

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

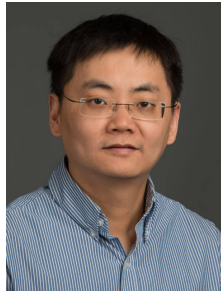
Faculty Coordinators



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*

The logo for the University of Wisconsin Eau Claire, featuring the text "University of Wisconsin" in a smaller font above "Eau Claire" in a larger, bold serif font, all in white on a dark blue rectangular background.

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

Weather Forecasting

Molecule Simulation

Airplane Design

Bridge Building

Designing New Chemicals

Natural Disasters

Self-Driving Cars

Oil / Gas Detection

3D / CGI Rendering

Drug Testing

Text To Speech

Rocket Science

Fire Suppression Strategies

Disease Detection

Modeling Outbreaks

Artificial Intelligence / Machine Learning

Space Photography

Deforestation Tracking

Historical Analysis

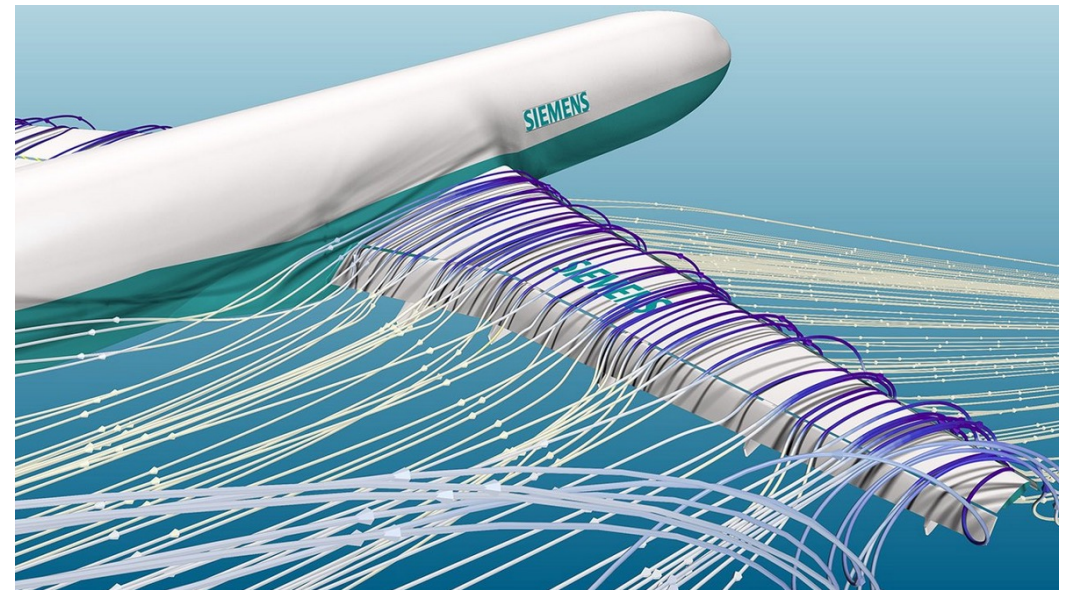
But why?

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

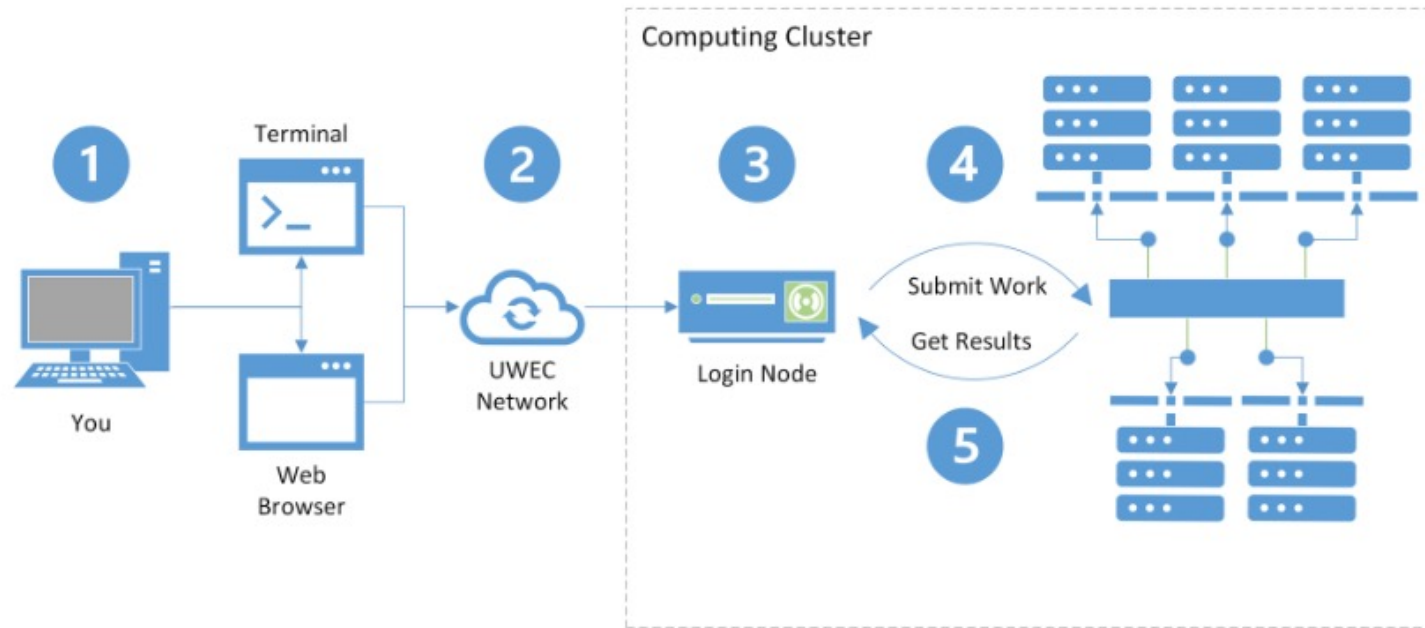
And it's free!



