

Introduction to TACC Computing Cluster



Scalable Computational Intelligence
Texas Advanced Computing Center (TACC)

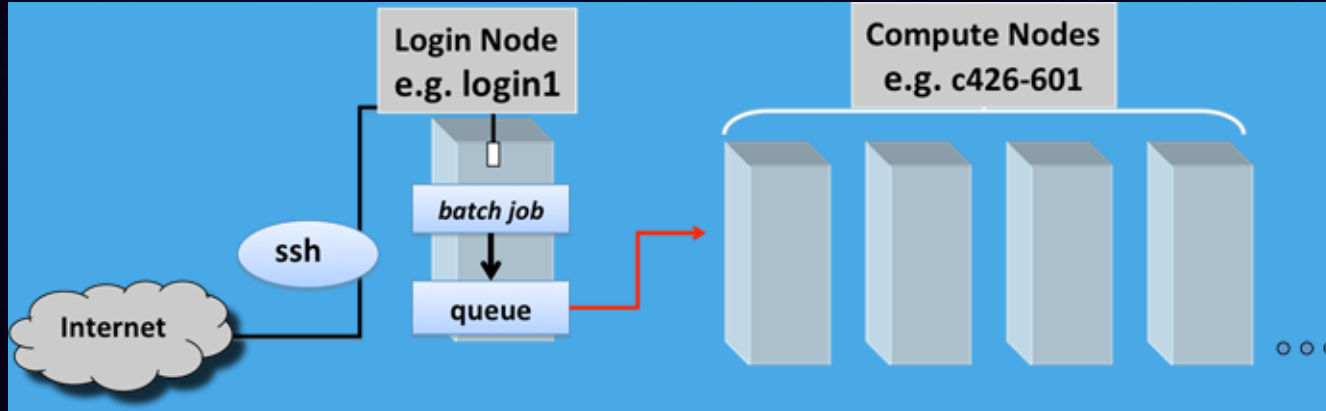
Overview

Practical introduction to using TACC resources

- Nodes and File system at TACC
- How to Remotely Access TACC
- Navigating the File System on TACC machines
- Hands On: Accessing TACC via TAP



Login vs Compute Nodes



Login Nodes

- Shared by multiple users
- Not meant for CPU or memory intensive jobs
- Meant for managing file and compiling code

Compute Nodes

- Where research computation occurs
- Training machine learning models, running simulations, etc.

Types of Compute Nodes: Partitions

- Compute nodes are divided into different pools called queues
 - For example here are a few queues on VISTA
 - Grace/Grace (gg)
 - Grace/Hoppersmall (gh)
 - Development Grace Hopper (gh-dev)
 - Refer to the user guide for the queue and accounting details



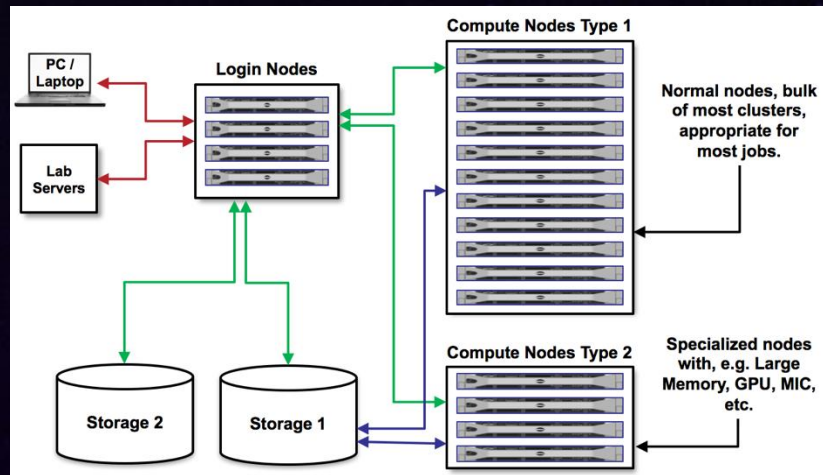
File Systems

Three (3) main file systems

- **\$HOME**
 - Quota (25G)
 - Backed up
 - Used for: small scripts, environment settings, and other routine file management task
- **\$WORK**
 - Quota (1TB)
 - Not Backed up
 - Used For: Intermediate staging/preparation of files, storing original datasets
- **\$SCRATCH**
 - No Quota
 - Not Backed up, subject to purge
 - Used for: High I/O bandwidth jobs

