AggieSTAAR Python Bootcamp

Tutorial 5: Computing Resources and Remote Access

TEXAS A&M UNIVERSITY

Computing Resources in Astronomy

Astronomers sometimes deal with large data products or complicated models. Computing resources can be essential to do your research efficiently.

Thankfully, TAMU has High Performance Computing Resources (HPRC) available upon request.

Remote Access

Depending on your advisor, you may need to access:

1. Grace or FASTER (HPRC)
2. Saire (Justin Spilker's personal machine)

which will require establishing a remote connection from your computer. There are two ways to do so:

1. Graphic User Interfaces (GUIs)
2. SSH (Secure SHell) connections through terminal

GUIs - Graphic User Interfaces

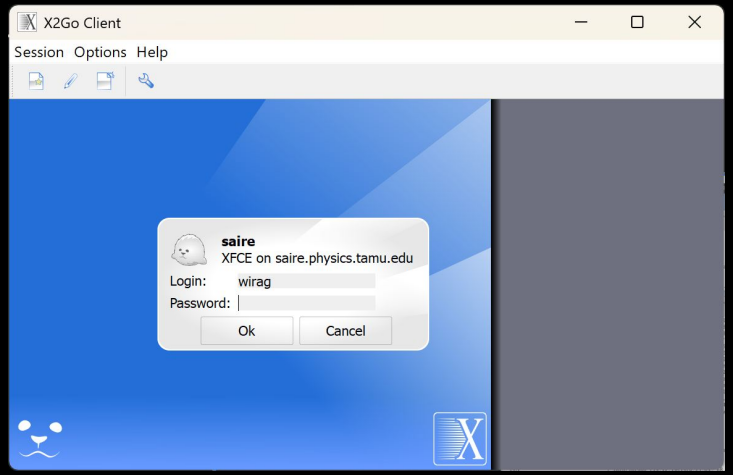
GUIs are user-friendly ways to execute commands

- File explorer (Windows) and Finder (Mac) are examples of these

If you're working with Justin Spilker, you will need to install x2go

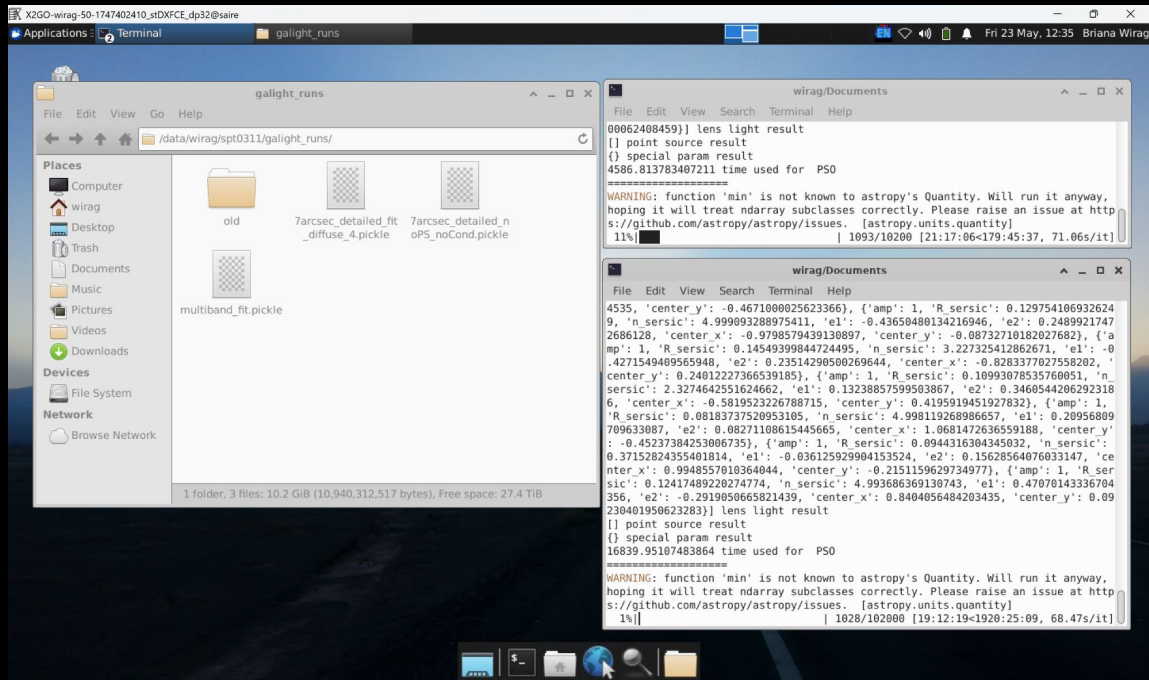
- X2go opens a window on your computer that is actually running on Saire

