



# Introduction to the Research Computing Center and High Performance Computing

Marcelina Nagales  
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# Agenda

- What is the Research Computing Center
- What is High Performance Computing (HPC)
  - HPC Definitions
- Accessing the HPC
- Support from RCC Team
- Research Computing Center Services and Updates
- More High Performance Computing Resources

## Bonus:

- Exercise/Hands-on Section



# What is High Performance Computing

**“High Performance Computing most generally refers to the practice of aggregating computing power in a way that delivers much higher performance than one could get out of a typical desktop computer or workstation in order to solve large problems in science, engineering, or business”**



# Why Use High Performance Computing

## Specialized Hardware

- Contains more processors than the average home computer
- Has AMD and Intel Processors
- Can house custom machines (via a research grant) with specialized hardware like special CPUs, DSPs, SSDs, GPUs

## Offload Your Work

- Takes pressure off your regularly used devices
- Scales computational processes not possible on home machines
  - parallel processes
- Runs repeatable tasks over a long period of time

# What is the FSU Research Computing Center (RCC)

- A unit of the FSU Information Technology Services department
- Originally a division of Scientific Computing back before 2013
- The team that hosts and administers the main supercomputing resource at FSU: the High Performance Computing system (HPC)





# RCC System Metrics

**649**  
Nodes

Beowulf Cluster  
AlmaLinux 8.6

**71**  
GPUs

NVIDIA:  
- GTX 1080 Ti  
- A4000  
- A4500  
- H100

**20,400**  
Processors

AMD, Intel

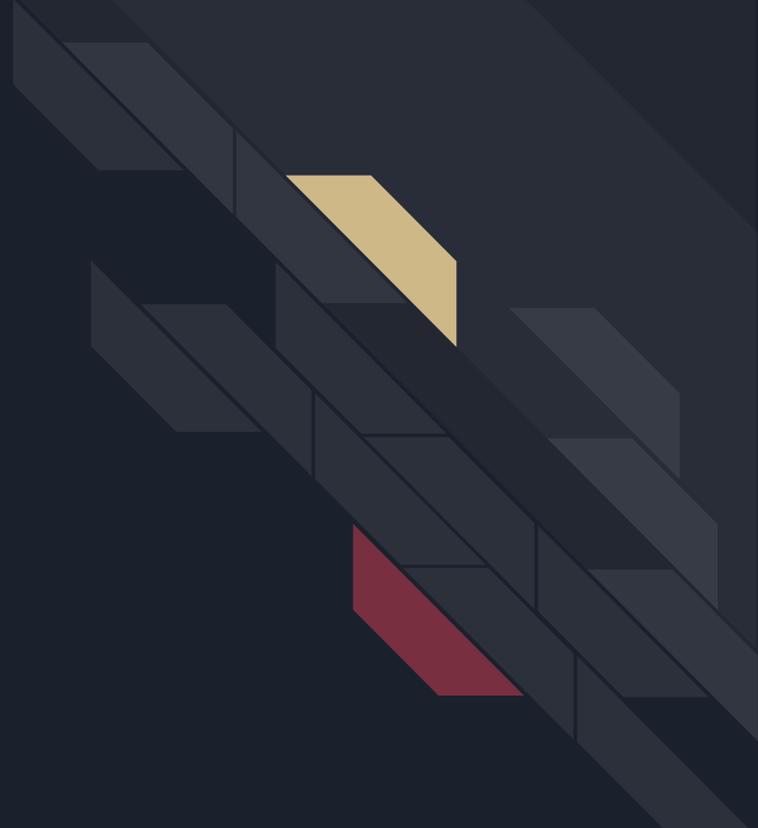
**975.168**  
TeraFLOPS

(Not Including  
GPUs)

