HPC Workshop 2023

INTRO TO HPC, COMPUTATIONAL SCIENCE, OPENONDEMAND, BASIC LINUX

Workshop Website

https://uwec.ly/hpcworkshop

Contains the schedule, presentations, and important links.

Who Are We?

Blugold Center for High Performance Computing

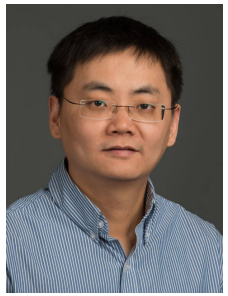
- Supercomputers: BGSC and BOSE
- Provide technical support
- Maintain clusters
- Promote supercomputing

The Team

Faculty Coordinators

Dr. Sudeep Bhattacharyay

Dr. Rahul Gomes



Dr. Ying Ma

System Administrator

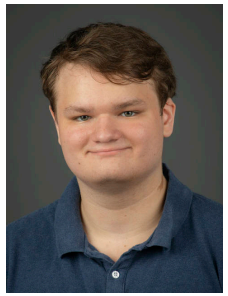
Tyler Bauer

Management

Kent Gerberich

Daren Bauer

Student Administrator Apprentices



Mitchell Ewan

Treesmorn Tanboonrith "Mammoth"

Jacob Weber

Who utilizes HPC at UWEC?

Classroom use
Research Projects
Departments
- Biology
- Chemistry & Biochemistry
- Computer Science
- Geography
- Materials Science & Biomedical Engineering
- Mathematics
- Physics
- *And More*

University of Wisconsin Eau Claire

Computational Science

What is computational science?

Using complex computation to solve complex problems:

- Algorithms
- Models (mathematical and scientific)
- Simulations

Impacted Fields + Applications

Wildfire Detection

Airplane Design

Behavioral Analysis

Modeling Big Bang

Financial Trends

Advertising

Cybersecurity

Urban Planning

Shopping Trends

Bridge Building

Weather Forecasting

Molecule Simulation

Airplane Design

Designing New Chemicals

Natural Disasters

Self-Driving Cars

Oil / Gas Detection

Fire Suppression Strategies

3D / CGI Rendering

Drug Testing

Text To Speech

Rocket Science

Disease Detection

Modeling Outbreaks

Artificial Intelligence / Machine Learning

Space Photography

Deforestation Tracking

Historical Analysis

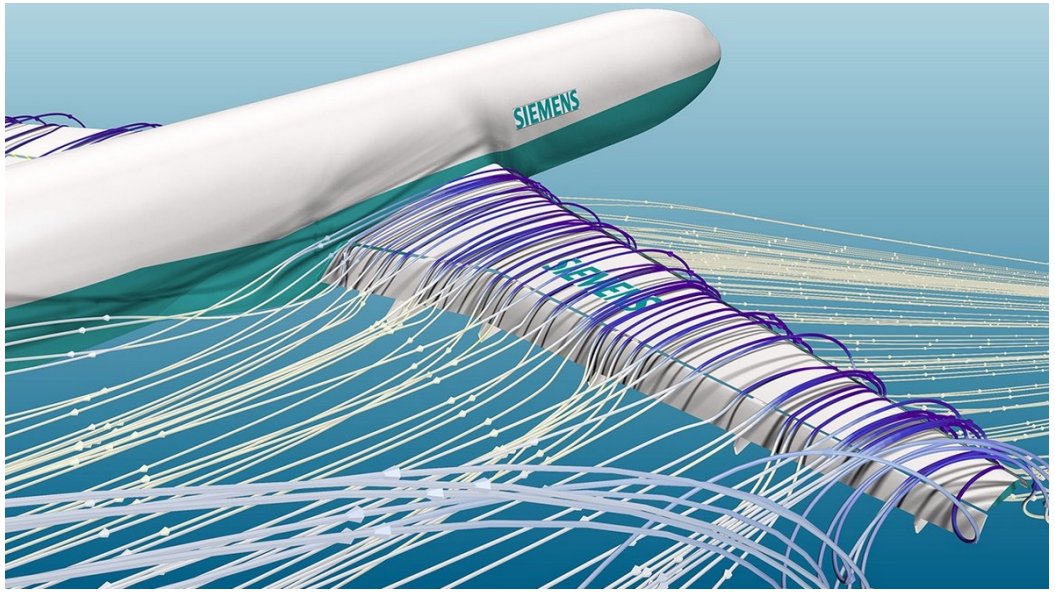
But why?

Testing complex machines is expensive:

- Design/engineering
- Material cost
- Labor/manufacturing cost
- Prototypes ($$$)

What should we do instead?

Simulate it!



Source: Ascend Tech

BGSC

Primarily used for classrooms
20 Machines

17 Nodes with
404 CPU Cores
1316GB of RAM
12 GPU cards

BOSE

Primarily used for research
60 Machines
You will be using this today!

56 Nodes with
3840 CPU Cores
16,750GB of RAM
12 GPU cards

What are computational resources?