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?



OPEN

 **nDemand**

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

University of Wisconsin-Eau Claire

Enter your UW-Eau Claire username and password below, then select the **Log In** button to continue.

[Forgot your password?](#)

Username

Password

Log In

LOGIN SERVICE

For security reasons, **completely close your web browser when you are done** accessing services that require you to log in.

Note: Be wary of any program or web page that asks you for your username and password. Secure UW-Eau Claire web pages that ask you for your username and password will generally have URLs that begin with "https://...uwec.edu". In addition, your browser should visually indicate that you are accessing a secure page.



Questions or Problems? Contact the [LTS Help Desk](#) at [715-836-5711](tel:715-836-5711) or helpdesk@uwec.edu.

Open OnDemand: Initial Setup

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

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  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  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](#)

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.

```

Welcome to BOSE
.....
.....
If you're reading this, it means you have been identified as a new user on the cluster.
To start using the cluster, please read and accept our terms of service.

If you have any issues, please contact BGSC.ADMINS@uwec.edu
.....
.....
Press enter to continue: 
```



Jupyter

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

Accessing Jupyter

OPEN

OnDemand

OnDemand provides an integrated, single access point for all of your HPC resources.

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

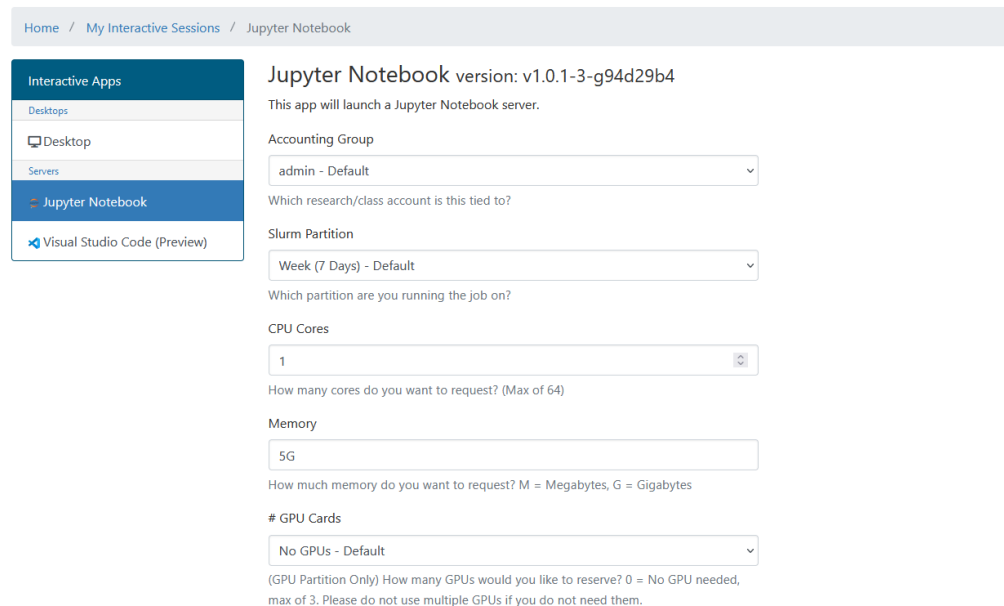


Visual Studio Code (Preview)