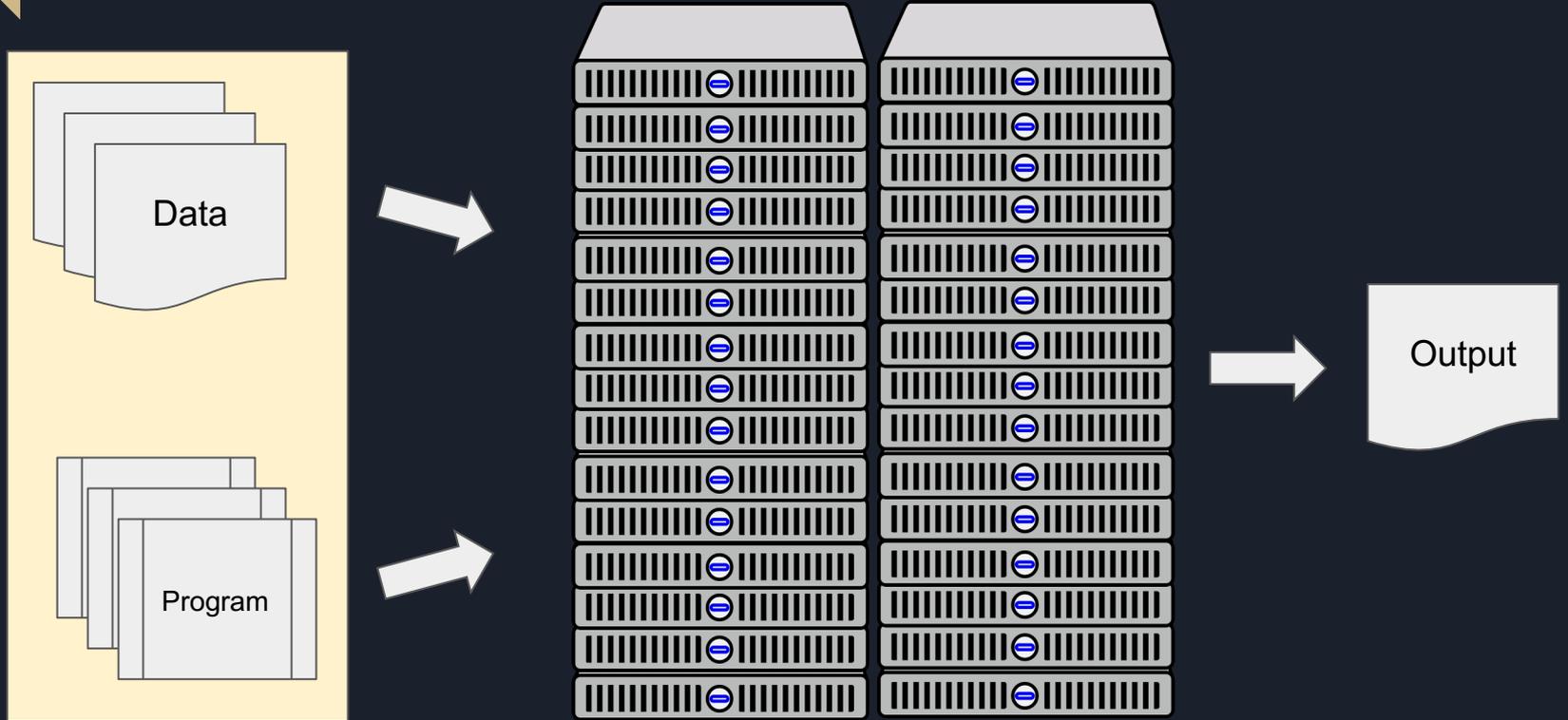
**30 million**  
jobs

Since 2008

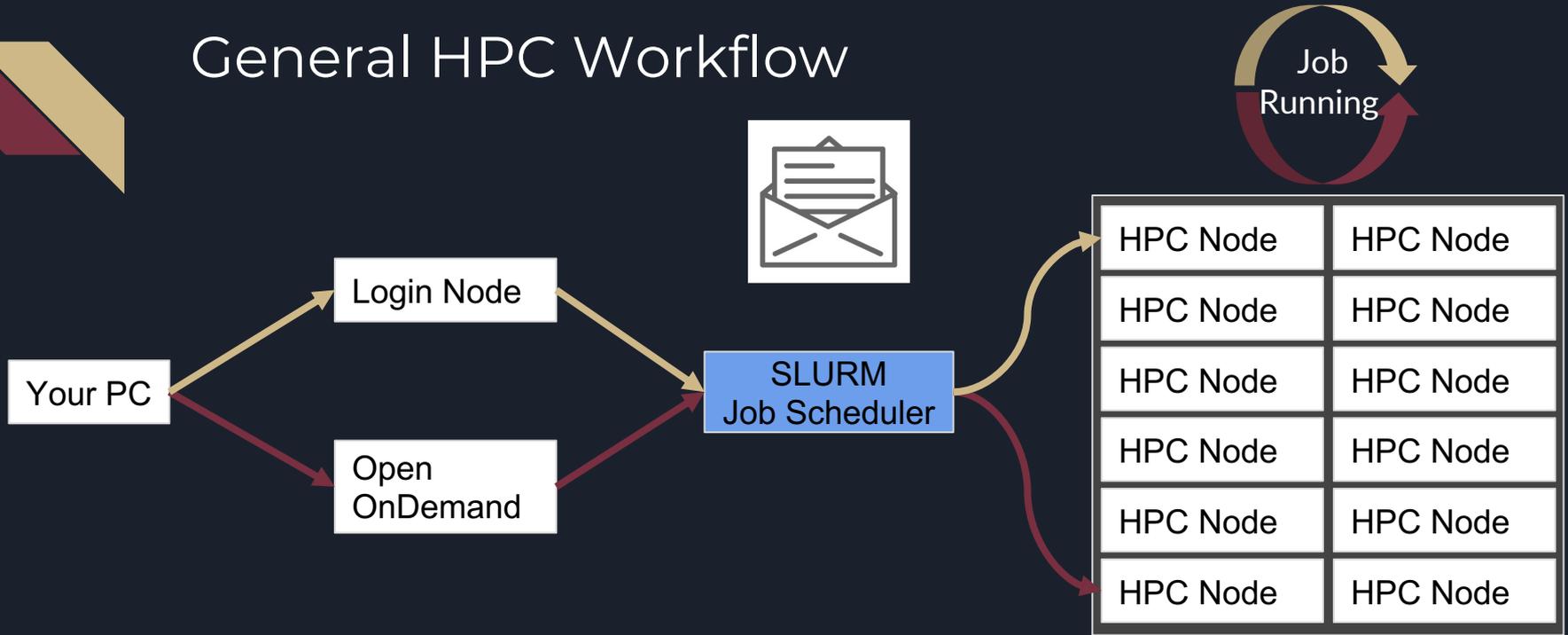
# HPC Definitions



# HPC Job



# General HPC Workflow



Data + Program =====> Output

- Output can be downloaded to your PC once program completes



# How HPC Works

**FSU's HPC is a shared resource for all FSU researchers**

## Job Scheduler: SLURM

- Directs jobs so they can be processed quickly and effectively
- Allocates resources to jobs so the cluster does not freeze up

## User Accounts

- Login and Home Directories

## Slurm Accounts

- Queues / Partitions
