HPC Workshop 2024

Upward Bound – Day 2

https://uwec.ly/hpcworkshop

Please log into your machine when you take a seat.

HPC Workshop: Last Week

Intro to computational science and HPC

Tyler Bauer
Blugold Center for HPC

Building “trees” in South African shrubs

Dr. Nora Mitchell
Biology

What stresses out California ground squirrels?

Dr. Jennifer Smith
Biology

HPC Workshop: Today

Coding in Python

Somin Lee
Blugold Center for HPC

How to engineer a super-bouncy ball

Dr. Ying Ma
Materials Science and Biomedical Engineering

The Lives of the Stars

Dr. Bill Wolf
Physics + Astronomy

SCIENCE • TECHNOLOGY • ENGINEERING + ARTS • MATHEMATICS

Panel Discussion on STEAM careers with:

Dr. Bill Wolf – Assistant Professor (Physics + Astronomy)

Dr. Jennifer Smith – Assistant Professor (Biology)

Dr. Kao Yang – Former Upward Bound and UWEC Graduate (Ph. D in Material Science)

Melody Manteufel – Outreach Counselor (Advising, Retention + Career Center)

Elaina Plonis – Research Student (Physics + Astrophysics Emphasis Major & Math + Computer Science Minor)

Workshop Website

https://uwec.ly/hpcworkshop

Contains the schedule, presentations, and important links.

https://ondemand.hpc.uwec.edu

You can also get to OnDemand from our webpage

OnDemand - Login

Welcome to BOSE!

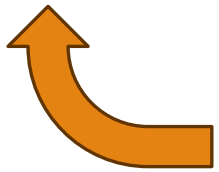
You appear to be a new member of the cluster, so there are a few steps you'll need to accomplish first before you're able to use this system.

1. Click this button to access the terminal / shell version of BOSE first.
2. You'll be asked to enter your UWEC password and trigger the Duo Authentication process.
3. Once logged in, go through and accept our Terms Of Service.
4. After you accept the terms, you can close out of that tab once you are presented with [username@bose ~].
5. Finally, click this button to log in again.

Already used BOSE and are getting this message, or this message isn't going away after going through the steps? Please contact us at BGSC.ADMINS@uwec.edu.

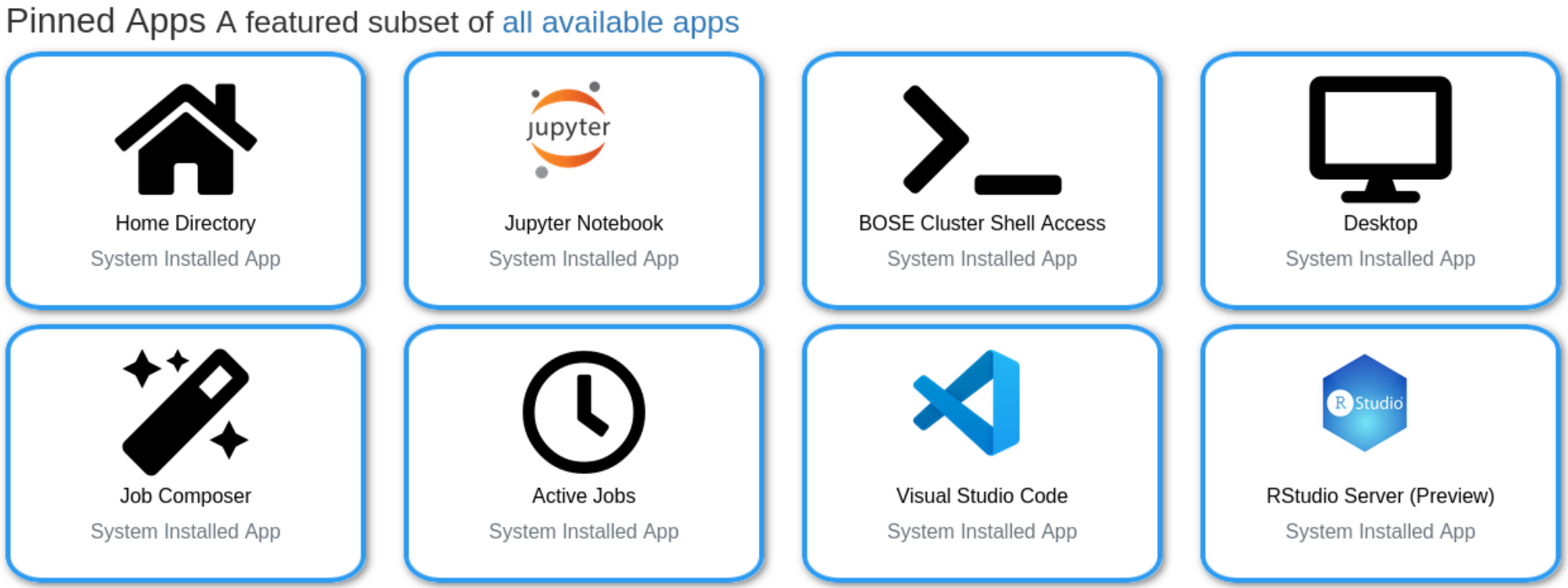
- Blugold Center for High Performance Computing