System Installed App

Creating a notebook

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



The screenshot shows a web interface for configuring a Jupyter Notebook. On the left is a sidebar with 'Interactive Apps' containing 'Desktop', 'Servers', 'Jupyter Notebook', and 'Visual Studio Code (Preview)'. The main area displays the following configuration options:

- Jupyter Notebook version:** v1.0.1-3-g94d29b4
- This app will launch a Jupyter Notebook server.**
- Accounting Group:** dropdown menu with 'admin - Default' selected.
- Which research/class account is this tied to?**
- Slurm Partition:** dropdown menu with 'Week (7 Days) - Default' selected.
- Which partition are you running the job on?**
- CPU Cores:** input field with '1' and a spinner icon.
- How many cores do you want to request? (Max of 64)**
- Memory:** input field with '5G'.
- How much memory do you want to request? M = Megabytes, G = Gigabytes**
- # GPU Cards:** dropdown menu with 'No GPUs - Default' selected.
- (GPU Partition Only) How many GPUs would you like to reserve? 0 = No GPU needed, max of 3. Please do not use multiple GPUs if you do not need them.**

Use these settings

Accounting Group: ub_workshop_2023

Slurm partition: Week

CPU Cores: 1

Memory: 5G

#GPU cards: No GPUs

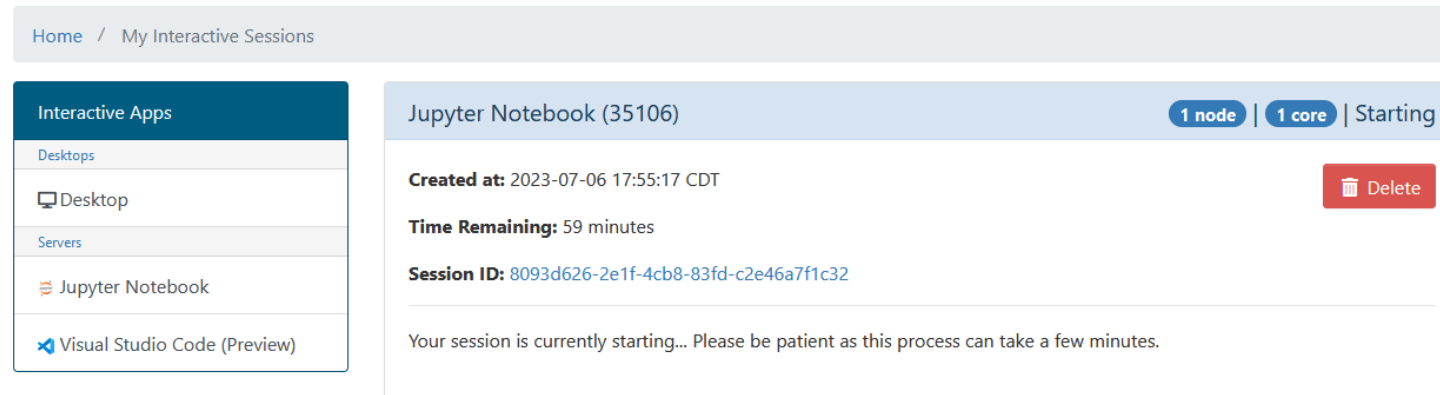
Number of Hours: 1

Working Directory: Leave empty

Then, click

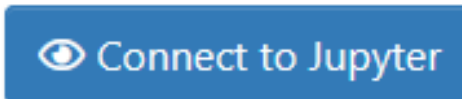
Launch

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



The screenshot shows a web interface for managing interactive sessions. At the top, there is a breadcrumb trail: "Home / My Interactive Sessions". On the left, a sidebar titled "Interactive Apps" contains a list of options: "Desktops", "Desktop" (with a monitor icon), "Servers", "Jupyter Notebook" (with a notebook icon), and "Visual Studio Code (Preview)" (with a VS Code icon). The main content area displays a session titled "Jupyter Notebook (35106)". To the right of the title, it shows "1 node | 1 core | Starting". Below the title, the session details are listed: "Created at: 2023-07-06 17:55:17 CDT", "Time Remaining: 59 minutes", and "Session ID: 8093d626-2e1f-4cb8-83fd-c2e46a7f1c32". A red "Delete" button with a trash icon is positioned to the right of the "Time Remaining" field. At the bottom of the session card, a message states: "Your session is currently starting... Please be patient as this process can take a few minutes."

