HPC Workshop 2023

Upward Bound – Day 2

https://uwec.ly/hpcworkshop

Please log into your machine when you take a seat.

Last Week…

Intro to HPC, Computational Science, Linux

Mammoth and Mitchell
Blugold Center for HPC

Informatics in music

Dr. Ben Fine
Computer Science

Building “trees” in South African shrubs

Dr. Nora Mitchell
Biology

SCIENCE • TECHNOLOGY • ENGINEERING + ARTS • MATHEMATICS

© Iowa PBS

Panel Discussion on STEAM careers with:

Tyler Bauer (Blugold Center for HPC)
Dr. Sudeep Bhattacharyay (Chemistry + Biochemistry)
Dr. Ben Fine (Computer Science)
Dr. Nora Mitchell (Biology)
Dr. Bill Wolf (Physics + Astronomy)

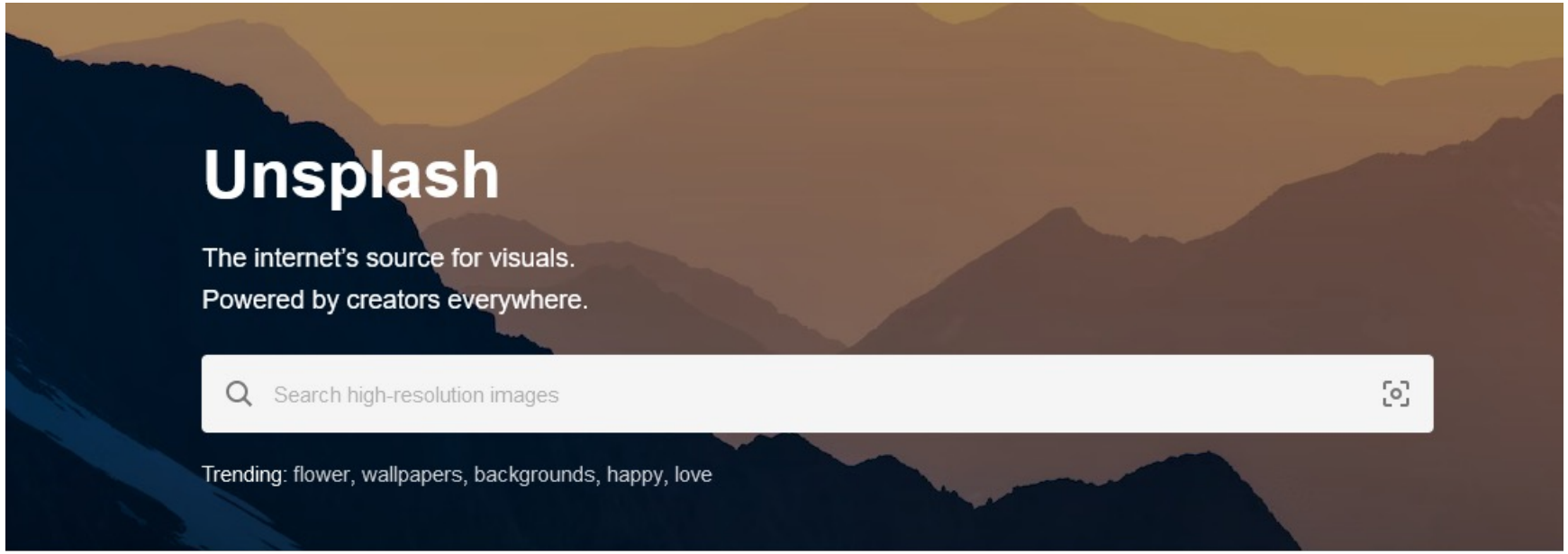
Task:
Our boss wants photos

Workshop Website

https://uwec.ly/hpcworkshop

Contains the schedule, presentations, and important links.

Photos from Unsplash.com



https://ondemand.hpc.uwec.edu

You can also get to OnDemand from our webpage

OnDemand - Login

Welcome to BOSE!

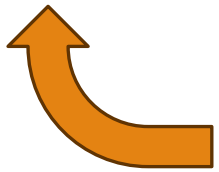
You appear to be a new member of the cluster, so there are a few steps you'll need to accomplish first before you're able to use this system.

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

Pinned Apps A featured subset of all available apps

Jupyter Notebook

System Installed App

BOSE Cluster Shell Access

System Installed App

Home Directory

System Installed App

Job Composer

System Installed App

Active Jobs

System Installed App

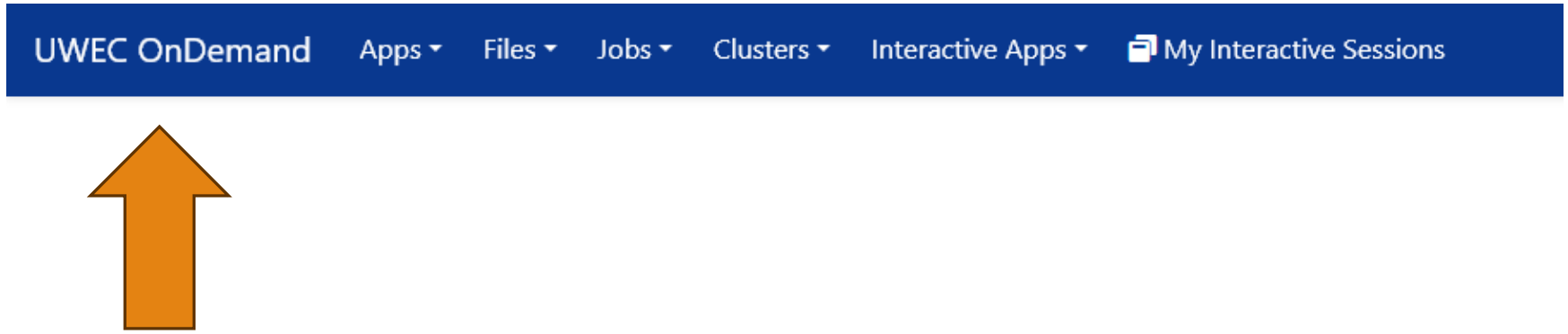
Desktop

System Installed App

Visual Studio Code (Preview)