"**Computational Resources**" are any resources available on the computer for software to take advantage of.

Examples of computational resources you will find in almost any computer:

- CPU Cores
- GPU Cards
- Random Access Memory (RAM)
- Storage Space

Managing computational resources

- How do you determine what jobs use what resources?
- How do you divide up nodes into groups?
- What happens if all the resources are in use, and someone wants to submit something?

Slurm Workload Manager

Open-source, scalable cluster resource manager and job scheduler.

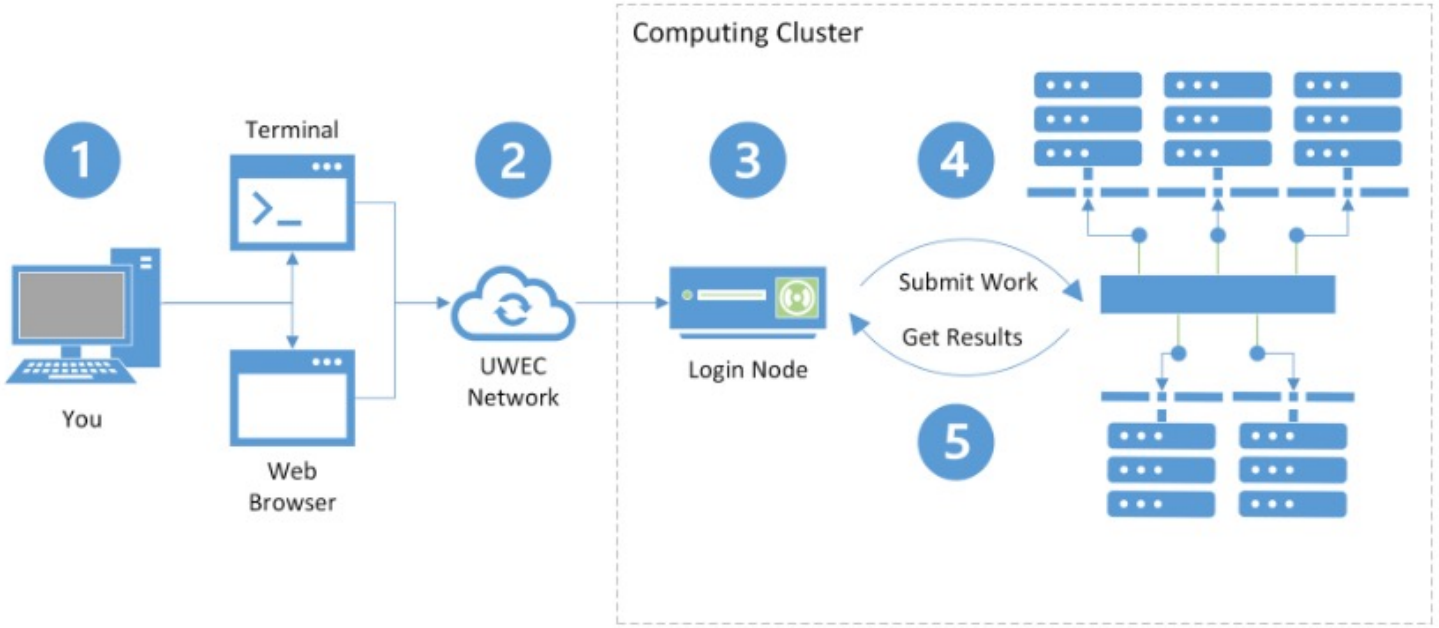
General-purpose, flexible, and stable

And it's free!

Slurm's functions

- 3 Main functions:
  - Allocate resources to jobs (CPU cores, memory, GPU if needed)
  - Start, run, and monitor jobs
  - Resolve situations where more resources than available are requested.
- Slurm also functions as a comprehensive logging system for all our jobs.
- Users can view detailed breakdowns of how their job utilized the requested resources while the job is running or after it has completed.

How do you interact with the supercomputer?



Introduction

About Open OnDemand

A web UI to access the cluster

Terminal:

- Hard to learn
- Unfamiliar
- Text-based

Open OnDemand:

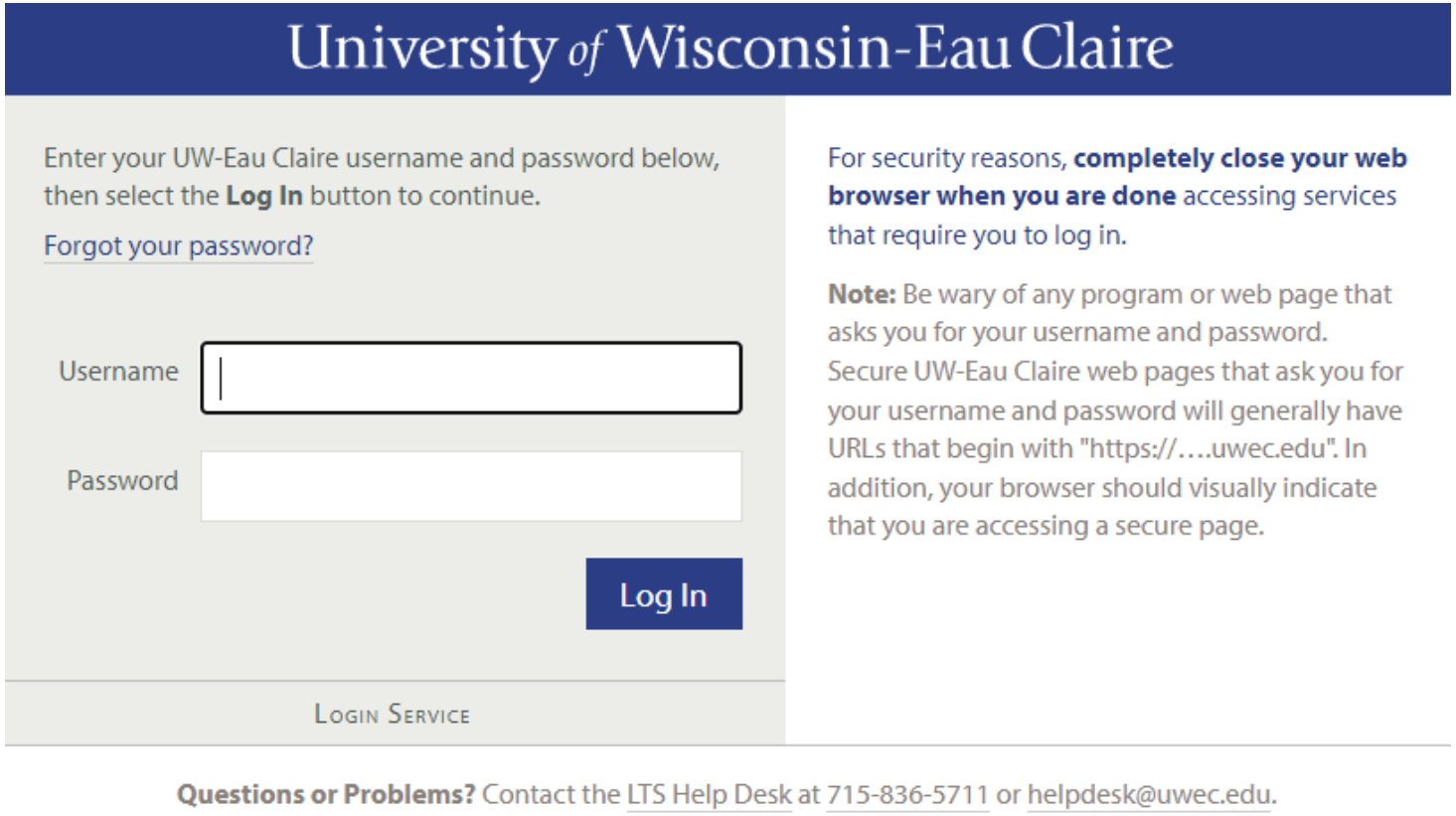
- Use your browser
- Navigate through files and folders in a GUI