HPC Website | HPC Wiki

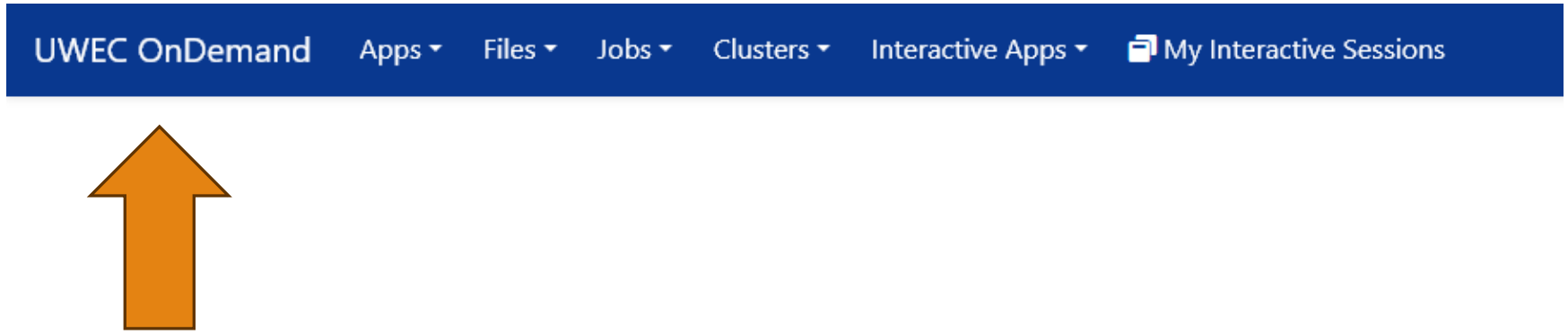


See this? Raise your hand and we'll catch you up.