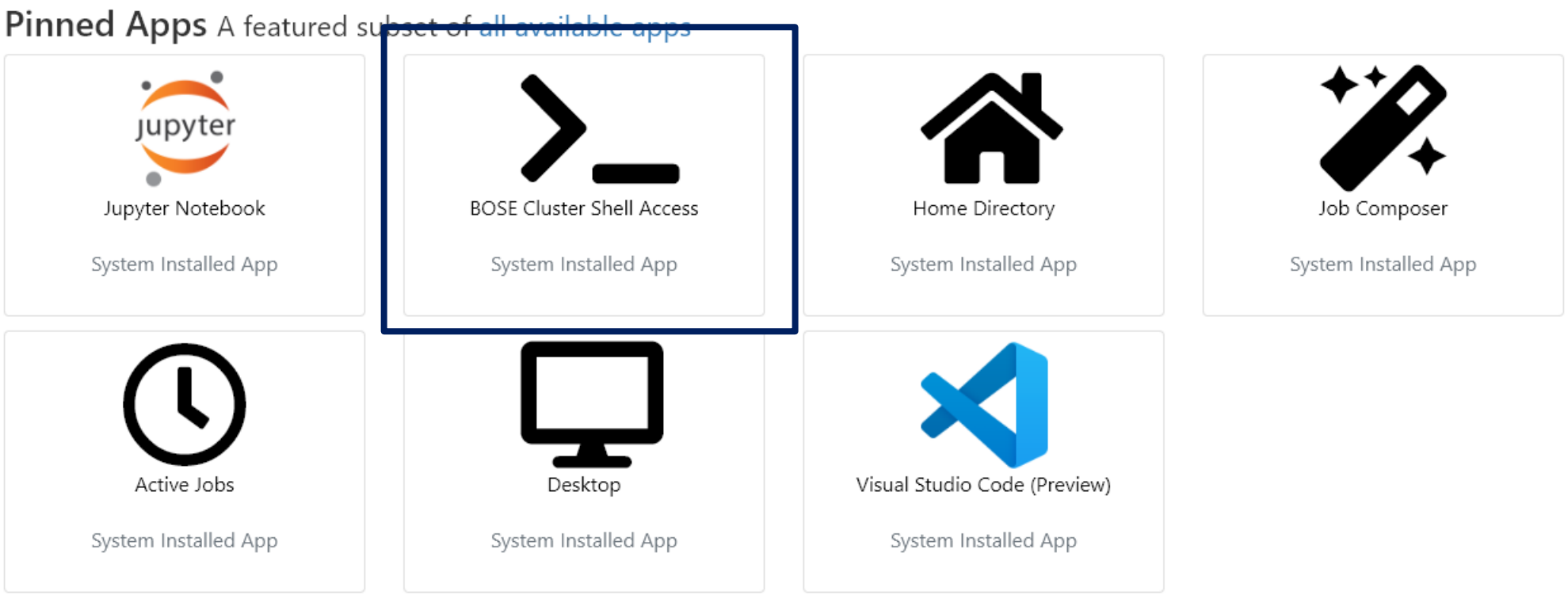
System Installed App

Lost? Go back to home!



Go Back Home (Dashboard)