- Collection of nodes that each user has access to



# General Access Slurm Accounts

[https://acct.rcc.fsu.edu/manage/hpc\\_partitions](https://acct.rcc.fsu.edu/manage/hpc_partitions)

Slurm Account	Default Runtime	Max Runtime	Max CPU Cores/Job	Max Jobs/User	Max Running Jobs/User
genacc_q	14 days	14 days	400	100	100
backfill	4 hours	4 hours	512	100	100
backfill2	4 hours	4 hours	512	100	100
condor	14 days	90 days	8	100	100
quicktest	10 minutes	10 minutes	8	2	1

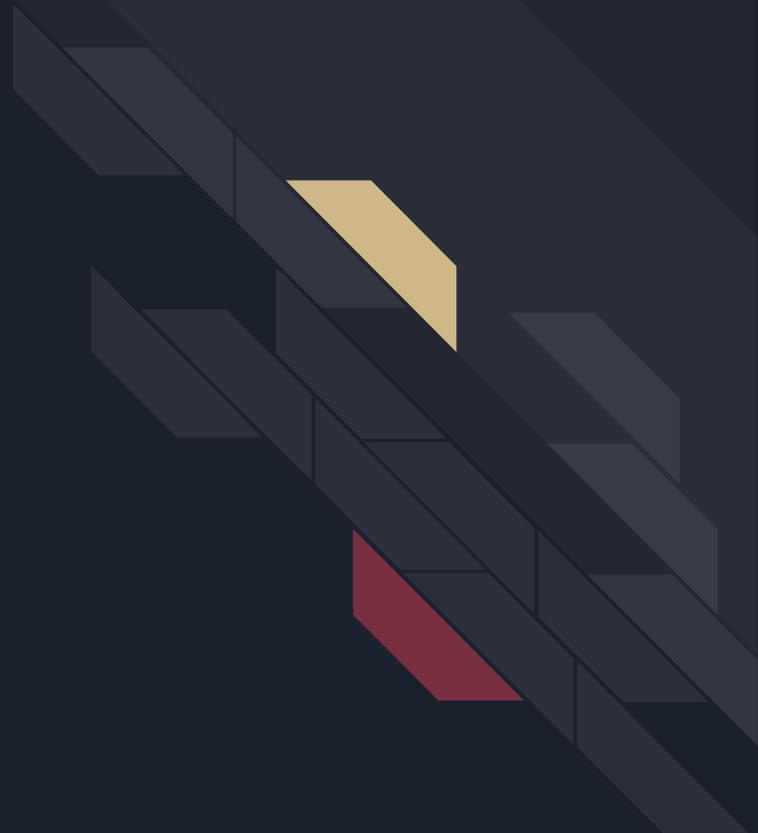
# SLURM Job Scheduler: How to Allocate Resources