OnDemand – Dashboard / Home

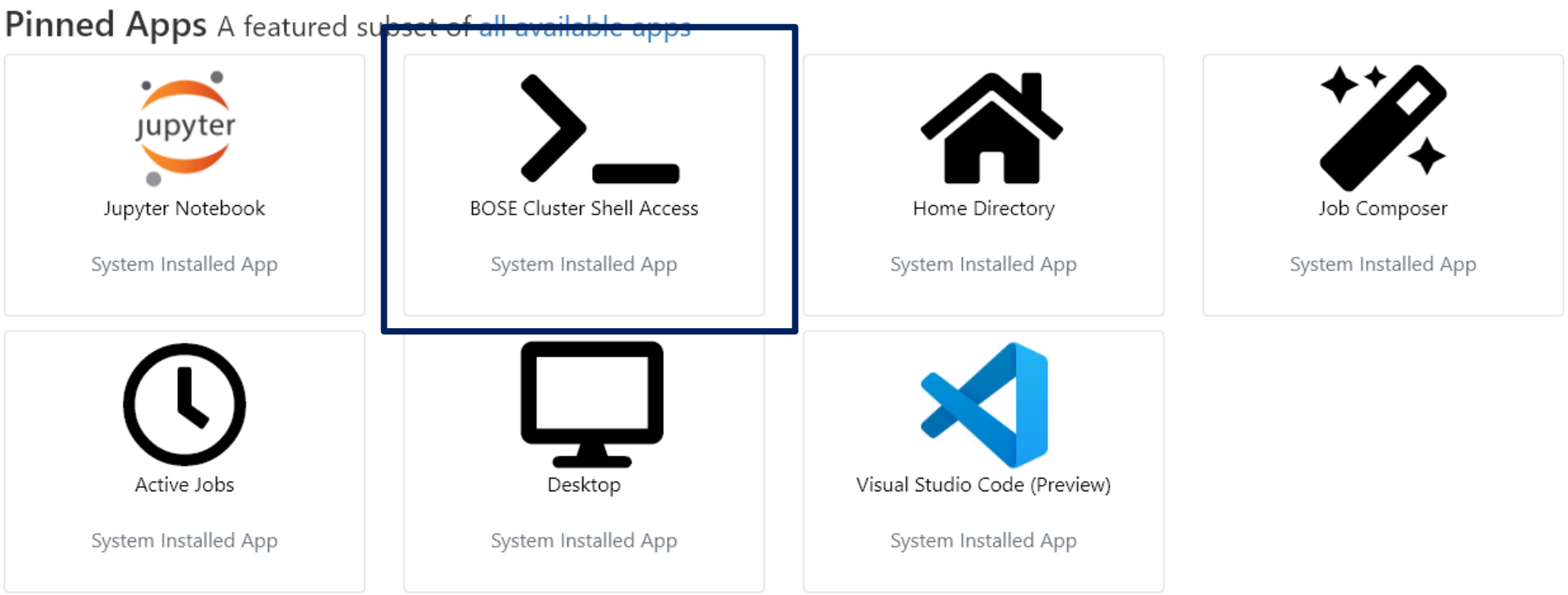