Refer to VISTA User Guide / TACC tutorials

- <https://docs.tacc.utexas.edu/hpc/vista/#system-filesystems>
- <https://docs.tacc.utexas.edu/tutorials/managingio/>

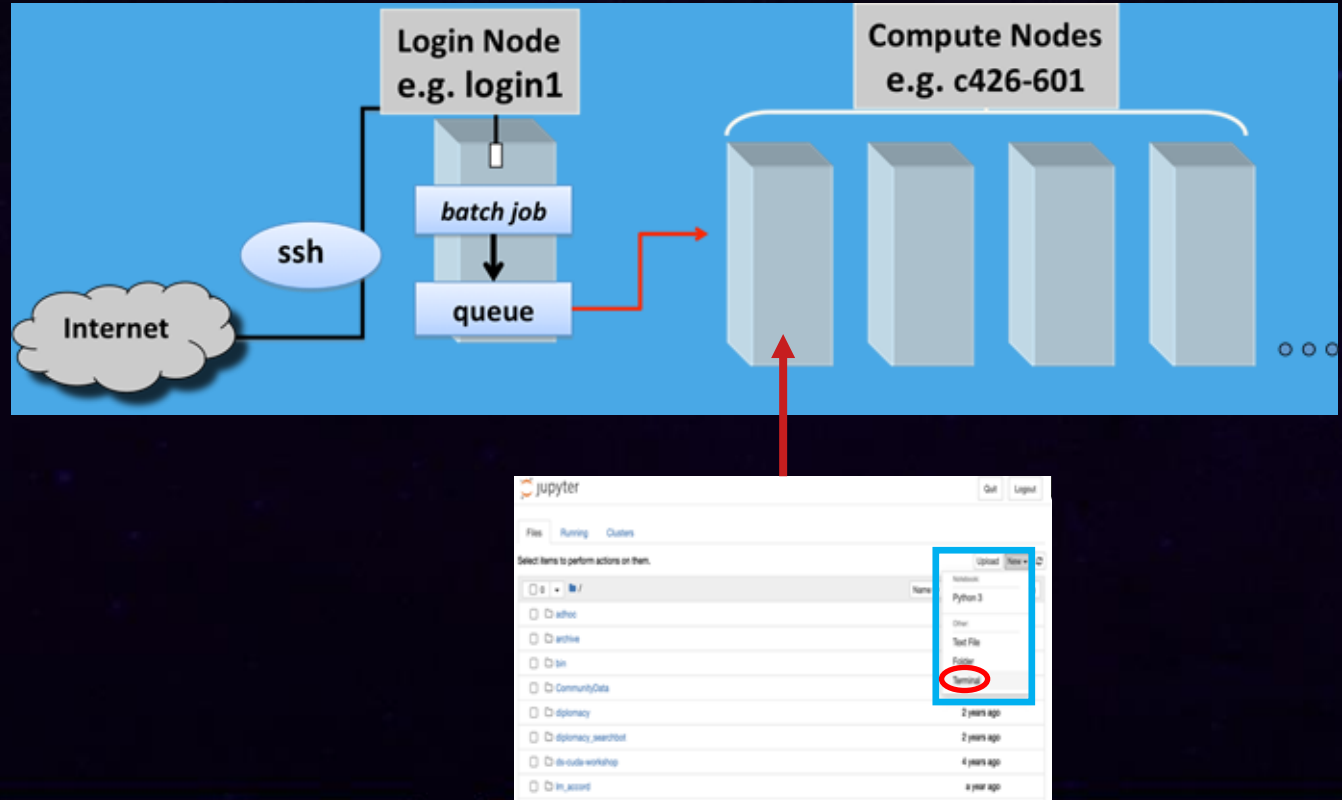


- **/tmp**
 - Each compute node comes with local storage (/tmp)
 - Fast I/O
 - **Temporary:** storage only last the duration of the job and should be copied for permanent storage

How to Remotely Access TACC

We will remotely access Frontera in two ways in this event:

1. SSH: Access login nodes via command line
2. TACC Analysis Portal: UI for accessing jupyter notebook session on a compute nodes



Accessing Compute Nodes

Let's assume we have logged into TACC via ssh and we are on a login node. How do we connect to a compute node?