OnDemand – Getting presentation files

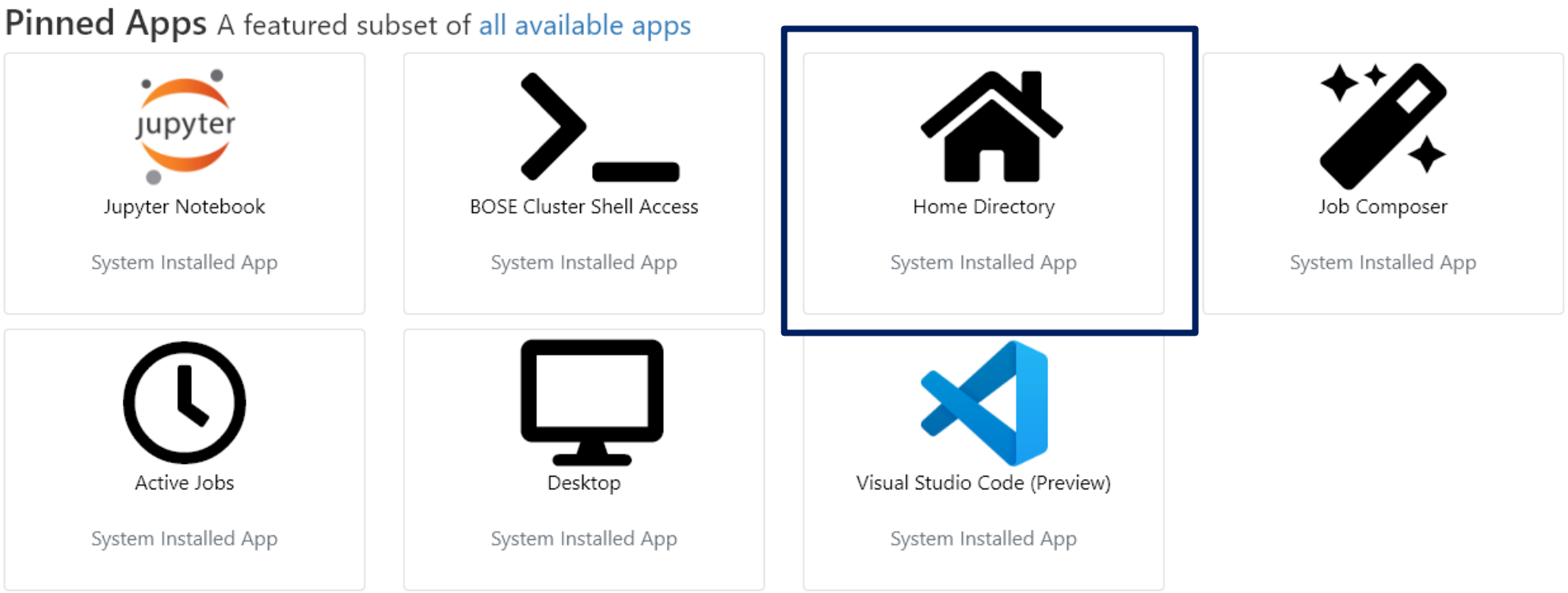


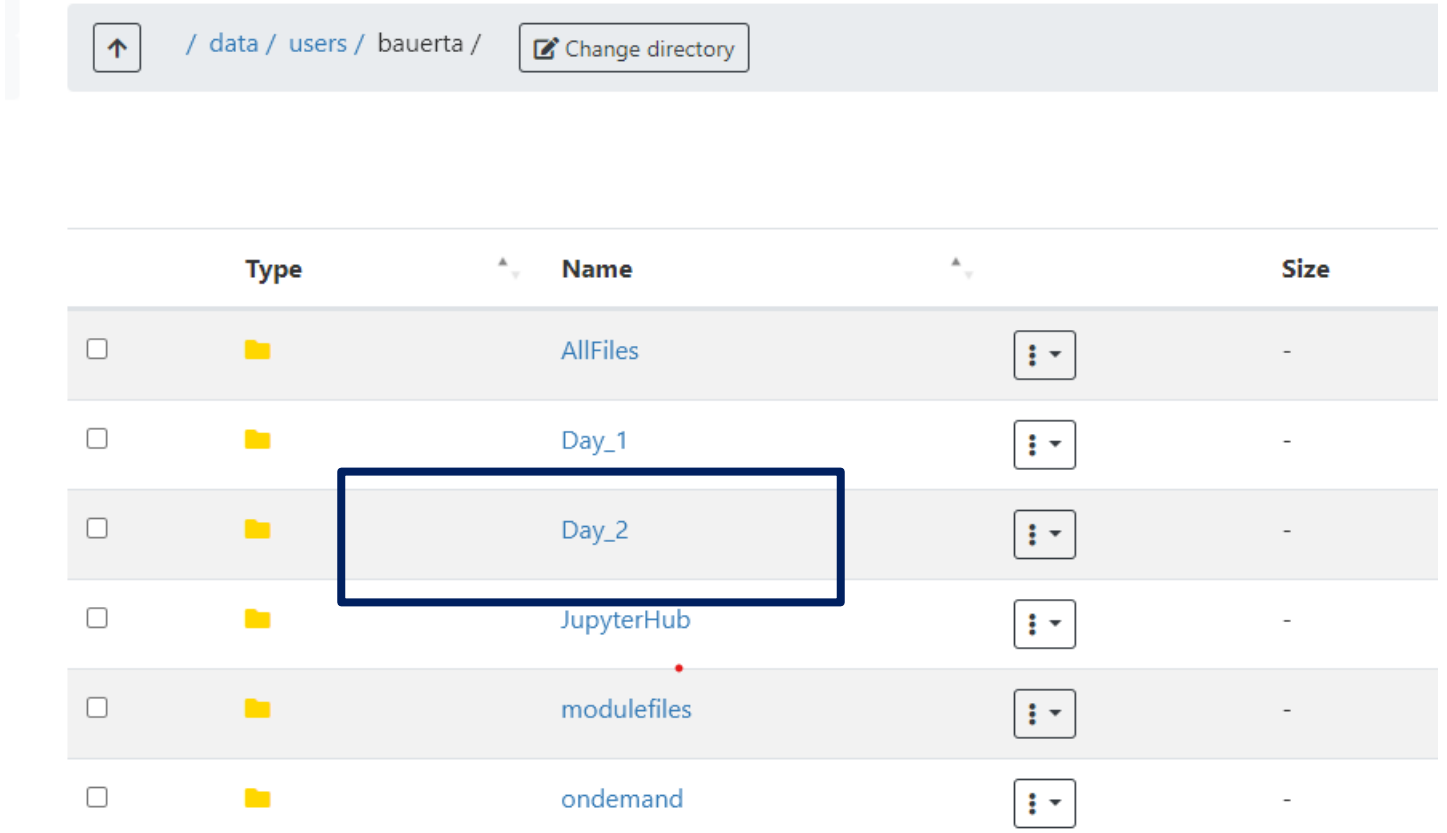
Type:

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

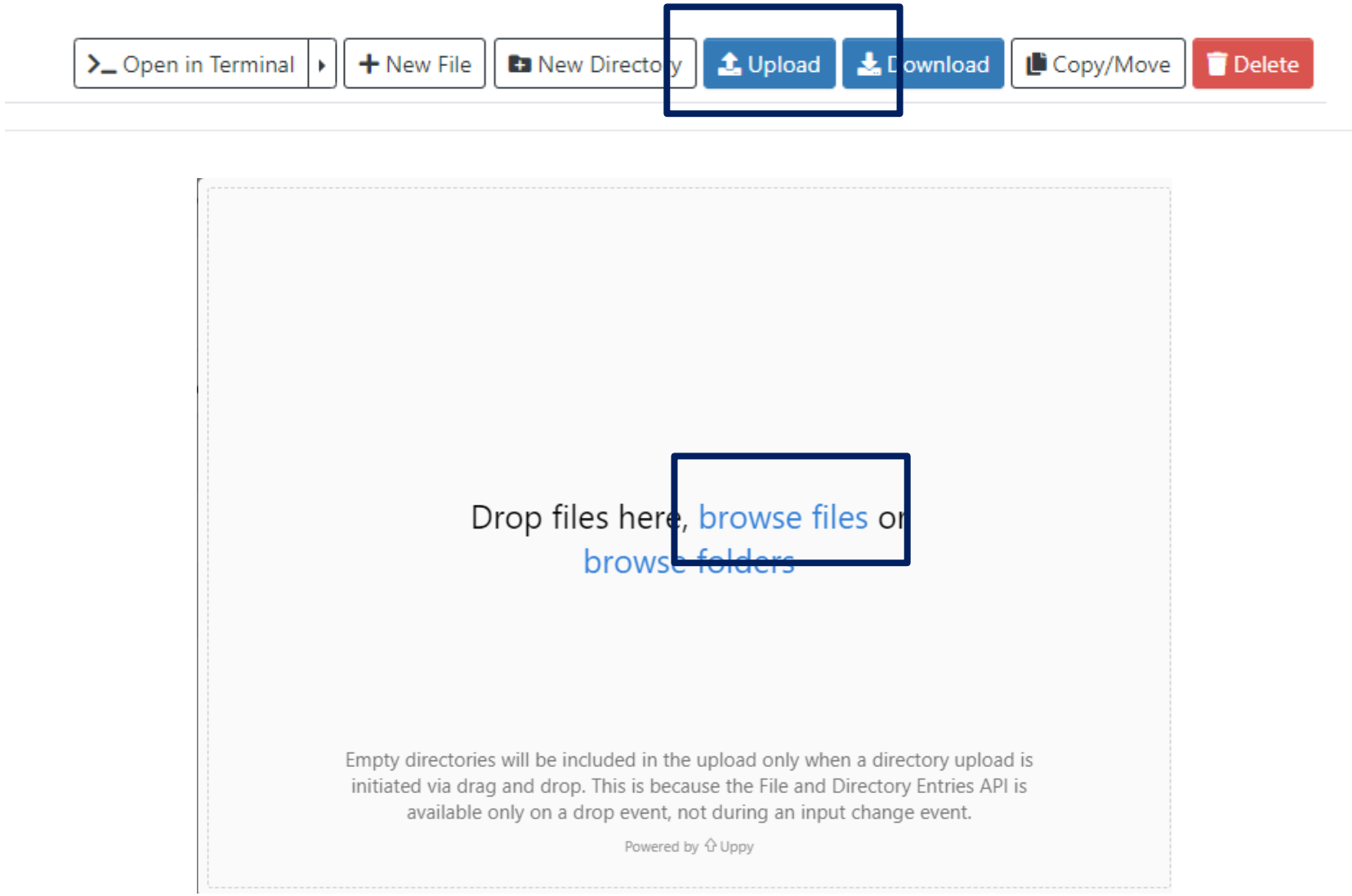
(You’ll be doing this in each session today)