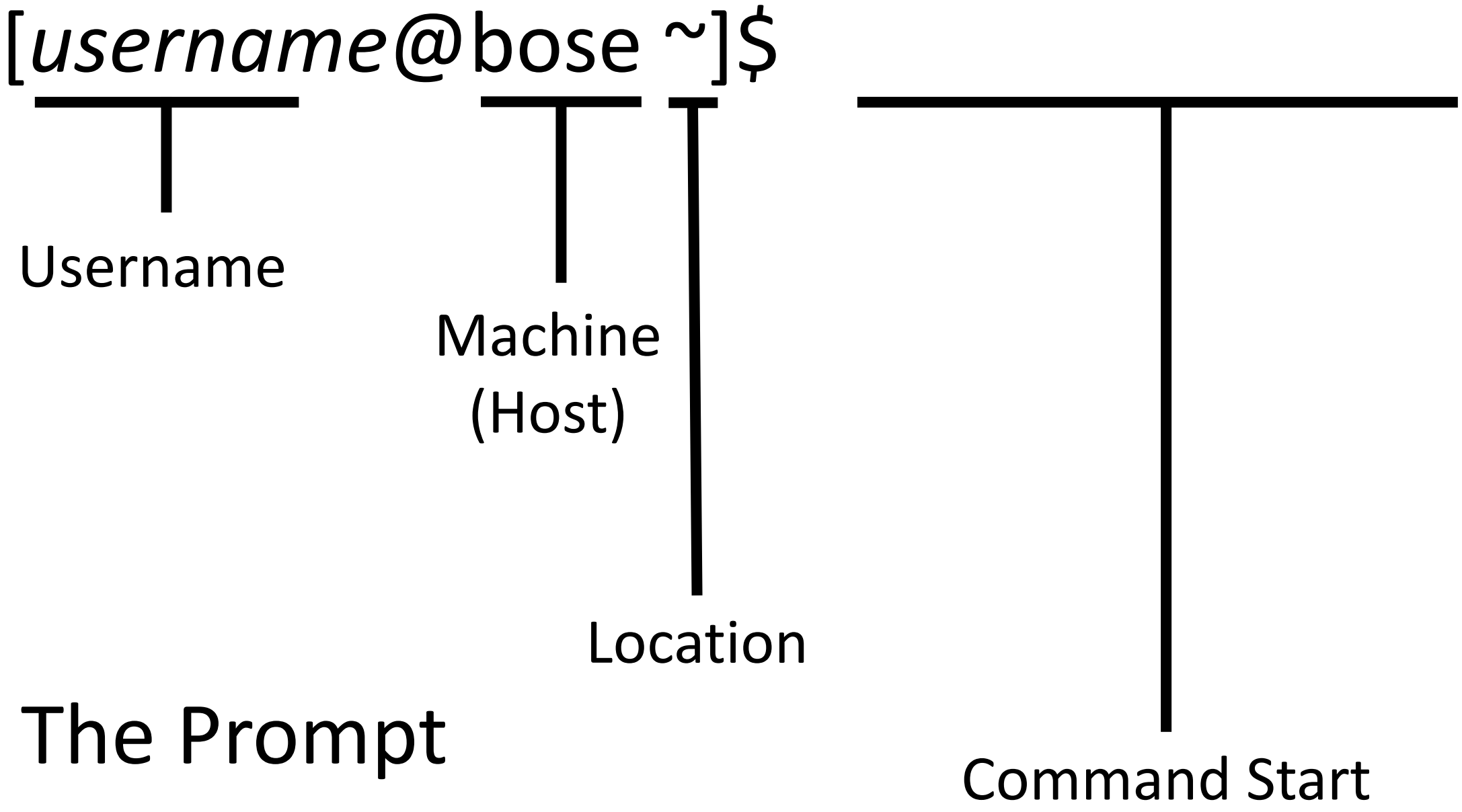
Lost? Go back to home!