- submit a batch job via the sbatch command
 - job waits in queue until resources are available
- activate an interactive session via **idev**
 - idev
 - Allows you to get a compute node for testing purposes
 - -m option lets you specify time in minutes
 - idev -m 30



Bash – basic file commands

- TACC machines use the Linux operating system
- Default shell and most popular is bash (Bourne Again Shell)

Command	Function
<code>pwd</code>	Shows absolute path of your present working directory
<code>ls <directory name></code>	Lists a directory (if mentioned) or present working directory
<code>mkdir <name></code>	Creates a new directory with mentioned name
<code>cd <name></code>	Changes working directory to name mentioned (or go to home directory if nothing is specified)
<code>cp <File1> <File2></code> <code>cp <File1> <Directory></code>	Makes a copy of File1 and names it File2 or makes a copy of the file with the same name in Directory1
<code>cp -r <directory1> <directory2></code>	Makes a copy of directory1 and all its contents into directory2
<code>mv <File1> <Directory></code> <code>mv <File1> <File2></code>	moves File1 to Directory1 or rename File1 to File2
<code>rm <File1></code> <code>rm -r <Directory1></code>	Removes a file or Remove a directory (add -f flag to force remove...be careful)



module

- On TACC Systems the module system helps setup or teardown useful packages that are supported by TACC, on the fly
- To find more information on a module
 - `module spider package-name`
- To load a module
 - `module load package-name`
 - `module load package-name/version.number`

Check out the User guide to learn more:

https://mod.readthedocs.io/en/latest/010_user.html



Hands on: Accessing TACC via the TACC Analysis Portal and Environment Setup

Development Environment

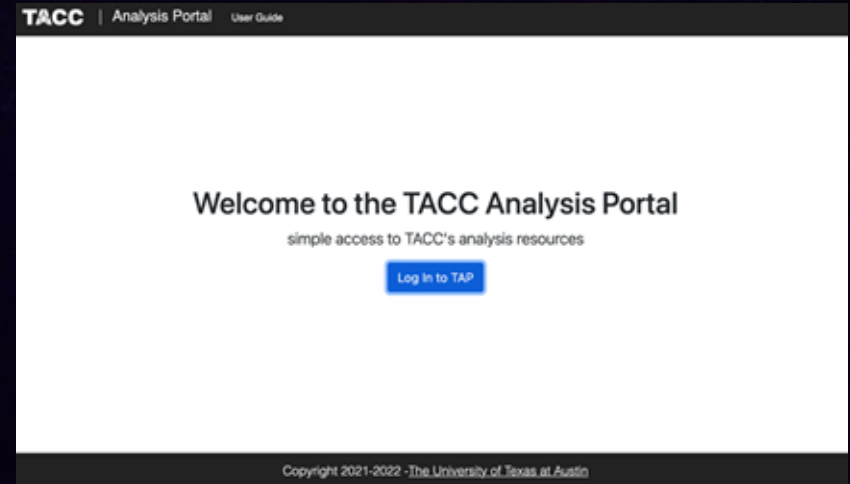


- ▶ Jupyter Notebook
 - ▶ <http://jupyter.org/>
 - ▶ Web application for creating and sharing computational documents.
 - ▶ It offers a simple, streamlined, document-centric experience.
 - ▶ Provides an interactive interface in the browser
 - ▶ Can view output and plots inline
 - ▶ Makes Iterative/Interactive Development easy
 - ▶ Can be turned into a pure script for non-interactive work



