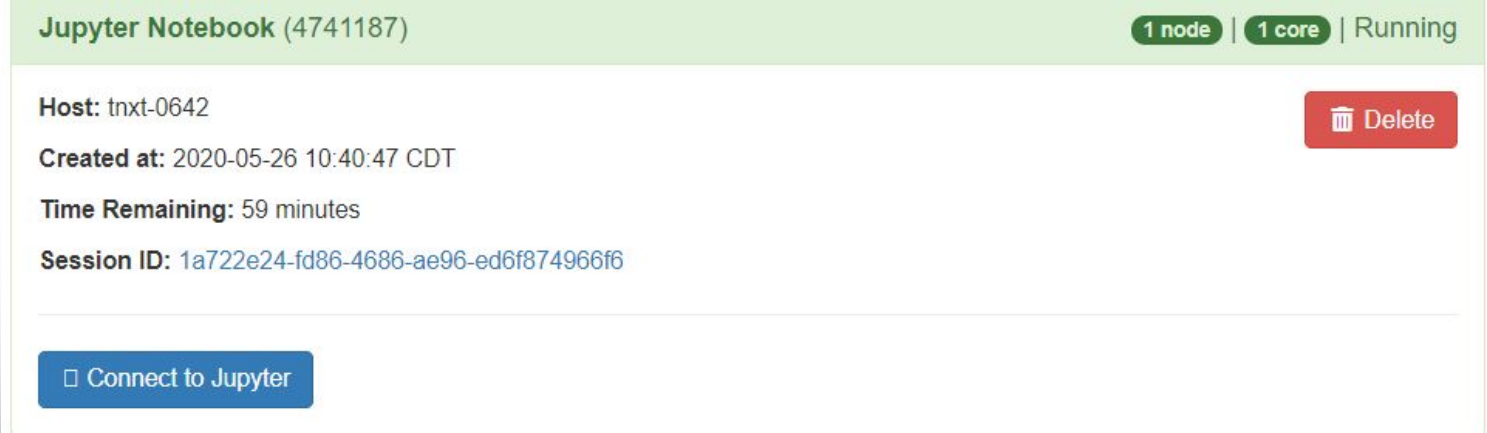
- Refer wiki link for more information:

https://hprc.tamu.edu/wiki/SW:Portal#Jupyter_Notebook

Launch Jupyter Notebook on HPRC Portal

Optional Environment Activation-Python

- Provide full path to to the activate command for your Python/3.6.6-foss-2018b environment in the "Optional Conda Environment to be activated"
- Jupyter notebook session with JobID (4741187 in this case) and session ID is active.
- Session ID can be used to trace logs



Launch Jupyter Notebook on HPRC Portal

Optional Environment Activation-Anaconda

- For creating virtual environment using Anaconda, create new directory under scratch and virtual environment my_notebook

```
module purge
module load Anaconda/3-5.0.0.1
conda create -n my_notebook
```

- Activate/Deactivate environment using the command mentioned below:
my_notebook-python-3.6.6-foss-2018b

```
Activate: source activate my_notebook
Deactivate: source deactivate
```

Launch Jupyter Notebook on HPRC Portal

Optional Environment Activation-Anaconda

- Activate virtual environment. Install notebook and conda packages

```
source activate my_notebook
conda install -c conda-forge notebook
conda install -c conda-forge package-name
```

- Refer wiki link for more information: https://hprc.tamu.edu/wiki/SW:Portal#Jupyter_Notebook

Using Jupyter Notebook on HPRC Portal

Using Jupyter Notebooks

- Default directory-user's home or directory pointing to virtual environment (optional)
- Create new file using New-> Python3
- If you are uploading existing .ipynb file, make sure the python version is similar

Using Jupyter Notebook on HPRC Portal

Using Jupyter Notebook-Basic Python

Exercise 1

- Create a new directory under pip_envs
- Create a new notebook inside it. Save the file.
- Print a message- Welcome to HPRC