Go Back Home (Dashboard)

OnDemand – Getting presentation files




[username@bose ~]$
Username
Machine
(Host)
Location
Command Start

The Prompt

Type:

getfiles 4 ← Means “get the files for session #4”

(You’ll be doing this in each session today)

Commands we'll be using:

ls - View files in current directory (l as in 'lamp')
pwd - Show where you currently are
cd - Change your directory
sbatch – Submit a job to our supercomputer

Check out the Linux Quick Guide on the website as a reference.

Let’s check those files out!

Type:

```
cd                  (Go back to home)
ls                  (Verify you see Day_2)
cd Day_2/Session_4      (Go to our session files)
ls                  (Verify you see runscript.sh)
```

Let’s run a program on a supercomputer!

Type:

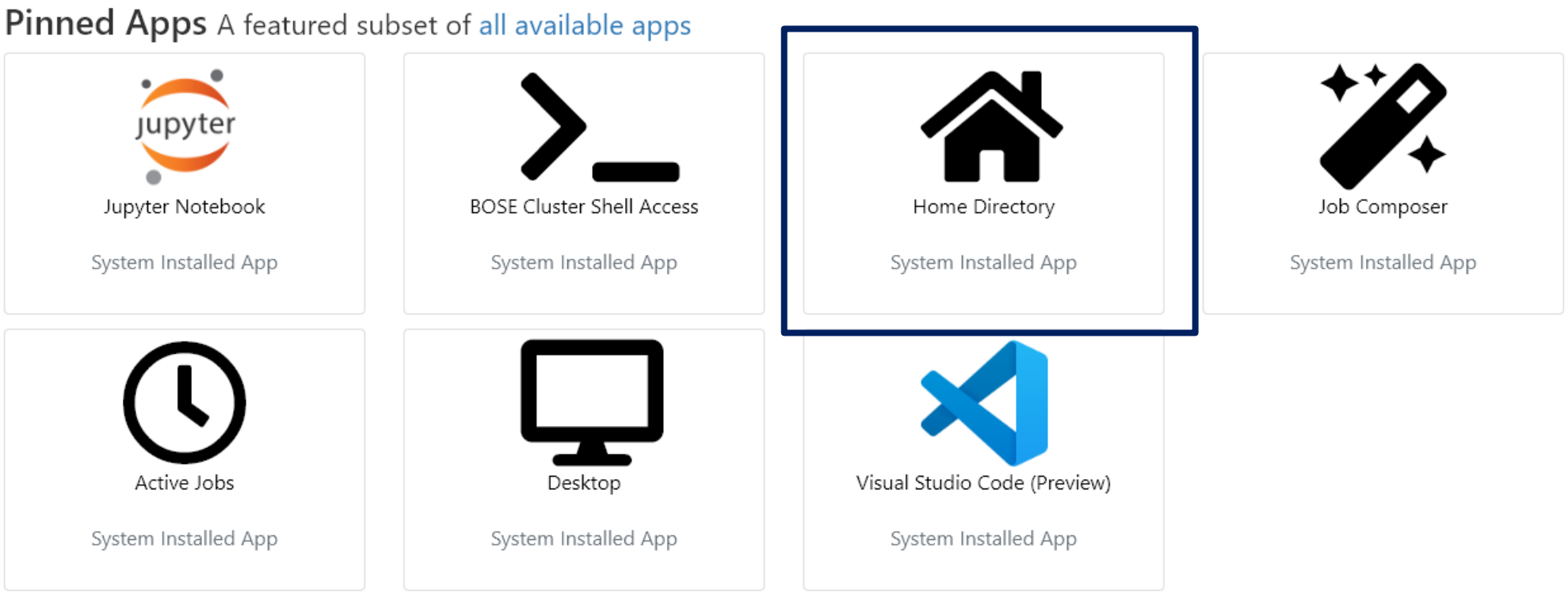
sbatch runscript.sh

Does it say “Submitted batch job #”?

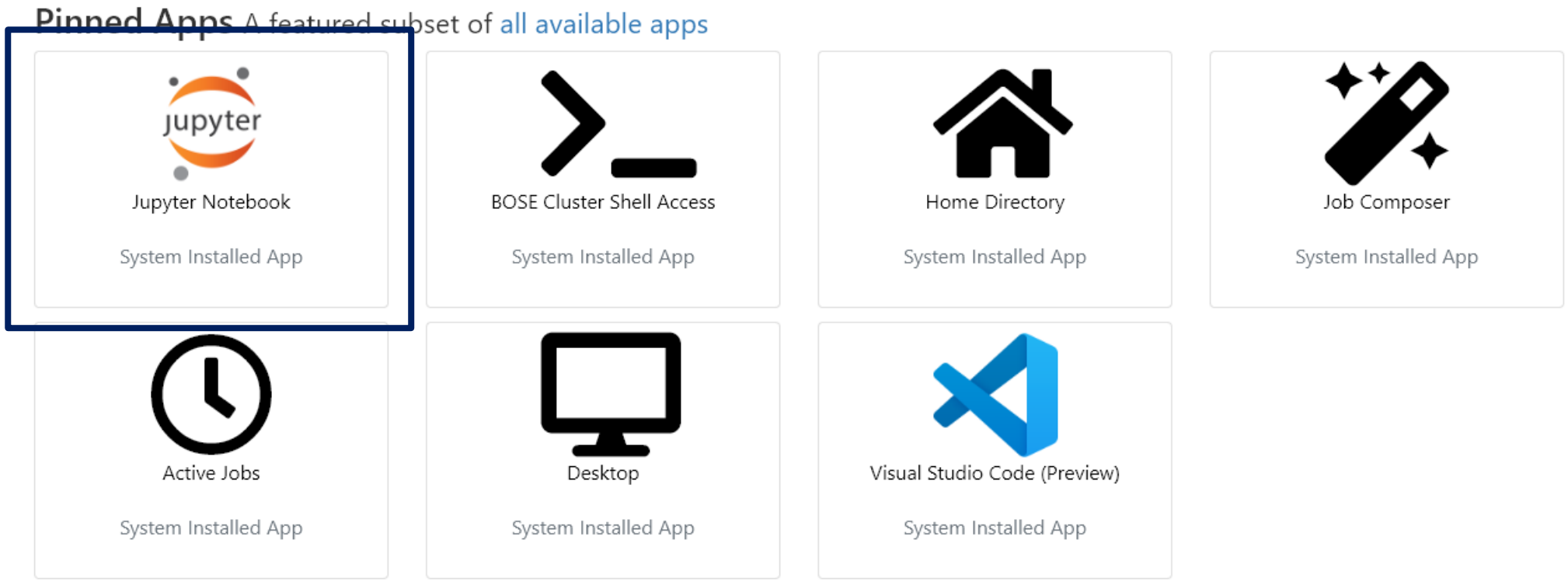
You did it!