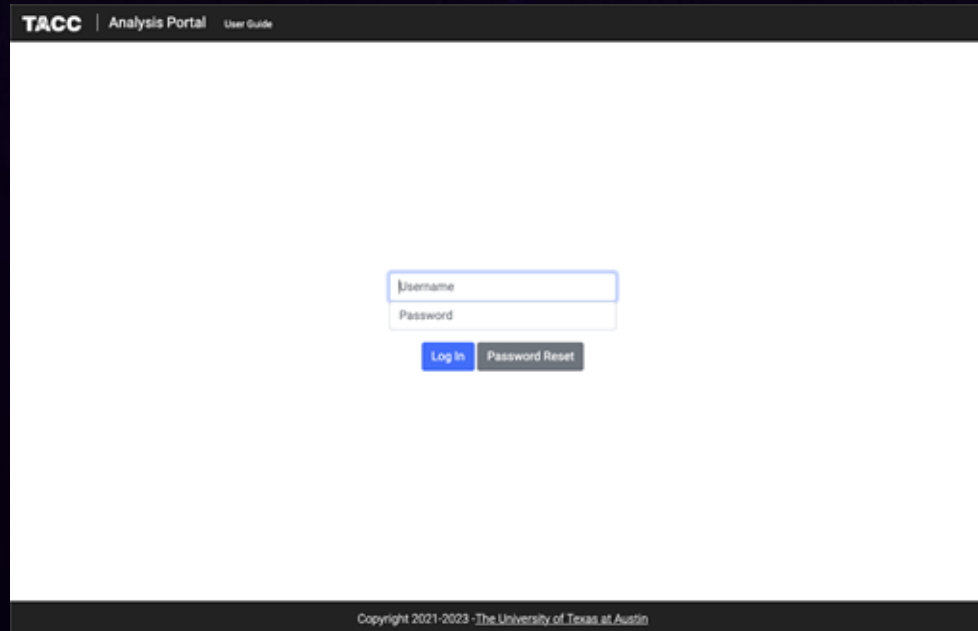
TACC Analysis Portal

- TACC Analysis Portal (TAP) provides access to interactive sessions on TACC machines
- Allows user to utilize web-based interactions on TACC computers
 - e.g. Jupyter notebook, Rstudio, remote linux desktop
- <https://tap.tacc.utexas.edu>



Login with your TACC account

- TACC Analysis Portal:
login with your TACC account credentials



The screenshot shows the TACC Analysis Portal login interface. At the top, a dark header bar contains the TACC logo, the text "Analysis Portal", and a link to the "User Guide". The main content area is white and features a centered login form. The form consists of two input fields: "Username" and "Password". Below these fields are two buttons: a blue "Log In" button and a grey "Password Reset" button. At the bottom of the page, a dark footer bar contains the copyright text: "Copyright 2021-2023 - The University of Texas at Austin".

Jupyter notebook: Accessing shell

TACC | Analysis Portal User Guide jrduncan Log Out

Submit New Job

System

Application

Select System

Project

Select System

Queue

Select System

Nodes

1

Tasks

1

Options

Job Name

20 characters max

Time Limit

H:M:S (default 2:0:0)

Reservation

reservation name

VNC Desktop Resolution

WIDTHxHEIGHT

Submit

Utilities

System Status

System	Status	Utilization	Job Count
Frontera	Open	99%	Running: 312 Queued: 1251
Lonestar6	Open	69%	Running: 135 Queued: 98
Longhorn	Open	74%	Running: 30 Queued: 40
Maverick2	Open	16%	Running: 4 Queued: 7
Stampede2	Open	96%	Running: 830 Queued: 736

Past Jobs

JNB-Frontera	03/18/2022	Details	Resubmit
JNB-Frontera	03/18/2022	Details	Resubmit
JNB-Frontera	03/18/2022	Details	Resubmit
JNB-Frontera	03/18/2022	Details	Resubmit
JNB-Frontera	02/21/2022	Details	Resubmit

Starting Jupyter notebook: Accessing shell

- TACC Analysis Portal:
Select the following options

The screenshot shows the 'Submit New Job' form in the TACC Analysis Portal. The following options are highlighted with red circles:

- System:** Vista
- Application:** Jupyter notebook
- Project:** Frontera-Training
- Queue:** gh
- Nodes:** 1
- Tasks:** 1
- Job Name:** 20 characters max
- Time Limit:** H:M:S (default 2:0:0)
- Reservation:** ML-Institute-Mon
- VNC Desktop Resolution:** WIDTHxHEIGHT

At the bottom of the form are two buttons: **Submit** and **Utilities**.

Waiting for Job to start (can take a minute)

TACC | Analysis Portal User Guide ngaffney

TAP Job Status

Job: Jupyter notebook on Frontera (6314485, 2024-05-13T13:42:05:00)
Status: PENDING
Refresh: in 41 seconds
Message:

TAP: Your script has been submitted to Frontera but it is not yet running.