Open OnDemand

Navigate to

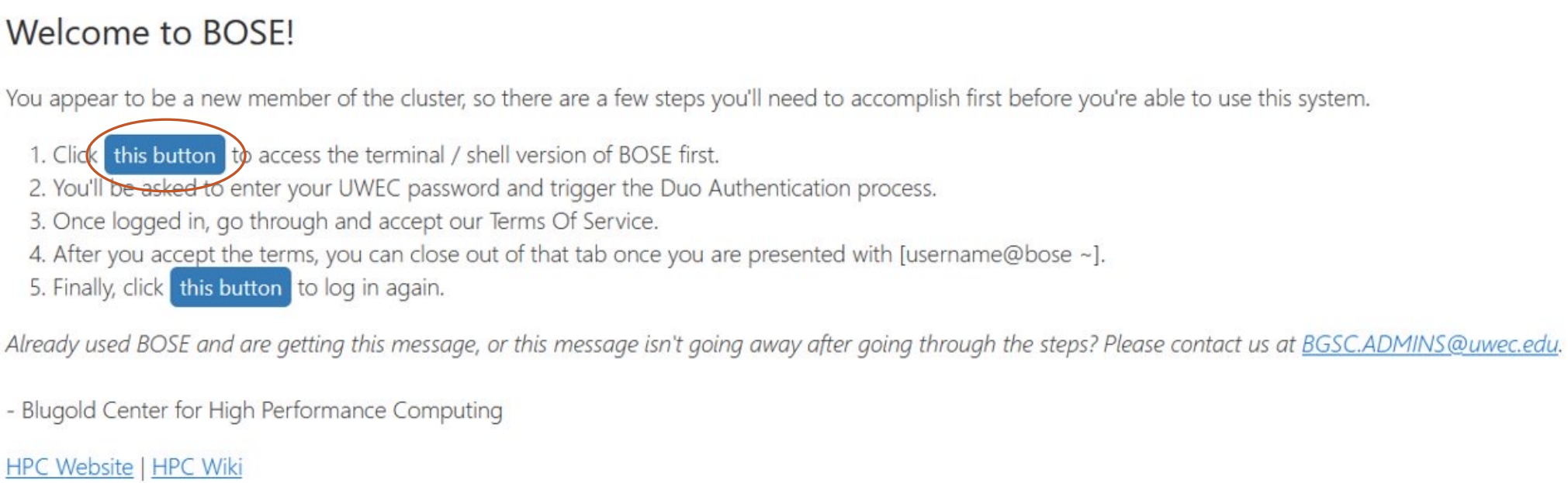
https://ondemand.hpc.uwec.edu

Open OnDemand



Open OnDemand: Initial Setup

This prompt will appear for first time users. Follow the instructions accordingly:



Open OnDemand: First Usage

Enter your password (No text will appear as you type, this is by design):

```
root@hedgieLaptop:~# ssh tanboont9801@hpc.uwec.edu -p 50022
ssh: Could not resolve hostname hpc.uwec.edu: No address associated with hostname
root@hedgieLaptop:~# ssh tanboont9801@bose.hpc.uwec.edu -p 50022
Password:
```

If your password is successful, then you must enter '1,' '2,' or '3' to select a method for DUO authentication

```
Enter a passcode or select one of the following options:

 1. Duo Push to XXX-XXX-9886
 2. Phone call to XXX-XXX-9886
 3. SMS passcodes to XXX-XXX-9886 (next code starts with: 1)

Passcode or option (1-3):
```