# Job Scheduler: SLURM



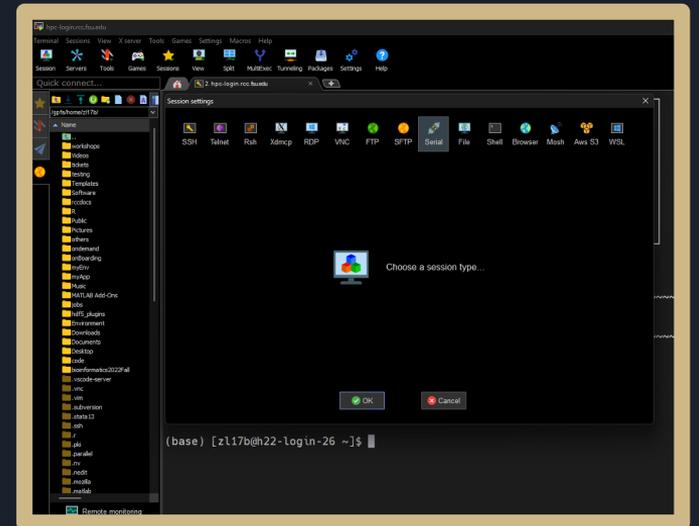
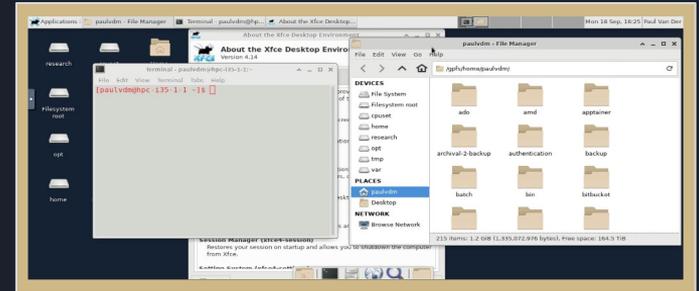
How to Access the HPC?





# Command Line Interface

- Connect using SSH (Secure Shell)
  - Linux Terminal
  - Mac Terminal
  - Windows PowerShell
  - PuTTY
  - Cygwin Emulator
  - **MobaXTerm Emulator**
- RCC uses Linux on all of our compute nodes and login nodes
  - RCC offers an Introduction to Linux Workshop