Using Jupyter Notebook on HPRC Portal

Jupyter Notebook- Familiarize the setup

- Jupyter server is up and running. Create notebook
  New->Notebook-> Python

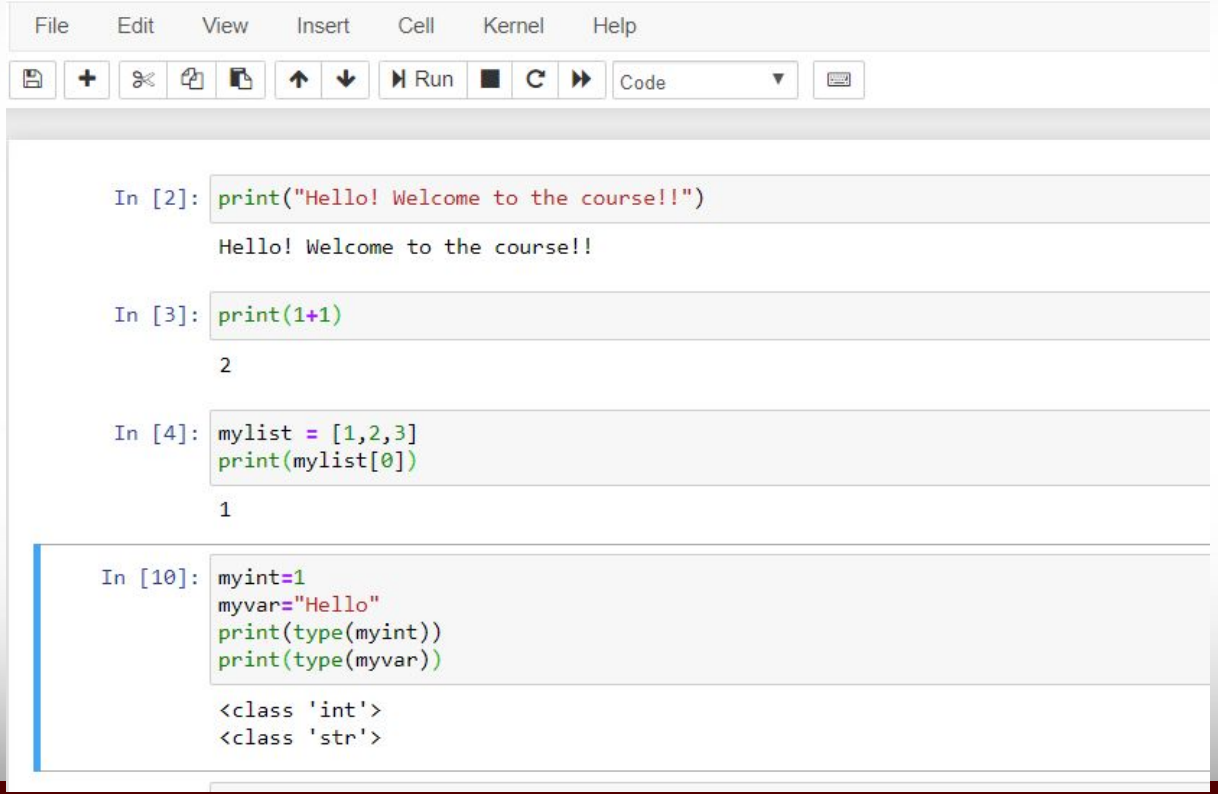
- Upload notebook(Python version must be same)
  Upload->Select notebook

- File naming convention
  All lowercase module names. Long module names can have words separated by underscores (really_long_module_name.py). CamelCase for class names