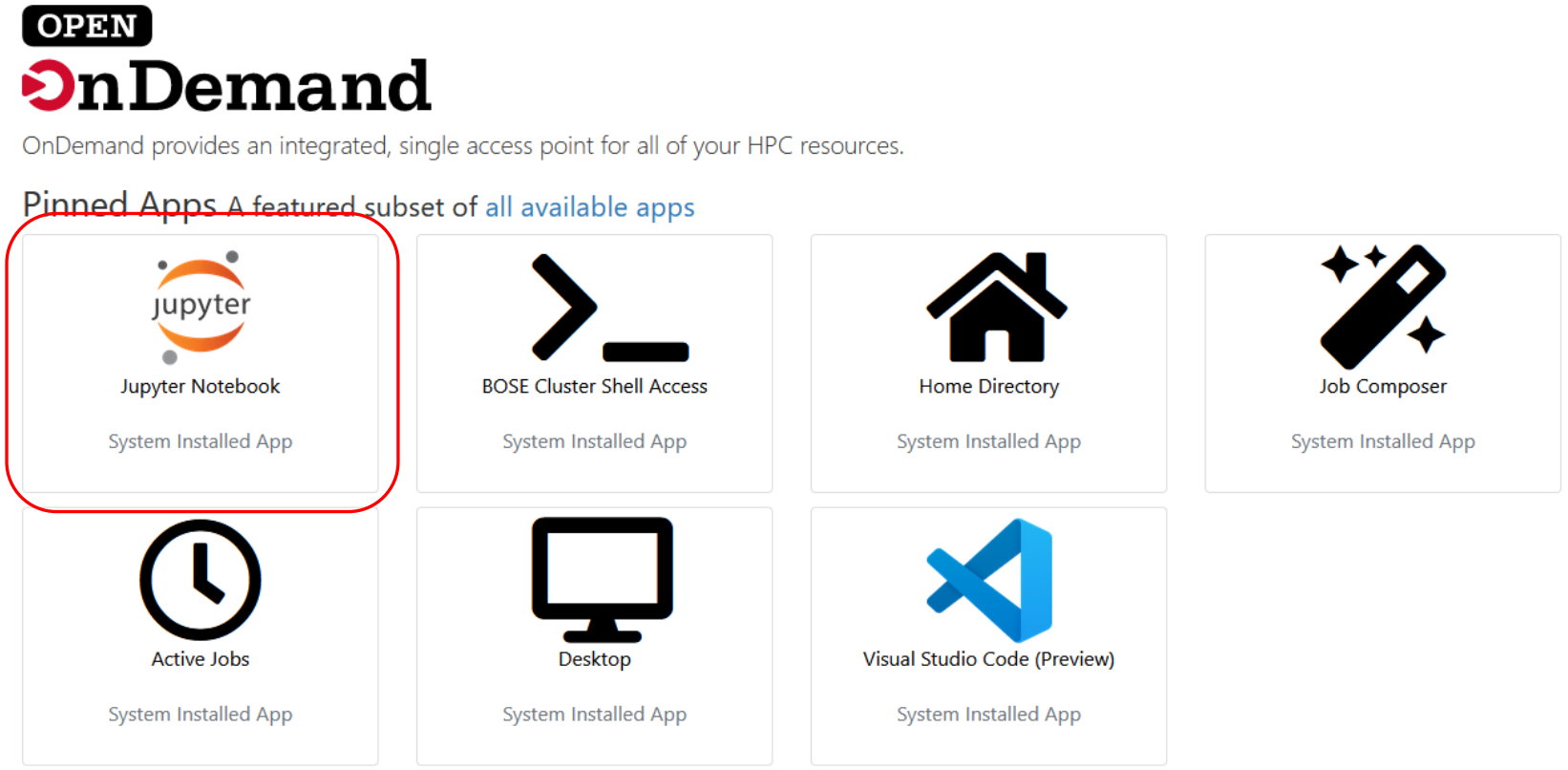
Open OnDemand

If you are logged in, your tab should look like this. Follow the instructions on-screen to read through the terms and conditions. After you are met with a prompt similar to '[username@bose~]' , setup is complete.

Jupyter

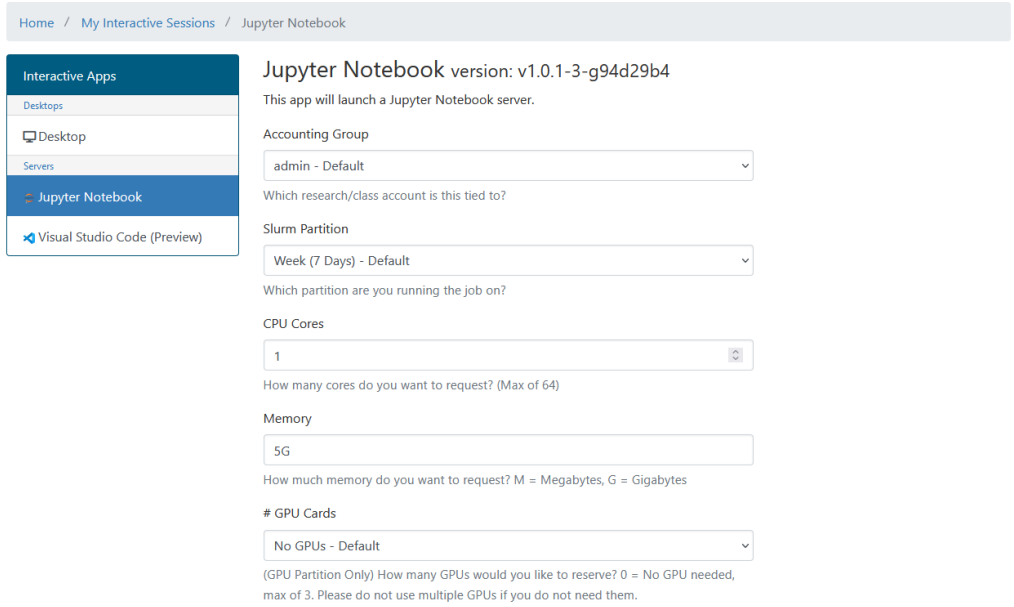
- Run code interactively
- Flexible
- Easy to learn and use