Let’s go check it out!

OnDemand – File Manager

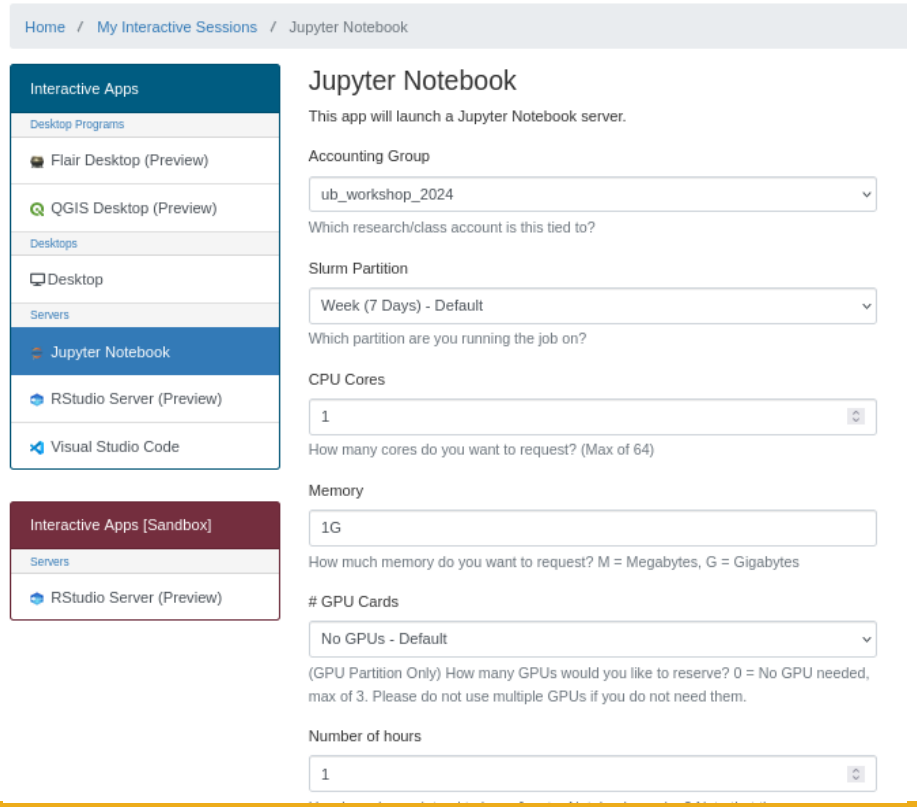


OnDemand - Jupyter



Creating a Notebook

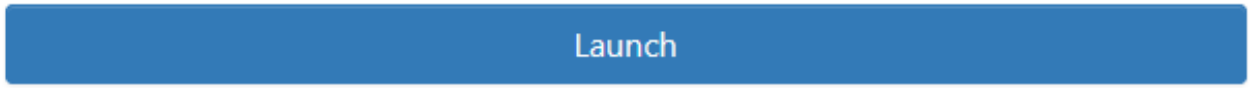
Once you click the Jupyter button, you should see something like this