`sinfo -p development` output is:

PARTITION	AVAIL NODES(A/I)
development*	up 390/4

Check Status

End Job

Show Output

Back to Jobs

Jupyter notebook: Accessing shell

TACC | Analysis Portal | [User Guide](#) | [jrduncan](#) | [Log Out](#)

TAP Job Status

Job: Jupyter notebook on Frontera (4175197, 2022-03-21T17:28-05:00)
Status: RUNNING
Start: March 21, 2022, 5:28 p.m.
End: March 21, 2022, 5:33 p.m.
Refresh: in 873 seconds
Message:

TAP: Your session is running at <https://frontera.tacc.utexas.edu:60752/?token=9cbad0f26752e7dd14fcf090d6a30b6ec5c15c63ed7d9e2b626f214712fb8b4d>

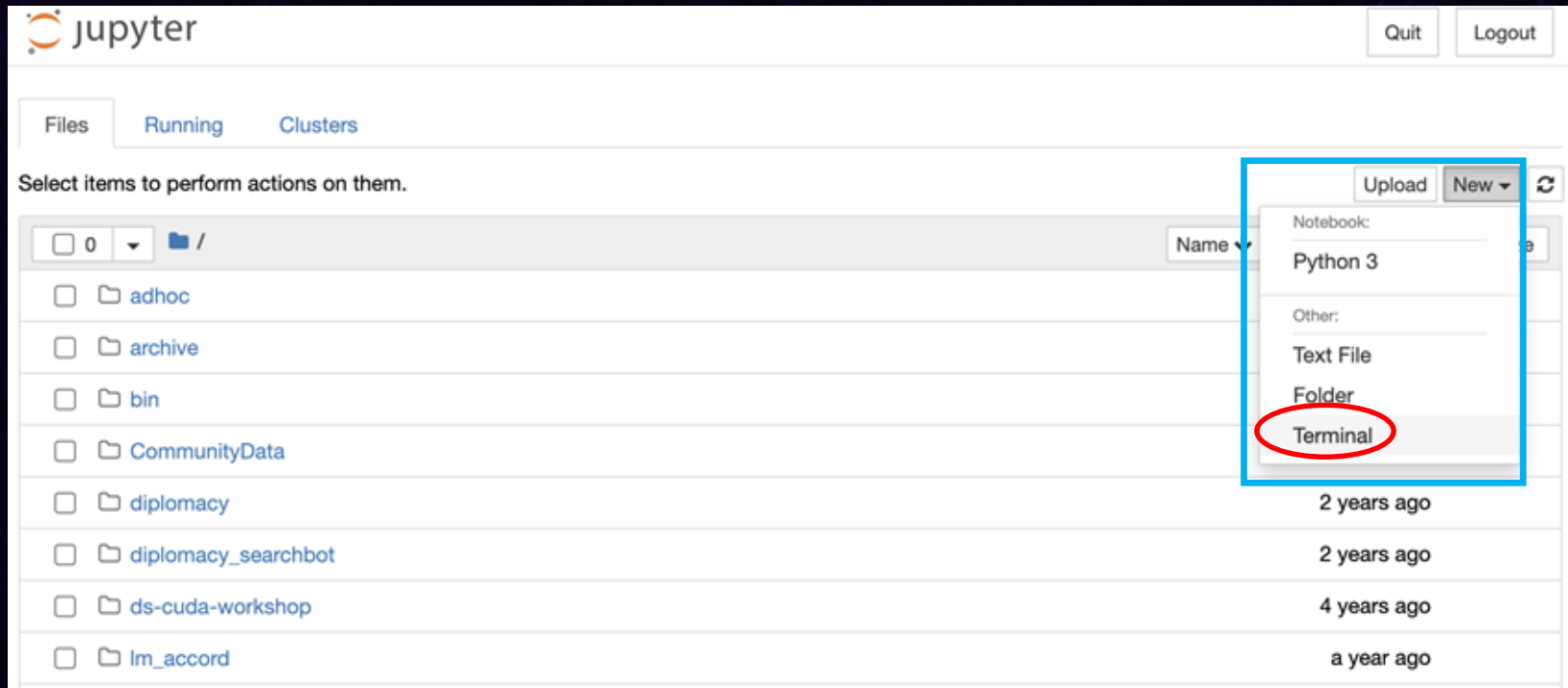
[Connect](#) [End Job](#) [Show Output](#) [Back to Jobs](#)



Setting up for the tutorial

- ▶ Note, the following setup only has to be done once.
- ▶ This is copying files into the right places so you can run these notebooks with us.