GUIs - Graphic User Interfaces



<- Launch from here in x2go

The remote window ->



SSH - Terminal

Another way to access Saire, and how you would connect to Grace, is through the terminal (Mac) or powershell/command line (Windows). You will initiate an SSH connection by typing the following:

- Saire: <username>@saire.physics.tamu.edu
- Grace: <username>@grace.tamu.edu

You will be prompted to enter your TAMU password (then DUO for Grace)

- NOTE: your password will NOT show up as you type, just trust the process

SSH - Terminal

```
(base) PS C:\Users\briwi> ssh wirag@saire.physics.tamu.edu

Texas A&M University

This computer system and the data herein are available only for authorized purposes by authorized users. Use for any oth
er purpose is prohibited and may result in disciplinary actions or criminal prosecution against the user. Usage may be s
ubject to security testing and monitoring. There is no expectation of privacy on this system except as otherwise provide
d by applicable privacy laws. Refer to University SAP 29.01.03.M0.02 Acceptable Use for more information.
wirag@saire.physics.tamu.edu's password:
```

Saire

```
(bhenv) PS C:\Users\briwi> ssh wirag@grace.tamu.edu
********************************************************************************
This computer system and the data herein are available only for authorized
purposes by authorized users. Use for any other purpose is prohibited and may
result in disciplinary actions or criminal prosecution against the user. Usage
may be subject to security testing and monitoring. There is no expectation of
privacy on this system except as otherwise provided by applicable privacy laws.
Refer to University SAP 29.01.03.M0.02 Acceptable Use for more information.
********************************************************************************

(wirag@grace.tamu.edu) Password:
(wirag@grace.tamu.edu) Duo two-factor login for wirag

Enter a passcode or select one of the following options:

 1. Duo Push to XXX-XXX-[redacted]
 2. Phone call to XXX-XXX-[redacted]

Passcode or option (1-2): 1
Success. Logging you in...
```

Grace

Running code on Grace

Grace has two primary directories:

- /home/user/<username>/ <- the default upon login
- /scratch/user/<username>/ <- NEED to work from here
  - Always run code from your scratch directory.

Once logged in, you'll need to set up virtual environments

```
*** Grace Terminal ***
cd /scratch/user/<username>          # change working directory to scratch
module load Anaconda3/2024.02-1      # load Anaconda to use conda commands
conda create --name my_env           # create env. called my_env (or whatever name)
conda activate my_env                # activate my_env before package installation
conda install python pip astropy…    # install necessary packages
### if conda DOESN'T work ###
pip install <package>                # some packages are only available with pip
```

Running code on Grace

Important: HPRC is a shared resource, so we cannot run code directly from the Grace terminal (or face the wrath of an angry email reminding you)

- Instead, we submit job requests so resources are allocated fairly. Your Grace account will be charged in SUs

```
#!/bin/bash

#SBATCH --job-name=ngc383                    # Job name
#SBATCH --time=2:00:00                       # Job time limit
#SBATCH --ntasks=48                          # Task/core, max cores per node is 48
#SBATCH --ntasks-per-node=48                 # Task/core per node (equal to ntasks for 1 node)
#SBATCH --mem=50G                            # Memory limit per node, max is 384GB
#SBATCH --output=out.%j                      # Outfile -- %J for unique job number
#SBATCH --account=<##>                       # Project account number associated with GRACE
```

Job specifications

```
module purge                                 # Purge all modules
module load Anaconda3/2024.02-1              # Load the Anaconda3 module
cd /scratch/user/wirag/ngc383                # Change directory
source activate bhenv                        # activate environment
python jam_optimization.py                   # Run script
conda deactivate                             # deactivate environment
```

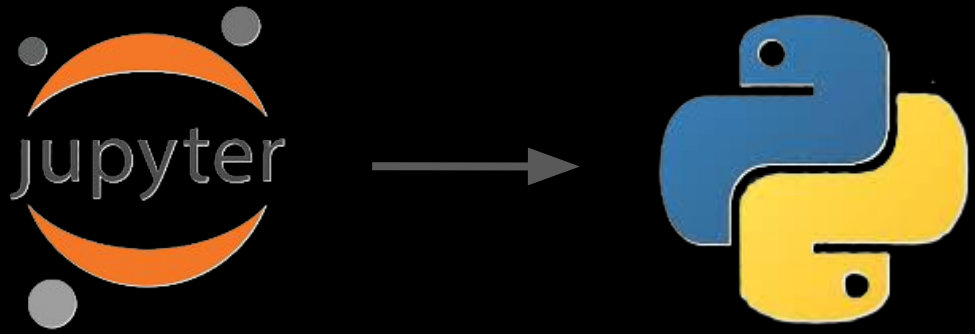
Example of executable terminal commands

Running code on Grace

We learned about Jupyter Notebooks (.ipynb files) in a previous tutorial. However, you may have noticed I was running a .py file