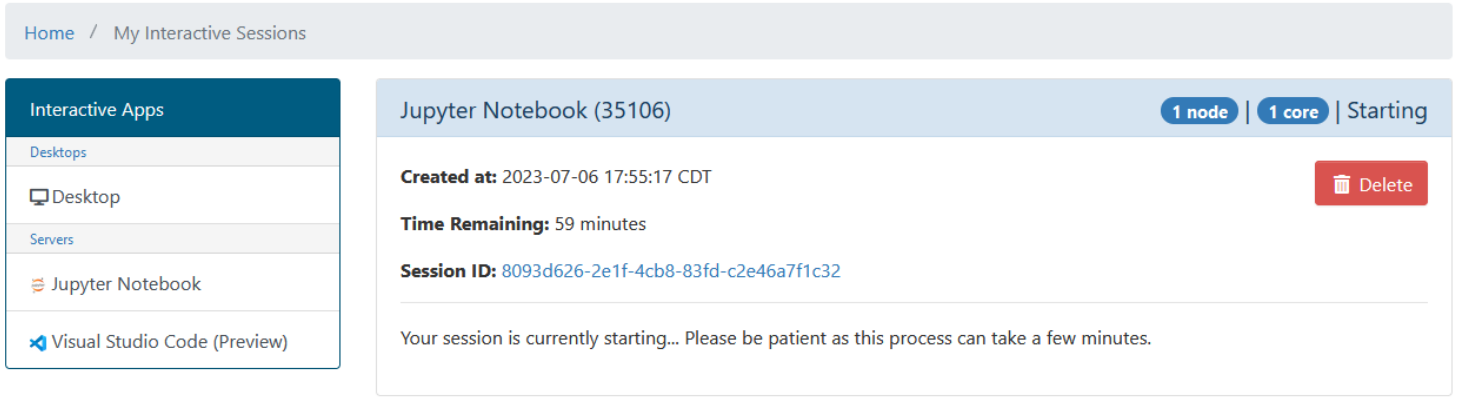
<u>Use these settings</u>

Accounting Group: ub_workshop_2024
Slurm partition: Week
CPU Cores: 8
Memory: 15G
#GPU cards: No GPUs
Number of Hours: 2
Working Directory: Leave empty

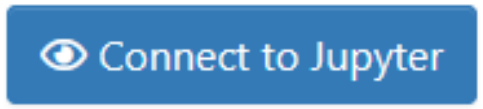
Then, click



Once you have created your notebook, you should see a screen like this

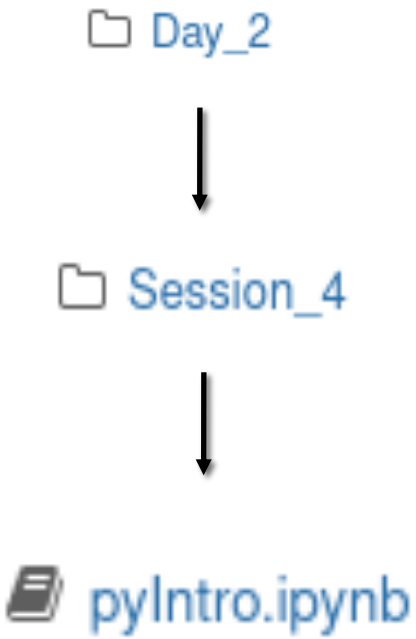


Once your notebook has started, click this button to access it:



Jupyter file view

You should now see a list of the files in your home directory. Open these folders:



Python

THE BASICS

What is Python?

- Increasingly popular programming language
- Considered easy to learn and understand
- Supports interactive programming (e.g. Jupyter)
- 137,000+ Libraries Available
  - Code created by other people to make everyone's life easier

What is it used for?

- Task Automation
- Artificial Intelligence, Machine Learning, Deep Learning
- Data Analysis
- Data Visualization
- Game Development
- Web Development

Jupyter Notebook

- Supports variety of languages: Python, R, Ruby, C++, Stata
- Cell-Based = Run blocks of code at a time rather than everything at once
- Visually see tables, images, graphs, 3D renderings

- **How To Use:**
  - Each piece of code is in a “Cell” that must be ran individually
  - Run a cell by clicking “Run” or pressing “Shift+Enter”
  - Wait for results – “In [*]” on left means running, a number means done.

Let’s code in Python!

Task 1: print() function

```
print("Hello, World!")

print("You can put any text here!")
```

Task 2: Variables

```
name = "Somin"
age = 24
is_student = True
```

Task 3: Display variables

```
print(name)
print(age)
print(is_student)
```

Make sure to press “Run” after each task!

Task 4: Display variable with string

```
print("My name is " + name)
```

Task 5: Arithmetic operations

```
#Addition
print(5 + 3)

#Subtraction
print(10 – 4)

#Multiplication
print(7 * 2)

#Division
print(8 / 2)

#Modulus (remainder)
print(9 % 4)
```

Make sure to press “Run” after each task!