Jupyter notebook: Accessing shell



The screenshot displays the JupyterLab web interface. At the top, the 'jupyter' logo is on the left, and 'Quit' and 'Logout' buttons are on the right. Below the logo, there are tabs for 'Files', 'Running', and 'Clusters'. A message 'Select items to perform actions on them.' is shown above a file browser. The file browser lists several folders: 'adhoc', 'archive', 'bin', 'CommunityData', 'diplomacy', 'diplomacy_searchbot', 'ds-cuda-workshop', and 'lm_accord'. On the right side of the file browser, there are buttons for 'Upload', 'New', and a refresh icon. A dropdown menu is open from the 'New' button, showing options: 'Notebook: Python 3', 'Other: Text File', 'Folder', and 'Terminal'. The 'Terminal' option is highlighted with a red circle. The background of the slide is a dark space with stars.

jupyter

Quit Logout

Files Running Clusters

Select items to perform actions on them.

0 /

adhoc

archive

bin

CommunityData

diplomacy

diplomacy_searchbot

ds-cuda-workshop

lm_accord

Upload New

Notebook:

Python 3

Other:

Text File

Folder

Terminal

2 years ago

2 years ago

4 years ago

a year ago

Jupyter notebook: Accessing shell (4)



The screenshot displays a Jupyter notebook interface. At the top left, the word "jupyter" is accompanied by its logo. At the top right, there is a "Logout" button. The main area is a terminal window with a black background and white text. The prompt "c161-092.frontera(226)\$" is visible at the top left of the terminal, indicating the user is logged into a shell on the "c161-092.frontera" host with PID 226.

```
jupyter
```

Logout

```
c161-092.frontera(226)$
```




One time installation

From the command line enter

```
/scratch/install
```

After running this enter **ls** and make sure you see an entry for **institute_summer_25**

Stop the Session

TACC | Analysis Portal | [User Guide](#) |  ngaffney | [Log Out](#)

TAP Job Status

Job: Jupyter notebook on Frontera (6301729, 2024-05-07T11:49-05:00)
Status: RUNNING
Start: 05/07/2024 11:49
End: 05/07/2024 13:49
Refresh: in 630 seconds
Message:

TAP: Your session is running at <https://frontera.tacc.utexas.edu:60069/?token=H7Y2iZVbCVPpJRn9-U9tArNnvynEX3D0tP29pqnM0Yc>

[Connect](#) [End Job](#) [Show Output](#) [Back to Jobs](#)

Back to the Jobs page

TACC | Analysis Portal | [User Guide](#) | [ngaffney](#) | [Log Out](#)

TAP Job Status

Job: Jupyter notebook on Frontera (6301729, 2024-05-07T11:49-05:00)
Status: RUNNING
Start: 05/07/2024 11:49
End: 05/07/2024 13:49
Refresh: in 630 seconds
Message:

TAP: Your session is running at <https://frontera.tacc.utexas.edu:60069/?token=H7Y2iZVbCVPpJRn9-U9tArNnvynEX3D0tP29pqnM0Yc>

[Connect](#) [End Job](#) [Show Output](#) [Back to Jobs](#)

- ▶ This is the end of the one time setup. Next we will make sure it worked and then get started with some notebooks about Python

Jupyter notebook: Accessing shell

- TACC Visualization Portal:
Go to <https://tap.tacc.utexas.edu>; Login with your training account credentials

The screenshot displays the TACC Analysis Portal interface. At the top, there's a header with the TACC logo, 'Analysis Portal', 'User Guide', a user profile 'jrduncan', and a 'Log Out' button. The main content is divided into three sections: 'Submit New Job', 'System Status', and 'Past Jobs'.

Submit New Job section includes:

- System: A dropdown menu with '---' selected.
- Application: A dropdown menu with 'Select System' selected.
- Project: A dropdown menu with 'Select System' selected.
- Queue: A dropdown menu with 'Select System' selected.
- Nodes: A numeric input field with '1' and a 'Tasks' input field with '1'.
- Options section with input fields for:
 - Job Name: '20 characters max'
 - Time Limit: 'H:M:S (default 2:0:0)'
 - Reservation: 'reservation name'
 - VNC Desktop Resolution: 'WIDTHxHEIGHT'
- 'Submit' and 'Utilities' buttons at the bottom.