- Running the cells **(Shortcut: Ctrl + Enter)**

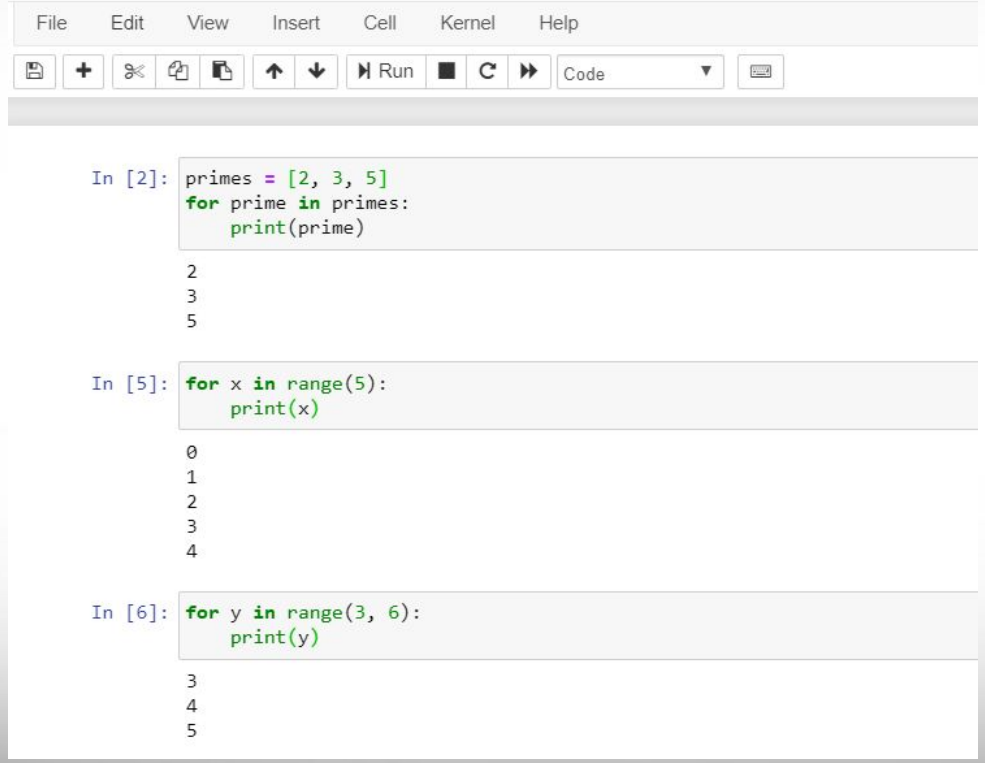
Using Jupyter Notebook on HPRC Portal

Jupyter Notebook- Running Python



Using Jupyter Notebook on HPRC Portal

Using Jupyter Notebook-Loops



Using Jupyter Notebook on HPRC Portal

Jupyter Notebook- Familiarize the setup

- **Kernel Attributes**

  -Restart

  -Interrupt

  -Change kernel (switch between various python versions)

  -Shutdown

  -List down all kernels available eg. Python 2, Anaconda 3

  -Remove specific kernels

```
jupyter kernelspec list
jupyter kernelspec remove <kernel-name>
```

Using Jupyter Notebook on HPRC Portal

Jupyter Notebook- iPython Shell Commands

- Print working directory-!pwd
- List files inside directory- !ls
- Change directory- %cd *newdir*
- Make directory- %mkdir *newdir*
- Copy file- %cp filename.ipynb newdir/
- Remove directory- rm -r *newdir*

Using Jupyter Notebook on HPRC Portal

Using Jupyter Notebook-Basic Python

Exercise 2

- Change the formatting as indicated below:

  Bold

  Italics

  Header1 format

  Include a link (https://hprc.tamu.edu/) next to the text

Using Jupyter Notebook on HPRC Portal

Jupyter Notebook- Markdown

- **Headers**

  # (Header 1, title) stands for html code <h1>Header 1,title<h1>

- **Line Break**

  The line breaks after using
 br tags and it is awesome

- **Inline Formatting**

  Bold: **HPRC
  Italics: *HPRC
  Horizontal Line: ***

- **Embed external link**

  Link to Google

  [section title](#section-title)

  [HPRC Link](https://hprc.tamu.edu/)

Using Jupyter Notebook on HPRC Portal

Jupyter Notebook- Markdown

- **Perform complex mathematical operations (‘$ math expression $’)**

$$\sqrt{k}$$

```
In [ ]: $\sqrt{k}$
```

- **Embed Python Code**

```
```Python
str = "This is block level code"
print(str)
```
```

Using Jupyter Notebook on HPRC Portal

Using Jupyter Notebook-Introduction to Numpy

In [9]:
```
# Create 2 new lists height and weight
height = [1.87,  1.87, 1.82, 1.91, 1.90, 1.85]
weight = [81.65, 97.52, 95.25, 92.98, 86.18, 88.45]

# Import the numpy package as np
import numpy as np

# Create 2 numpy arrays from height and weight
np_height = np.array(height)
np_weight = np.array(weight)

# Calculate bmi
bmi = np_weight / np_height ** 2

# Print the result
print(bmi)
# For a boolean response
bmi > 25

# Print only those observations above 23
bmi[bmi > 25]
```

```
[23.34925219 27.88755755 28.75558507 25.48723993 23.87257618 25.84368152]
```