OnDemand – File Manager

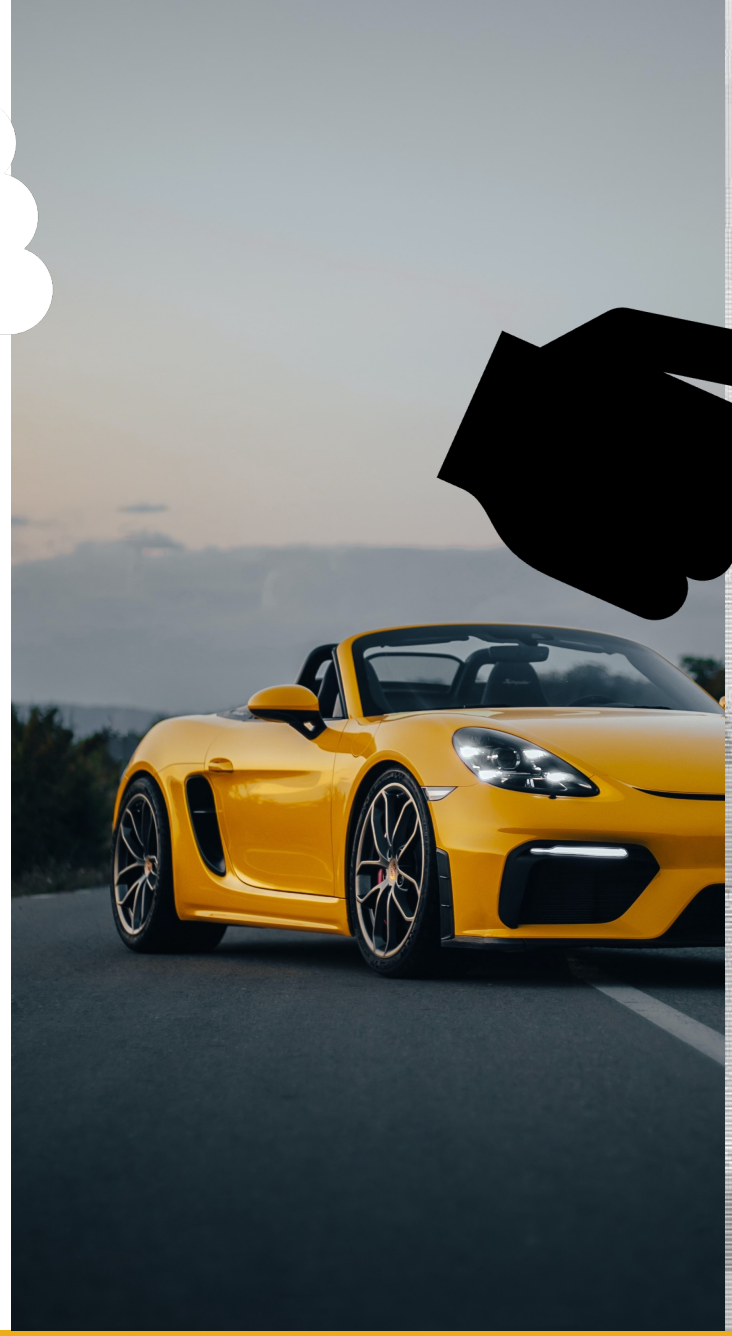


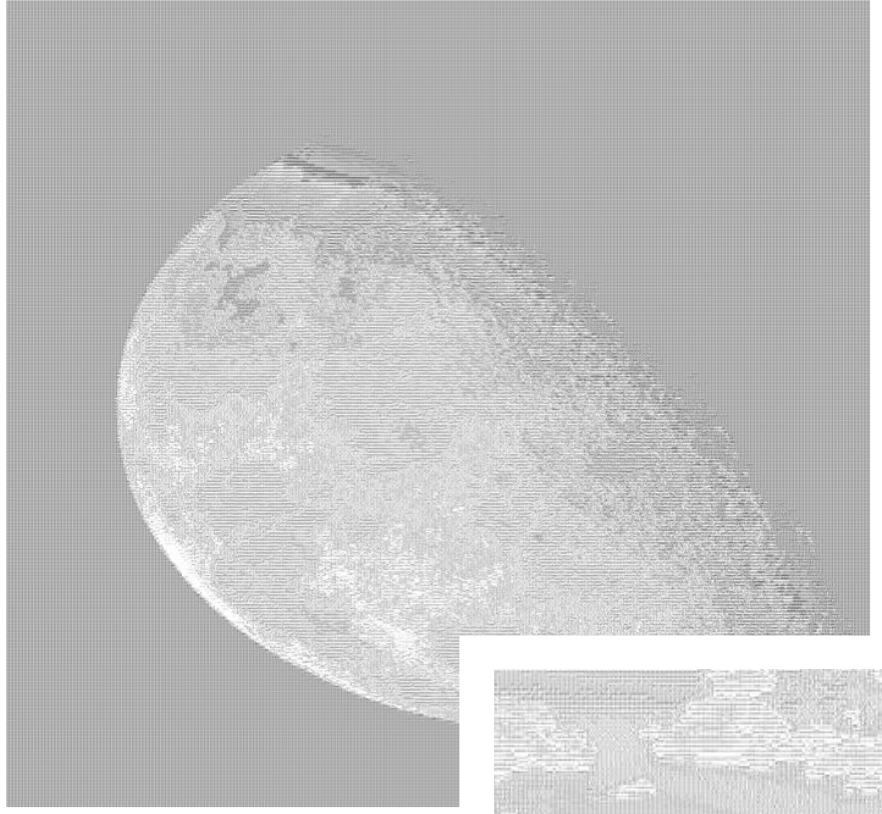


Go to Day_2 → Session_4 → myphotos



Upload your images from Unsplash





New Task:
Our boss wants text art (aka ASCII)

Python

THE BASICS

What is Python?

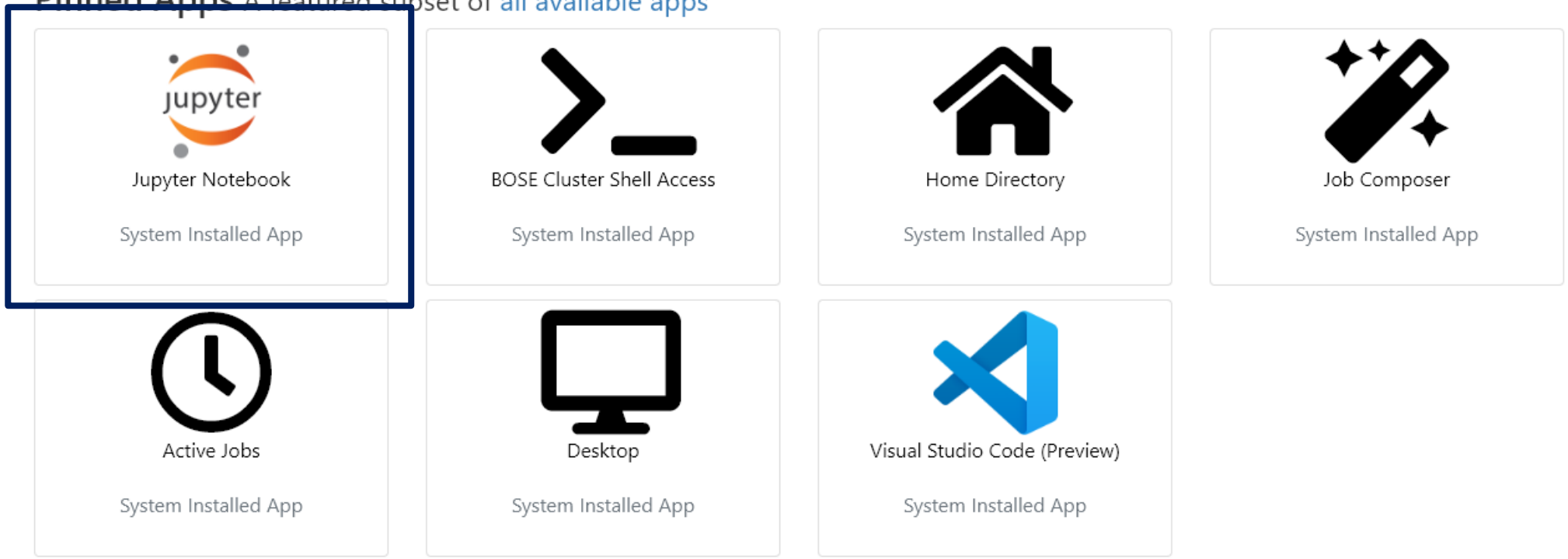
- Increasingly popular programming language