System Status section shows a table of system resources:

System	Status	Utilization	Job Count
Frontera	Open	99%	Running: 312 Queued: 1251
Lonestar6	Open	69%	Running: 135 Queued: 98
Longhorn	Open	74%	Running: 30 Queued: 40
Maverick2	Open	16%	Running: 4 Queued: 7
Stampede2	Open	96%	Running: 830 Queued: 736

Past Jobs section shows a list of jobs with columns for job name, date, and a 'Details' link. A red circle highlights the 'Resubmit' button for the first job (JNB-Frontera, 03/18/2022).

Job Name	Date	Details	Resubmit
JNB-Frontera	03/18/2022	Details	Resubmit
JNB-Frontera	03/18/2022	Details	Resubmit
JNB-Frontera	03/18/2022	Details	Resubmit
JNB-Frontera	03/18/2022	Details	Resubmit
JNB-Frontera	02/21/2022	Details	Resubmit

Jupyter notebook: Accessing shell

TACC | Analysis Portal | [User Guide](#) | [jrduncan](#) | [Log Out](#)

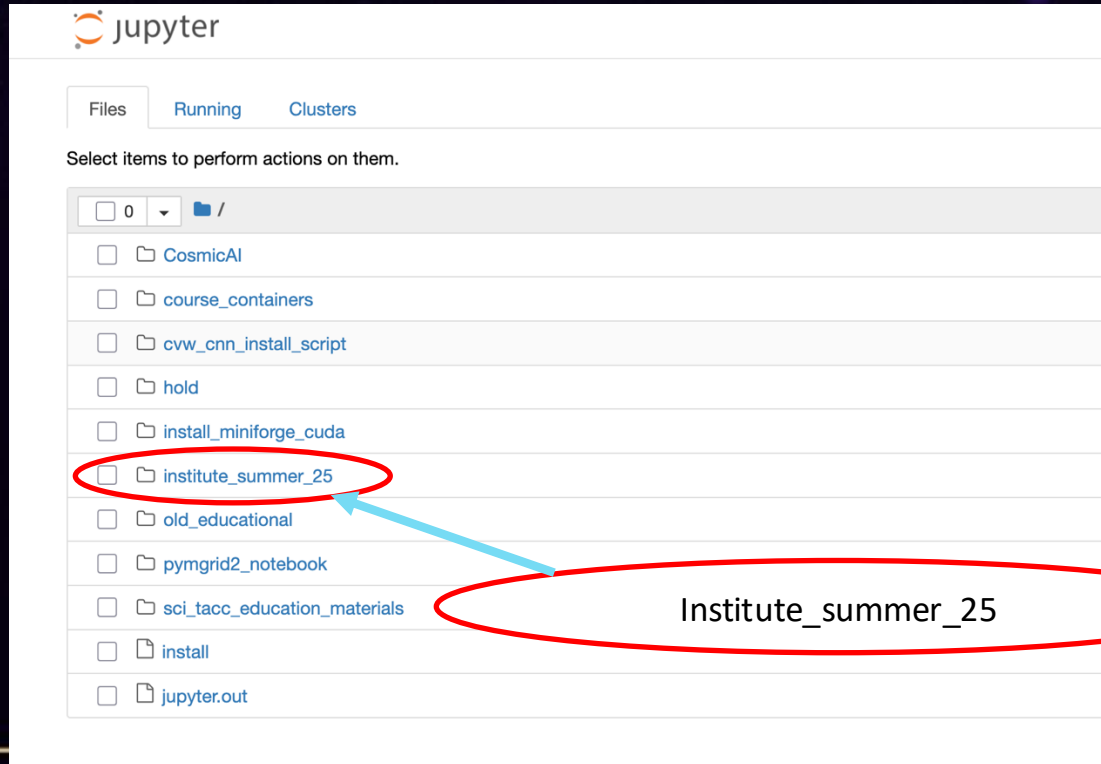
TAP Job Status

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[Connect](#) [End Job](#) [Show Output](#) [Back to Jobs](#)

Jupyter notebook: Accessing New Python Notebook



The screenshot shows the Jupyter web interface. At the top, there's a header with the Jupyter logo and the word "jupyter". Below this, there are tabs for "Files", "Running", and "Clusters". The "Files" tab is selected. A message says "Select items to perform actions on them." Below this is a file browser showing a list of files and folders. The folder "institute_summer_25" is highlighted with a red circle. A blue arrow points from this folder to a larger red circle containing the text "Institute_summer_25".