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:

📁 Day_1



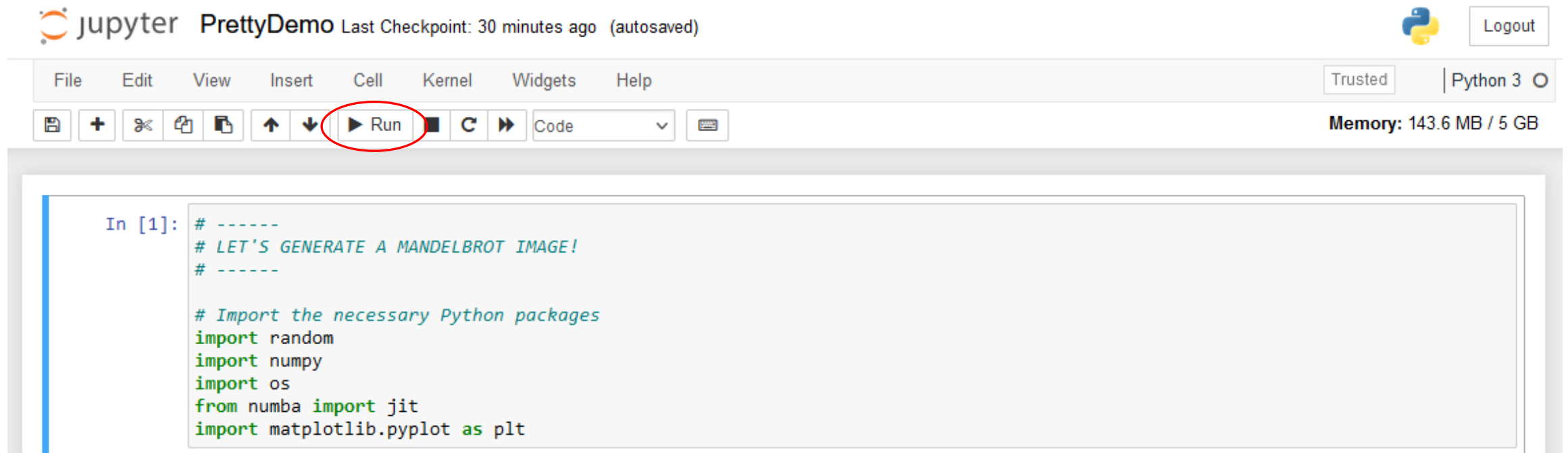
📁 Session_1



📄 PrettyDemo.ipynb

Create Mandelbrot images

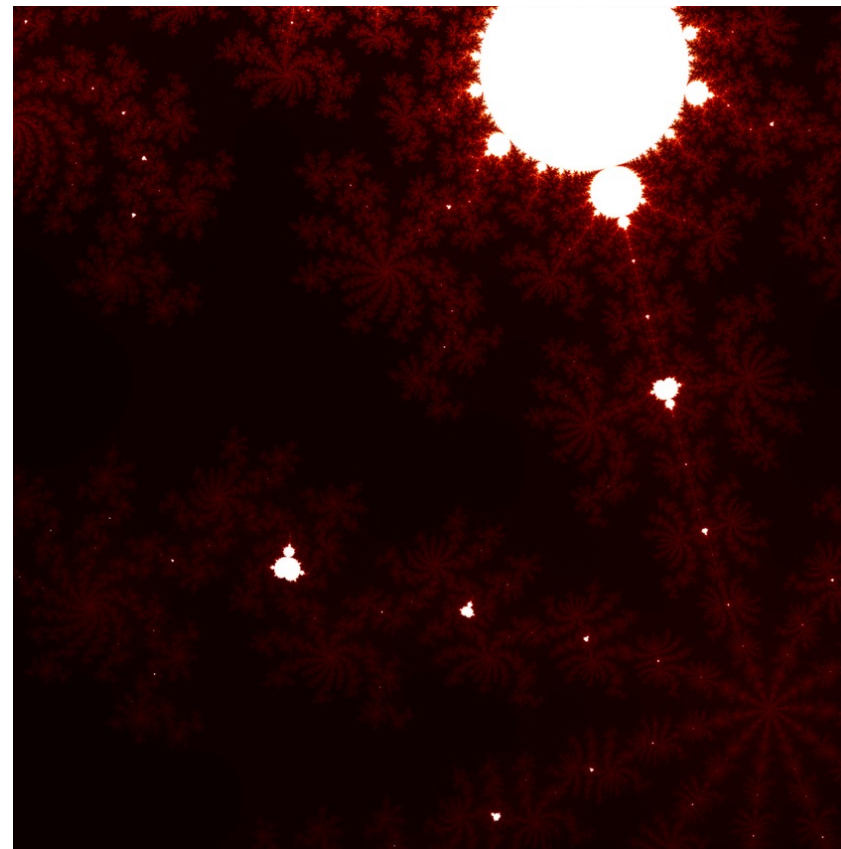
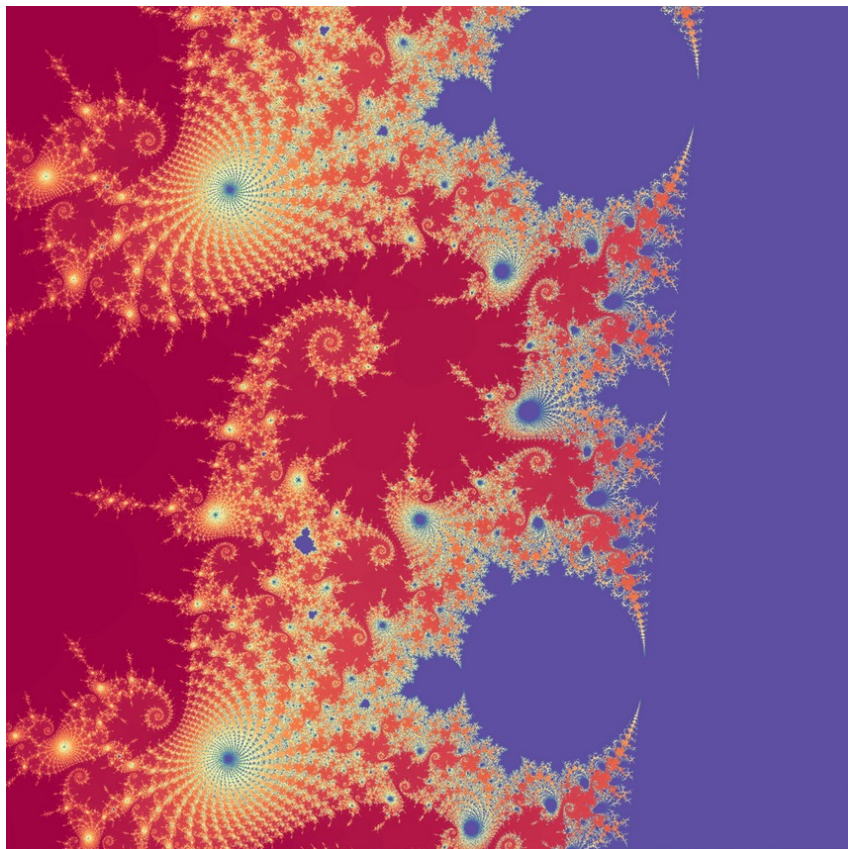
Each Cell contains a section of code. To use this demo, run them in order.

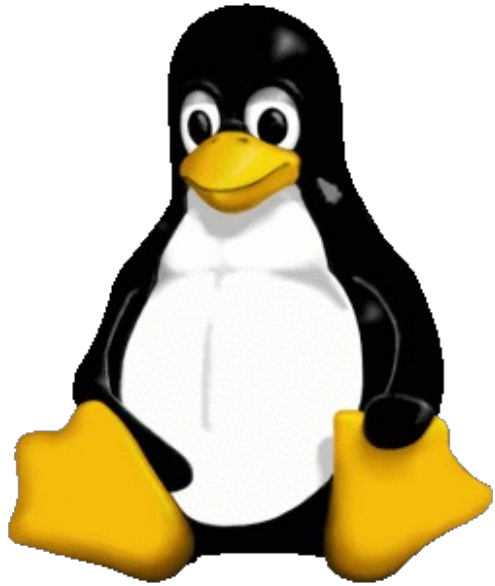


The screenshot shows the Jupyter Notebook interface. At the top left, it says "jupyter PrettyDemo Last Checkpoint: 30 minutes ago (autosaved)". On the top right, there is a Python logo and a "Logout" button. Below this is a menu bar with "File", "Edit", "View", "Insert", "Cell", "Kernel", "Widgets", and "Help". To the right of the menu bar, it says "Trusted" and "Python 3". Below the menu bar is a toolbar with various icons, including a "Run" button (a play icon) which is circled in red. To the right of the toolbar, it says "Memory: 143.6 MB / 5 GB". The main area of the notebook contains a code cell with the following text:

```
In [1]: # -----  
# LET'S GENERATE A MANDELBROT IMAGE!  
# -----  
  
# Import the necessary Python packages  
import random  
import numpy  
import os  
from numba import jit  
import matplotlib.pyplot as plt
```

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 yourscripname.sh` (to submit your job to the node)

`myjobs` (to view your submitted job status)