Accessing Jupyter



Creating a notebook

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



Use these settings

Accounting Group: ub_workshop_2023

Slurm partition: Week

CPU Cores: 1

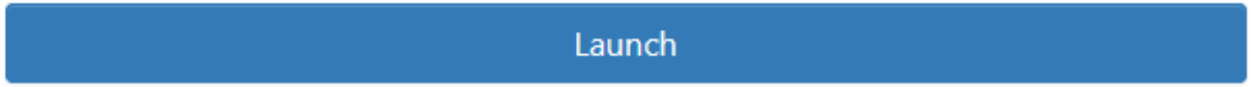
Memory: 5G

#GPU cards: No GPUs

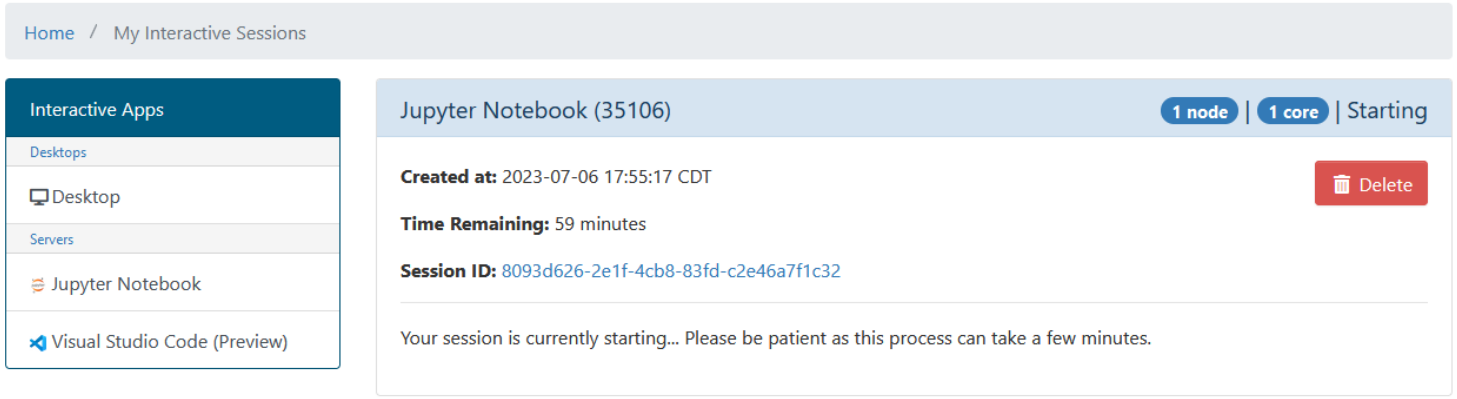
Number of Hours: 1

Working Directory: Leave empty

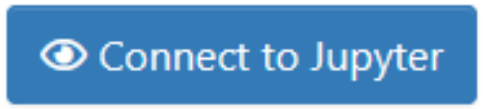
Then, click



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

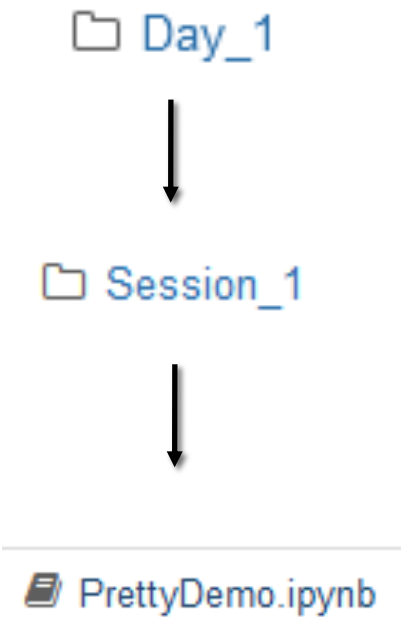


Once your notebook has started, click this button to access it:



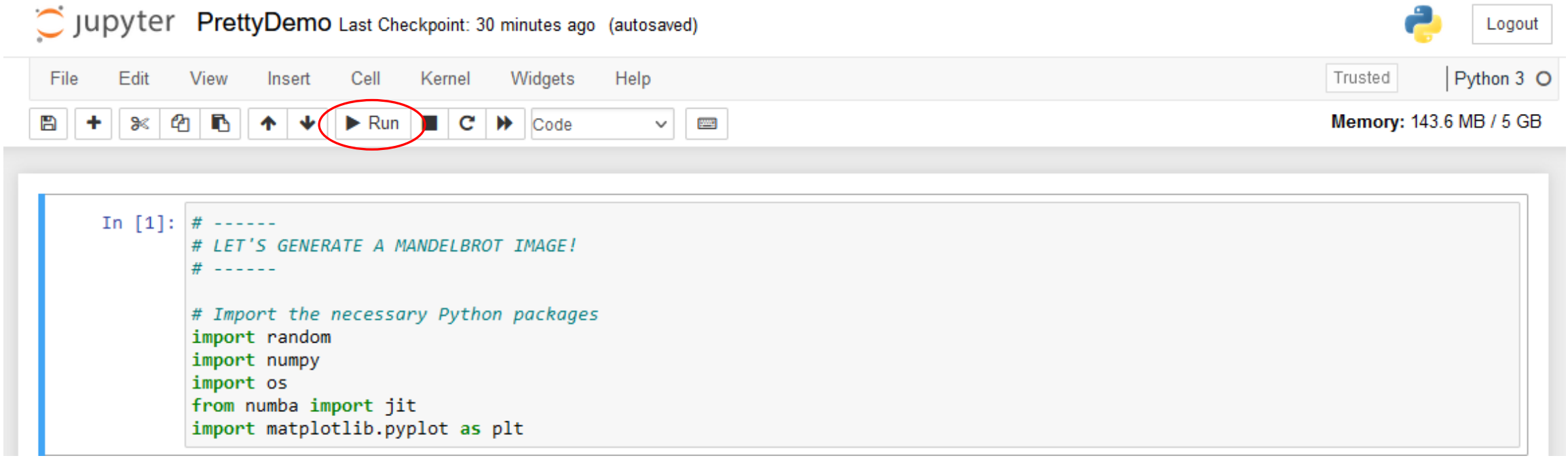
Jupyter file view

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

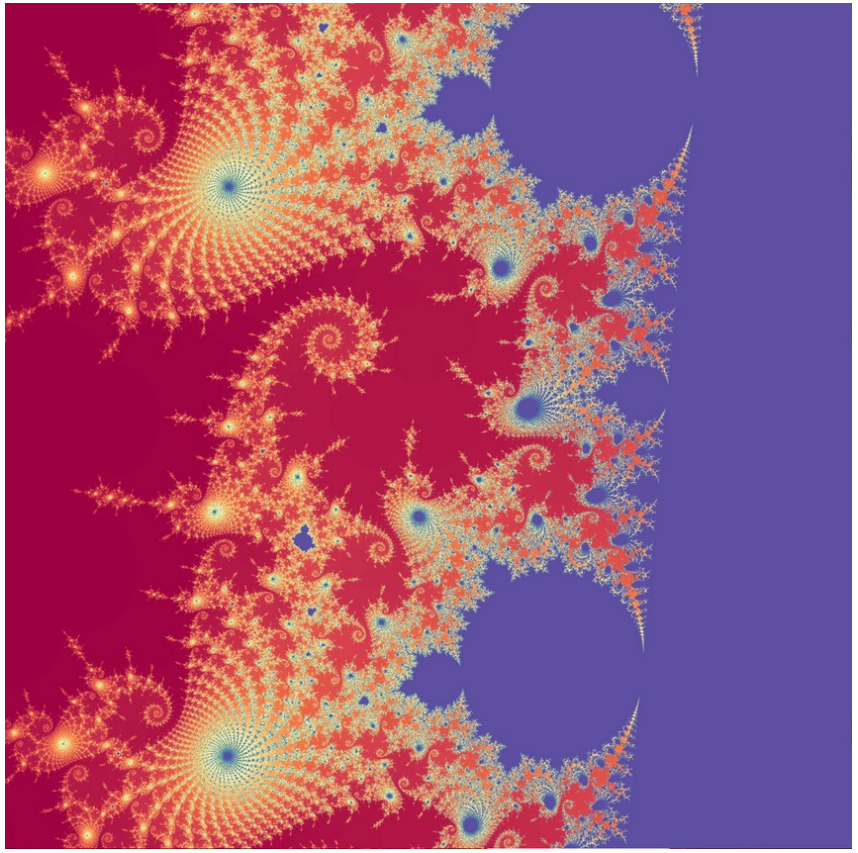


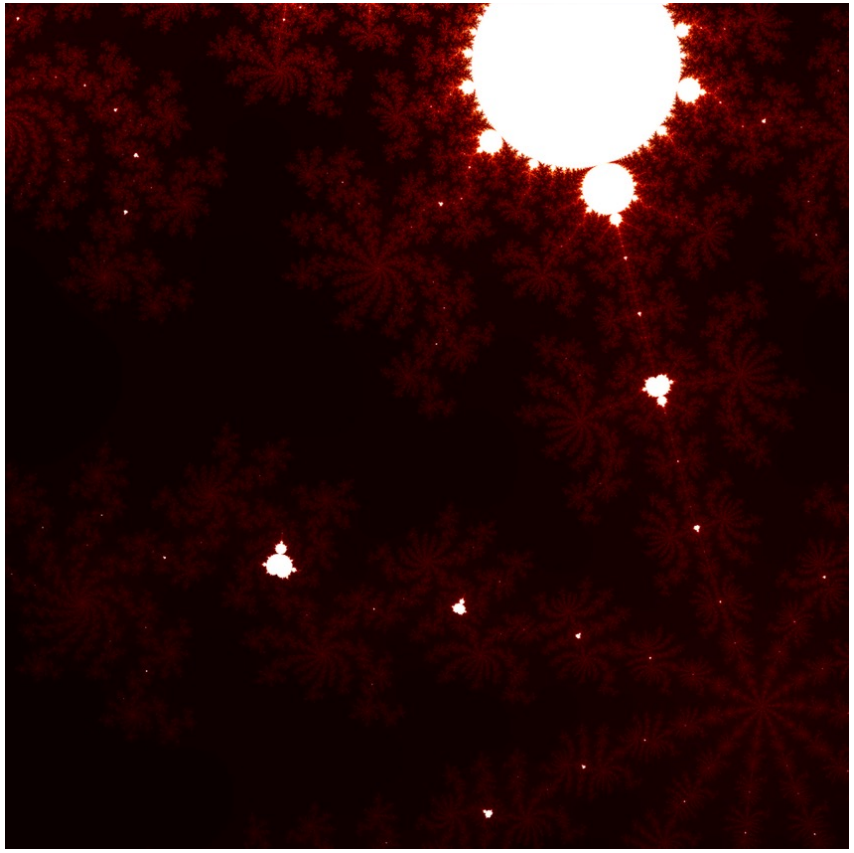
Create Mandelbrot images

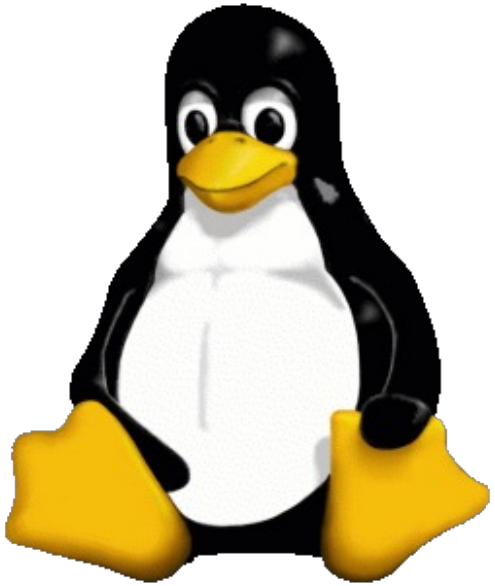
Each Cell contains a section of code. To use this demo, run them in order.