Files Running Clusters

Select items to perform actions on them.

0 /

- ☐ CosmicAI
- ☐ course_containers
- ☐ cvw_cnn_install_script
- ☐ hold
- ☐ install_miniforge_cuda
- ☐ **institute_summer_25**
- ☐ old_educational
- ☐ pymgrid2_notebook
- ☐ sci_tacc_education_materials
- ☐ install
- ☐ jupyter.out

Institute_summer_25

Jupyter Notebook: Open Existing File

- Click on the [institute_summer_25](#) directory in the list
- Click on **KNNs** directory in the list
- Click on the file notebook file [intro_sklearn.ipynb](#)
- A Jupyter notebook should launch in a new tab
- Check to make sure you can run this notebook in the containerized kernel



Thanks!!

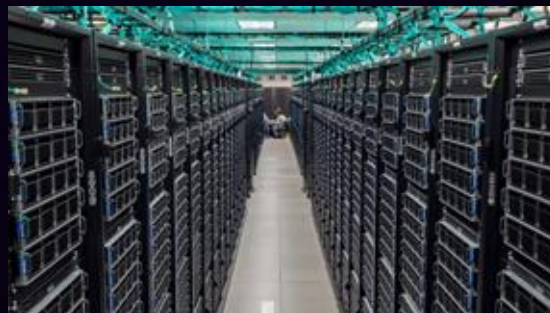
- Any Issues on TACC Systems that we can not help you with?
 - Open a ticket at <https://tacc.utexas.edu/about/help/>



Supplemental Slides

File Transfer Mechanisms

- Copying files from your local machine to TACC system
- Mac/OSX or Linux
 - Open Terminal window
 - Use scp (Secure Shell Copy)
 - Copies over ssh connection
 - -r option for recursive



```
scp <local file name> user@frontera.tacc.utexas.edu
```

```
scp -r <local folder name> user@frontera.tacc.utexas.edu:
```

File Transfer Mechanisms (2)

- Copying files from your local machine to TACC system
- Windows
 - Download WinSCP (<https://winscp.net>)
 - Double click installer
 - Choose “Explorer” Option
 - Hostname: `frontera.tacc.utexas.edu`
 - Username: `username`
 - TACC Code: <Use Code from your credentials handout>
- Drag and Drop Files/Folders to copy to Stampede2



Command Line Editing

- Often will be required
 - Working with code
 - Editing configuration files
 - Writing Bash Scripts
 - TACC Systems: Writing job submission scripts
- Vim
 - Vi Improved
- Emacs
- Nano
 - Simple, Easy to use



module

- On TACC Systems the module system helps setup or teardown useful packages that are supported by TACC, on the fly
- To find more information on a module
 - `module spider package-name`
- To load a module
 - `module load package-name`
 - `module load package-name/version.number`
- [Learn more here](#)

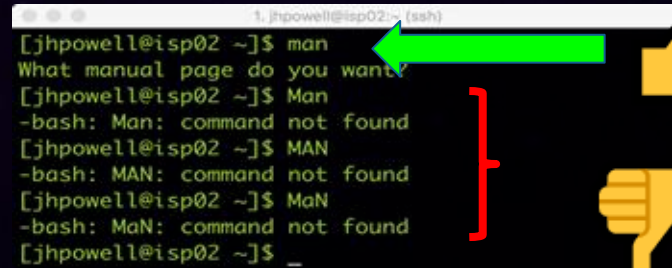


Linux/bash

- TACC machines use the Linux operating system
- Default shell and most popular is bash (Bourne Again Shell)
- Bash features auto completion of commands with tab key
- Bash commands are case sensitive

Example:
The “**man**”
command

`man` \neq `Man` \neq `MAN`



A terminal window titled '1. jhpowell@isp02:~ (ssh)' showing the following commands and outputs:

```
[jhpowell@isp02 ~]$ man  
What manual page do you want?  
[jhpowell@isp02 ~]$ Man  
-bash: Man: command not found  
[jhpowell@isp02 ~]$ MAN  
-bash: MAN: command not found  
[jhpowell@isp02 ~]$ MaN  
-bash: MaN: command not found  
[jhpowell@isp02 ~]$ _
```

A green arrow points to the first 'man' command, and a red bracket groups the subsequent 'Man', 'MAN', and 'MaN' commands.