Task 6: String Operations

```
#Concatenation
first_name = "Somin"
last_name = "Lee"
full_name = first_name + " " + last_name
print(full_name)

#Repetition
laugh = "Ha" * 3
print(laugh)
```

Make sure to press “Run” after each task!

Task 7: Import module

```
import random
```

Task 8: Set variables

```
# The computer picks a random number between 1 and 10
number_to_guess = random.randint(1, 10)

# Variable to store the user's guess
guess = 0
```

Make sure to press “Run” after each task!

Task 9: While loop and if statement

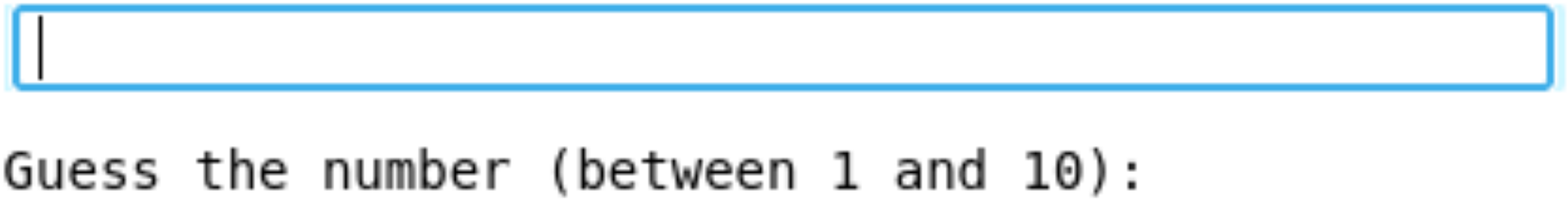
```
print("Guess the number:")

# Loop until the user guesses the correct number
while guess != number_to_guess:
    guess = int(input())          # Get user input and convert it to integer

    if guess < number_to_guess:   # If user guess is lower than the number

        print("Too low! Try again:")
    elif guess > number_to_guess:  # If user guess is higher than the number
        print("Too high! Try again:")

    else:                         # not lower & not higher? guess is correct
            print("Congratulations! You guessed it!")
```

Make sure to press “Run” after each task!

You created a game!

Once you have run the last two cells that you coded, you should see a screen like this.

Type in your guess in the box and play the game!



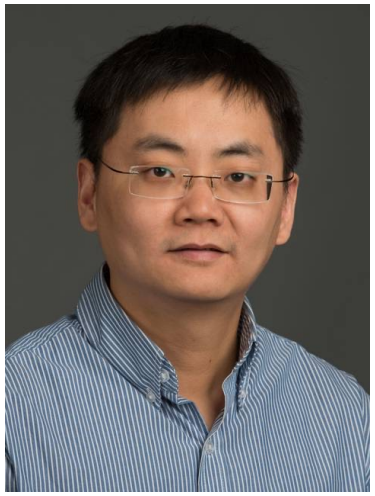
We Did It!

Any Questions?

Today's Schedule

Time	Who	What
9:00 – 10:15	Blugold Center for HPC	Recap of June 21st and coding in Python
10:30 – 11:45	Dr. Ying Ma	How to engineer a super-bouncy ball
11:45 – 12:45	LUNCH	LUNCH
12:45 – 2:00	Dr. Bill Wolf	The Lives of the Stars
2:15 – 3:15	Workshop Faculty + Guests	Careers in STEAM in Phillips Hall 265

Next Up



How to engineer a super-bouncy ball

Dr. Ying Ma, Ph.D.
Materials Science and Biomedical Engineering
Associate Professor

Pull up the website if you haven't already!

Website: https://uwec.ly/hpcworkshop

Lunch Break

BE BACK BY 12:45PM

Next Up

The Lives of the Stars

Dr. William Wolf, Ph.D.
Physics and Astronomy
Assistant Professor

Pull up the website if you haven't already!

Website: https://uwec.ly/hpcworkshop

Next Up – Panel Discussion

Let’s move to room 265!