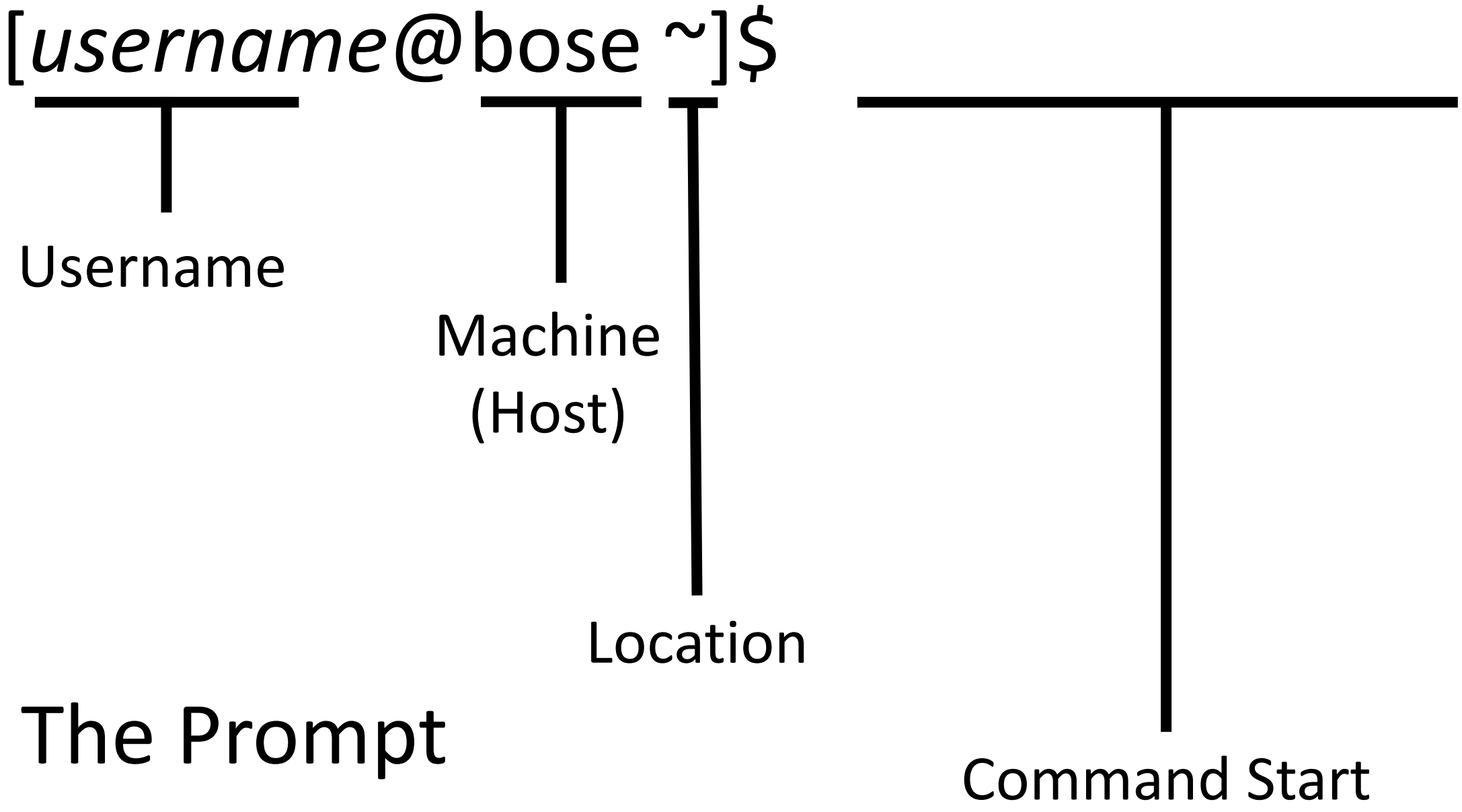
The result!







Basic Linux Commands


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

The Prompt

What is Linux?

Why Linux?

What is a command line interpreter?

Show the directory (folder) and files

1. ls (All lower case. No space before and after “ls”)

2. ls -l (All lower case. There is a single space between “ls” and “-l”)

Note: The differences between these 2 is that “ ls –l ” shows a list format with more information

Change the current directory

cd (All lower case. No space before and after)

Show the current working path

pwd (All lower case. No space before and after)

Note: “ pwd ” stands for **print working directory**

Creating a folder (directory)

mkdir (All lower case. No space before and after)

Slurm commands for your job/s

sbatch yourscriptname.sh (to submit your job to the node)

myjobs (to view your submitted job status)