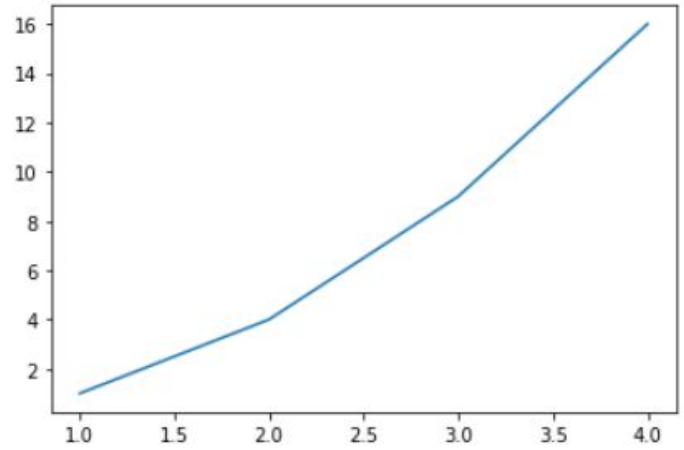
Out[9]:
```
array([27.88755755, 28.75558507, 25.48723993, 25.84368152])
```

Using Jupyter Notebook on HPRC Portal

Using Jupyter Notebook-Introduction to Matplot

```
In [5]: %matplotlib inline
        import matplotlib.pyplot as plt
        import numpy as np
        plt.plot([1, 2, 3, 4], [1, 4, 9, 16])
```

```
Out[5]: [<matplotlib.lines.Line2D at 0x2b6ecfe8a908>]
```



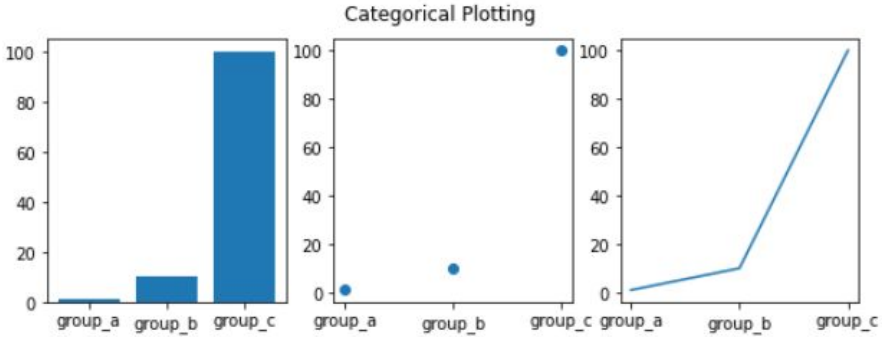
Using Jupyter Notebook on HPRC Portal

Using Jupyter Notebook-Introduction to Matplot

```
In [6]: names = ['group_a', 'group_b', 'group_c']
        values = [1, 10, 100]

        plt.figure(figsize=(9, 3))

        plt.subplot(131)
        plt.bar(names, values)
        plt.subplot(132)
        plt.scatter(names, values)
        plt.subplot(133)
        plt.plot(names, values)
        plt.suptitle('Categorical Plotting')
        plt.show()
```



Using Jupyter Notebook on HPRC Portal

Final Steps

- **Logging Out:**
  To properly log out the portal,follow the below mentioned steps:
  - log out the portal by clicking 'Log out' from the top navigation bar
  - close the browser to completely terminate the session

- **Clean up:**
  The portal stores temporary files for interactive apps in *$SCRATCH/ondemand/data/sys/dashboard.*
- Use the below mentioned command on cluster to clean up after completing the simulations on Jupyter Notebooks.

```
rm -rf $SCRATCH/ondemand/data/sys/dashboard/batch_connect/sys/*
```

- **Saving the files:**
  Notebooks will be saved in the default directory (home or virtual environment)

Continued Learning

Intro to HPRC Video Tutorial Series

HPRC's Wiki Page