- Since we access Grace through SSH, and to comply with the resource allocation system, we must run python scripts

Notebooks are great for testing code locally (on your computer) so you don’t eat up your SUs on Grace



Running code on Grace

After running your code, you'll need to transfer any outputs to your local computer for analysis.

```
*** Local Terminal ***
scp <username>@grace.tamu.edu:/scratch/user/<un>/path_to_files/files /Local/path
```

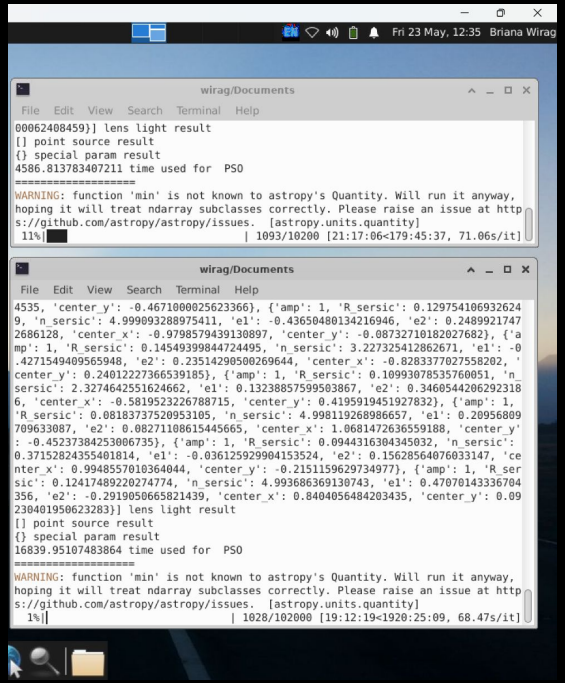
OR

```
*** Local Terminal ***
cd /Local/path
scp <username>@grace.tamu.edu:/scratch/user/<un>/path_to_files/files .
```

The period means "current directory", you can double check what that is by typing pwd into the terminal

Running code on Saire

Since we can access Saire through SSH or a GUI, we can run both scripts and notebooks.



After connecting with x2go, you can run scripts as normal

- Can run code from /home/<username>
- Store data/files in /data/<username>

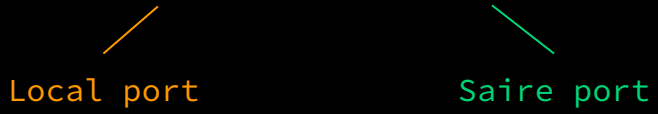
Any code started in a terminal this way will continue to run in the background

Running code on Saire

Running notebooks in x2go can be quite laggy. Thankfully, we can open a local browser that's running the remote notebook

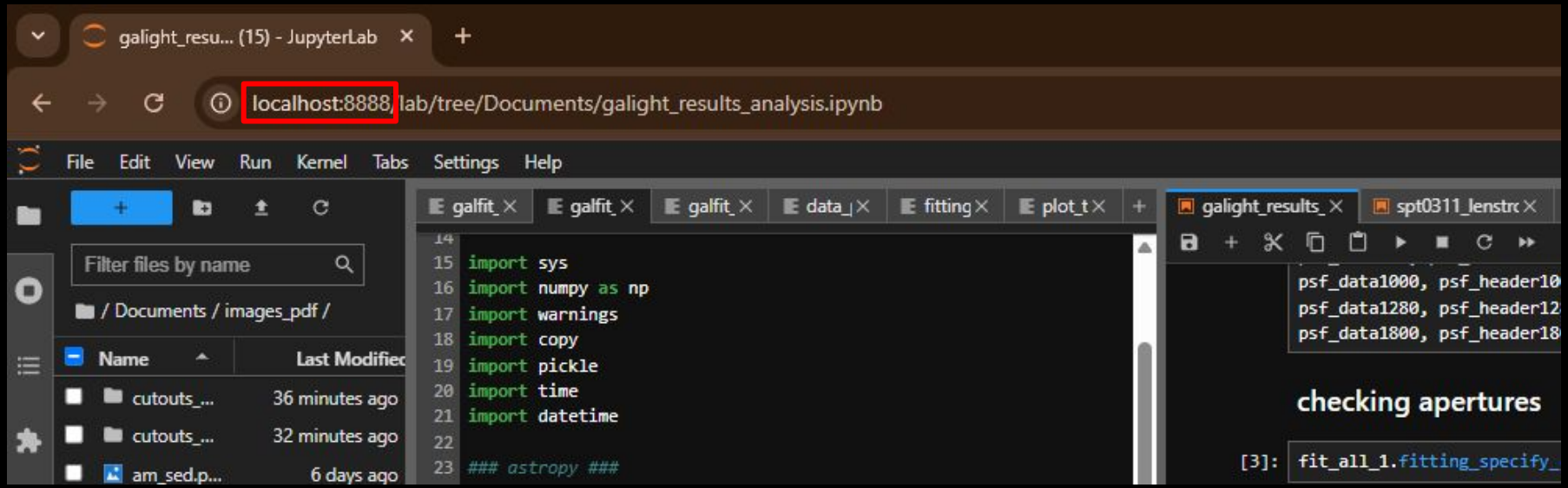
```
*** Saire Terminal ***
ssh <username>@saire.physics.tamu.edu
*** enter password ***
jupyter lab --no-browser --port=8889 #or another Saire port

*** Local Terminal ***
ssh -N -f -L localhost:8888:localhost:8889 <username>@saire.physics.tamu.edu
```