- Considered easy to learn and understand
- Supports interactive programming (e.g. Jupyter)
- 137,000+ Libraries Available
  - Code created by other people to make everyone's life easier

What is it used for?

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

OnDemand - Jupyter

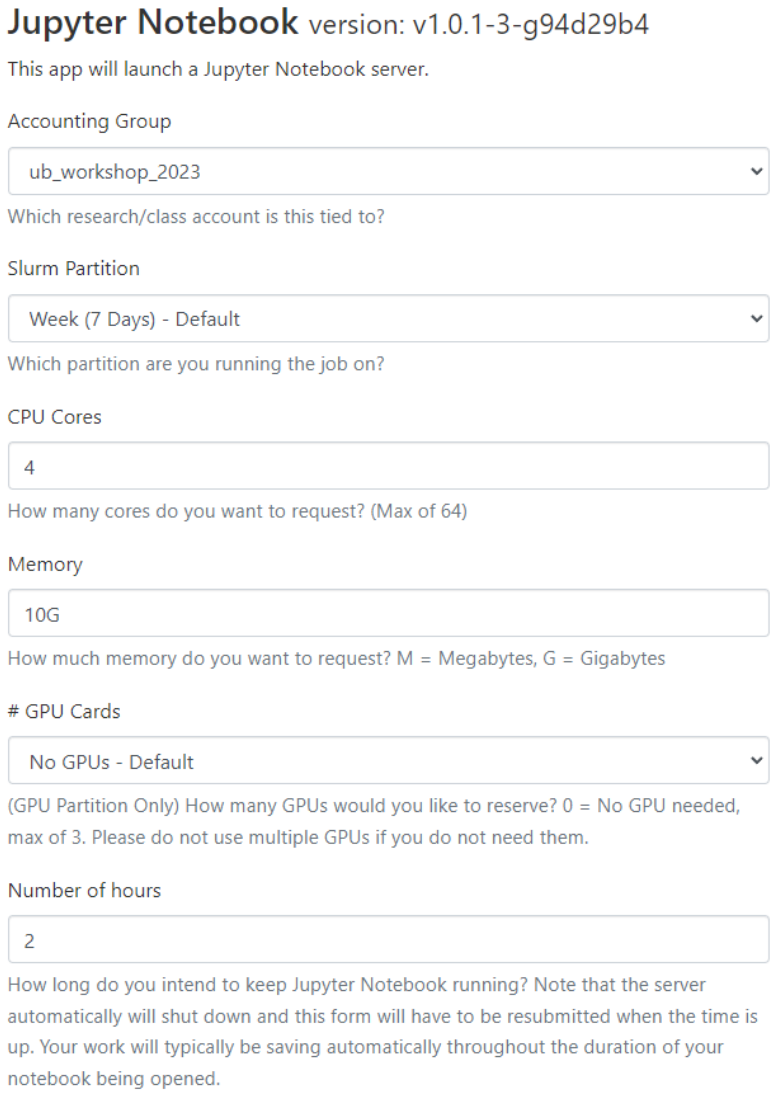
Pinned Apps A featured subset of all available apps



https://ondemand.hpc.uwec.edu

Initial Steps

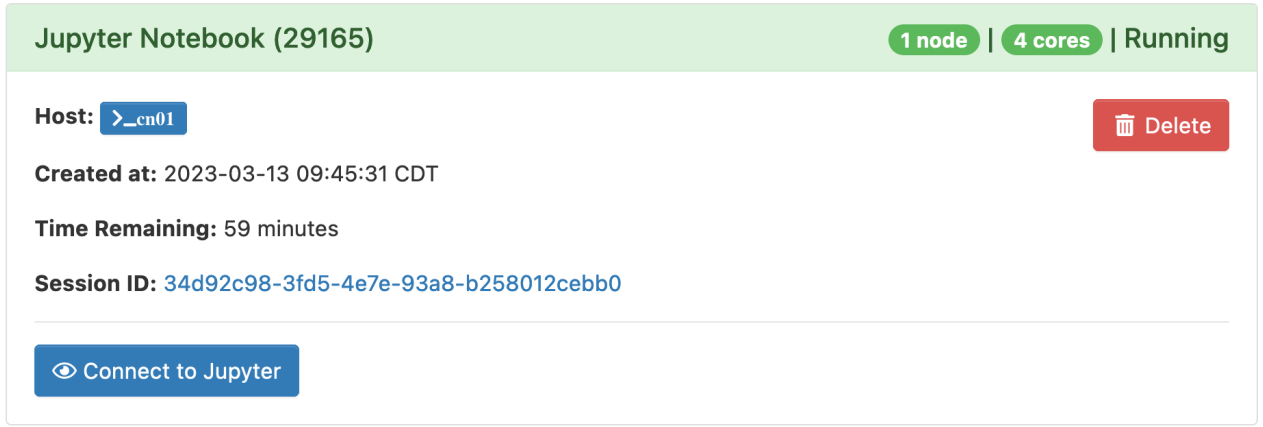
- Choose these Settings:
  - Account Group: ub_workshop_2023
  - Slurm Partition: Week (7 Days) – Default
  - CPU Cores: 4
  - Memory: 10G
  - # GPU Cards: No GPUs – Default
  - Number of Hours: 3
  - Working Directory (Leave empty)
- Hit ”Launch”



https://ondemand.hpc.uwec.edu

Initial Steps

- Wait until Running…. Then hit “Connect to Jupyter”
- Click on your ”Day_2” Folder
- Click on your “Session_4” Folder
- Click on “DoWork.ipynb”
- You’re in a Jupyter Notebook!



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: Variables

```
name = "Tyler"
```

Task 2: Display Our Name

```
print (“My name is “ + print)
```

Make sure to press “Run” after each task!

Task 3: Get Photos

```
# How many photos do we want to process?
numPhotos = 3

# Find photos to change
photoList = findPhotos(numPhotos)

print("Photos Found: ", photoList)
```

Make sure to press “Run” after each task!

Task 4: Loops

```
# Loop through and process our images
for photoFileName in photoList:
   print(photoFileName)
```

← Put a space before “print”

Make sure to press “Run” after each task!

Task 4: Loops

```
# Loop through and process our images
for photoFileName in photoList:
   print(photoFileName)
   runPhoto(photoFileName)

print("All Done!“)
```

← Put a space before “print”

← Put a space before “runPhoto”

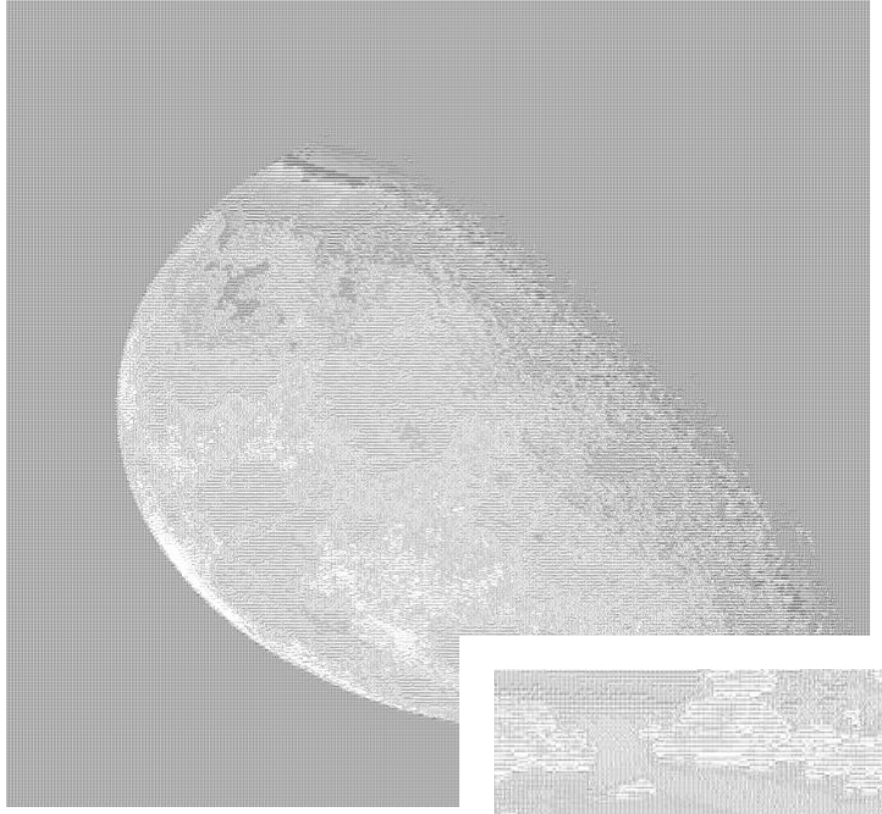
← DON’T put a space before “print”

Make sure to press “Run” after each task!