Then type localhost:8888 into a browser on your computer (it may ask for a token, which will be in the Saire Terminal)

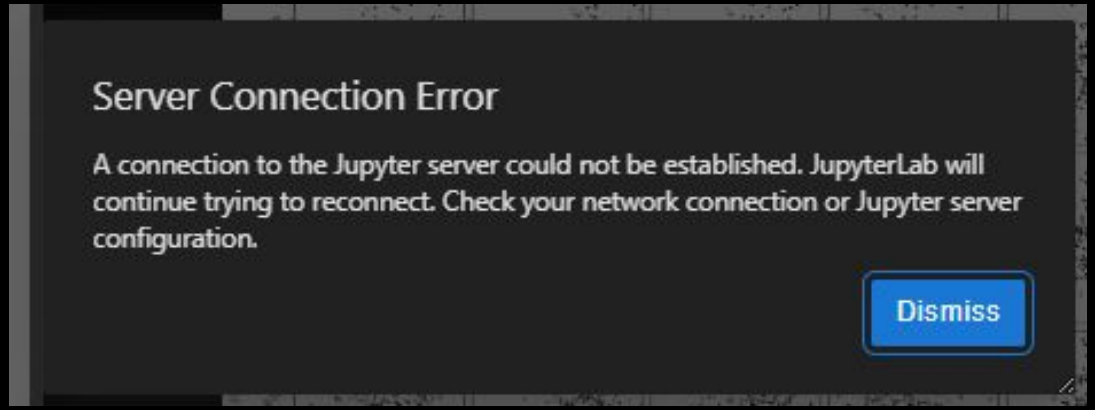
Running code on Saire



This will look the exact same as normal Jupyter, but all of this is actually running on Saire

- Configuration will be preserved after disconnecting

Running code on Saire



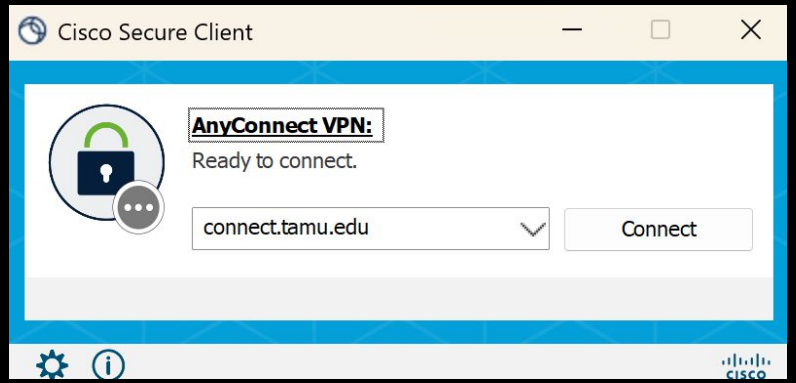
Unlike running scripts in x2go, if the ssh connection breaks, the notebooks do NOT continue running, so you will need to re-establish the connection and restart the notebook

- This happens if you're inactive for too long or lose internet connection

Remote Access From Home

Everything mentioned thus far is assuming you are connected to TAMU wifi

- If you need to access these resources from home, you will need to install the TAMU VPN (here)
- Follow the instructions under “**Getting Started**”



Additional Resources

- Check out the TAMU HPRC website for more information about Grace
  - Includes more detailed explanations and examples than what was presented here
- If working with Justin Spilker, go to this Evernote page for more information about Saire
- When in doubt, look it up or ask for help :)