Boss approves!

But we have a new problem…

What if there are thousands of photos?
That’ll take too long!



New Task:
Make it *faster*

What do we do?

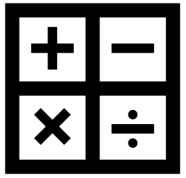
Any ideas?

BOSE

- 61 total machines
  - 4 GPU (12 total graphics cards)
  - 2 Large Memory
- 3,904 total cores
  - 61 x 64 cores
- ~18 TB total RAM
  - 57 x 256 GB
  - 3 x 1 TB

Processor / CPU

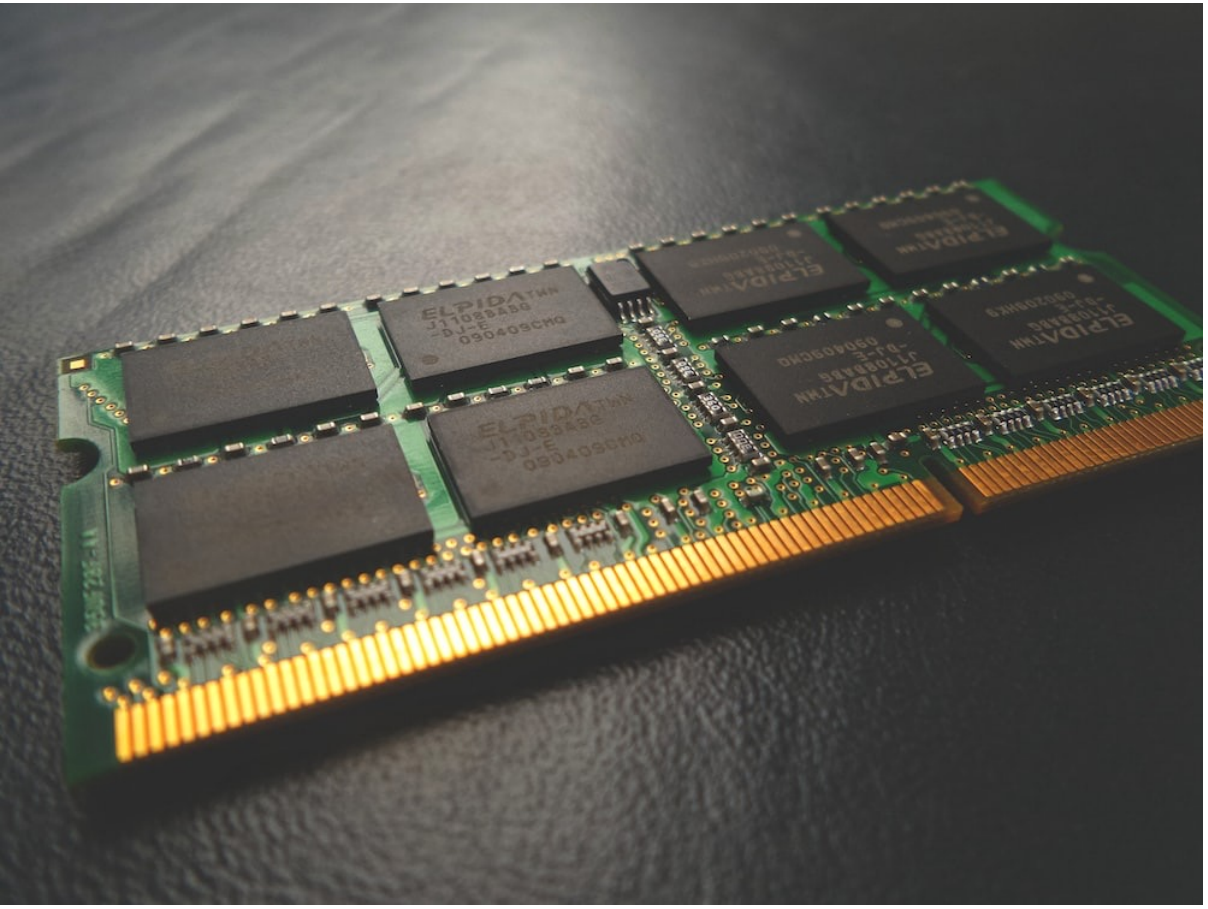
Brains of a computer



Runs instructions
like 1+1 = 2

Can do multiple things at once through its use of “cores”

Memory / RAM



Short term memory – not permanent

Works with the CPU to store what is actively being worked on

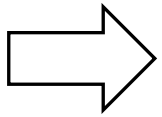
Very fast

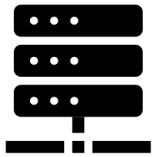
Personal

Supercomputer

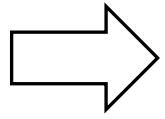
Supercomputing Cluster

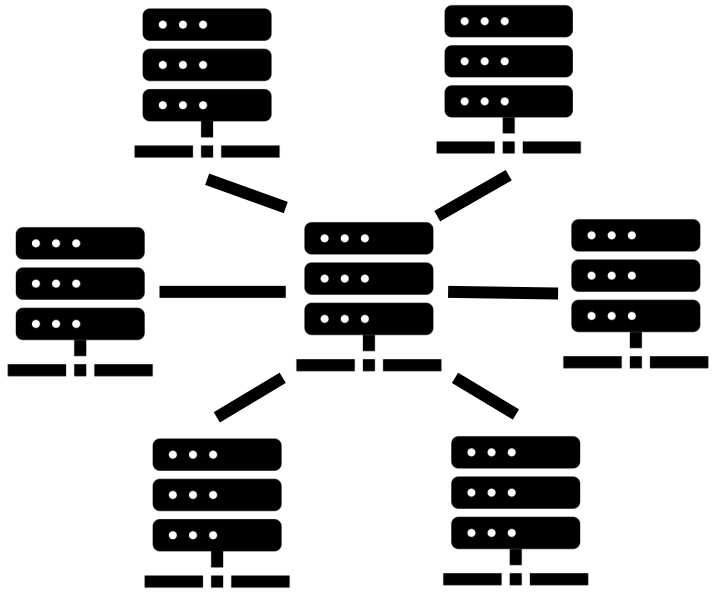
4-core CPU
16GB RAM





32-core CPU x 2
256GB RAM

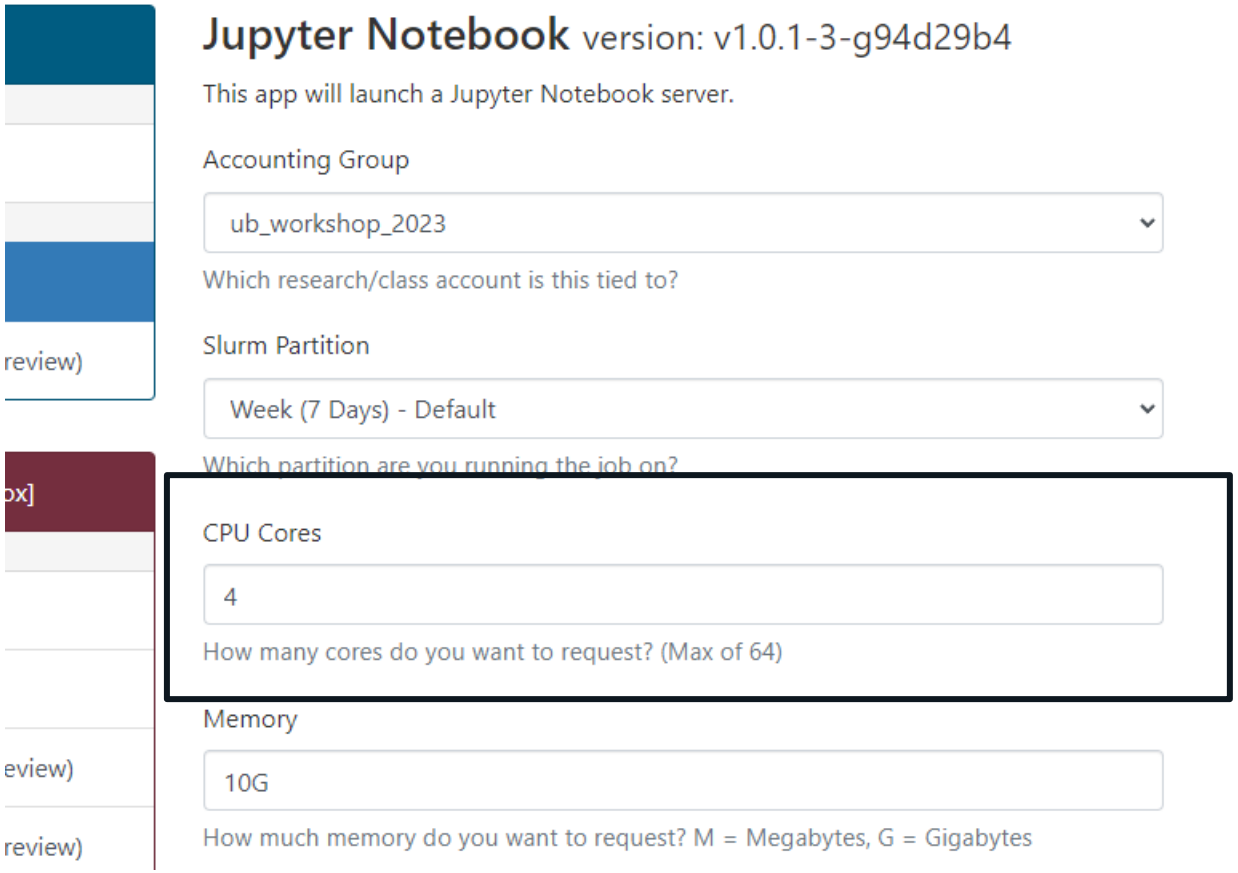




One

Many

High-Performance Computing



Remember this?

We planned ahead and already requested four CPU cores for our program.

That means we can do four images at once!

But we have some more coding to do…

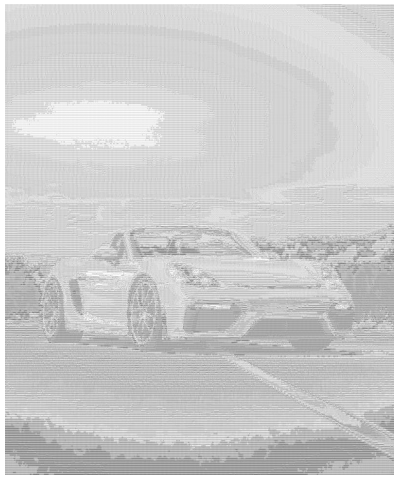
Let’s do more coding!

Task 5: Multiprocessing

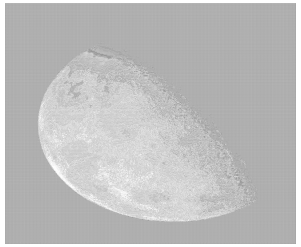
```
# Define a new list of photos
photoList = findPhotos(10)

# Use all the cores!
from multiprocessing.pool import Pool
p = Pool(int(os.environ.get('SLURM_CPUS_ON_NODE')))
p.map(runPhoto, photoList)

print("All Done!")
```

Uploading using OnDemand

Python using Jupyter



Running on Supercomputer (High-Performance Computing)



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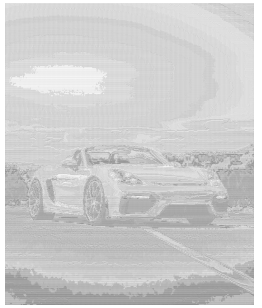

+

We Did It!

Any Questions?

Today's Schedule

Time	Who	What
9:00 – 10:15	Blugold Center for HPC	Coding with Python
10:15 – 11:30	Dr. Sudeep Bhattacharyay	The molecular machines in us
11:45 – 12:30	LUNCH	LUNCH
12:45 – 2:00	Dr. Rahul Gomes	When computers think like us
2:30 – 3:15	Faculty + Research Students	Panel discussion on careers in STEM education

Next Up

The Molecular Machines In Us

Dr. Sudeep Bhattacharyay, Ph.D.
Chemistry + Biochemistry
Professor

Pull up the website if you haven't already!

Website: https://uwec.ly/hpcworkshop

Lunch Break

BE BACK BY 12:45PM

Next Up

When Computers Think Like Us

Dr. Rahul Gomes, Ph.D.
Computer Science
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 102!