# Graphical Interface: Open OnDemand

- **GUI Applications**

- RCC Desktop
- MATLAB
- STATA
- VisIt
- Spyder

- **Servers**

- Jupyter Notebooks
- RStudio Server

## **Digital Humanities**

- Agisoft Metashape
- Meshroom

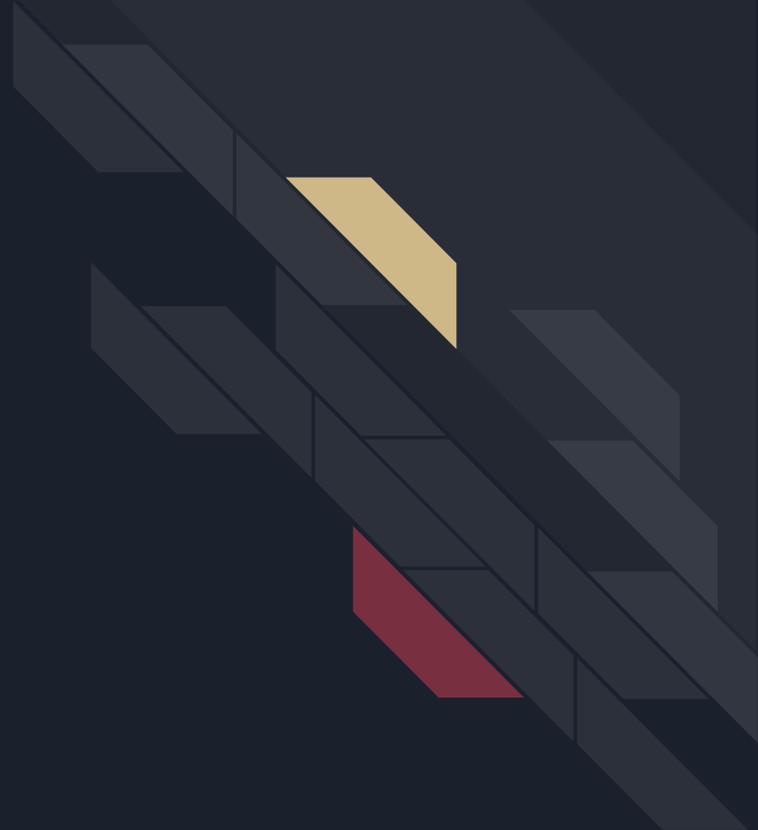
## **Visualizations**

- OpenRefine
- Paraview
- PyMol
- VMD
- xmgrace

<https://rcc.fsu.edu/docs/oo>

[d](#)

# Submitting Jobs to the HPC System



# Submitting Jobs to the HPC System

## Resource Allocation:

- Open OnDemand
  - Lay of the Land
  - File Manager
  - Job Parameters
- Command Line
  - Sbatch Script Parameters

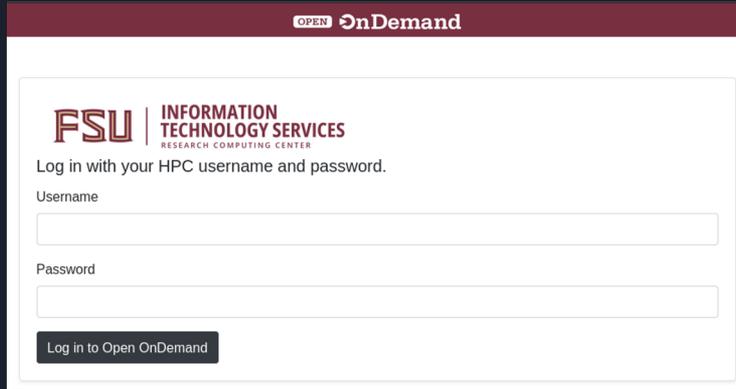
Required parameters - like postage or recipient address

Optional parameters - like the return address

^^ some have default values



# Open OnDemand Interactive Jobs



OPEN OnDemand

**FSU** | INFORMATION TECHNOLOGY SERVICES  
RESEARCH COMPUTING CENTER

Log in with your HPC username and password.

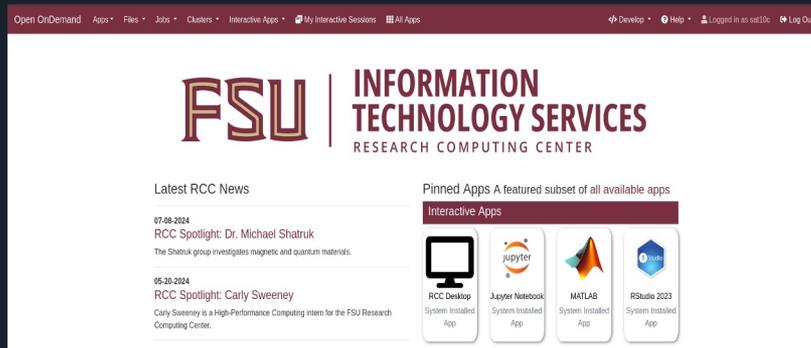
Username

Password

Log in to Open OnDemand

## Login Page

- Click the Link: [ood.rcc.fsu.edu](https://ood.rcc.fsu.edu)
- Login Credentials: Your RCC Account details



Open OnDemand Apps Files Jobs Clusters Interactive Apps My Interactive Sessions All Apps

Develop Help Logged in as sst10c Log Out

**FSU** | INFORMATION TECHNOLOGY SERVICES  
RESEARCH COMPUTING CENTER

Latest RCC News

07-08-2024  
RCC Spotlight: Dr. Michael Shatruk  
The Shatruk group investigates magnetic and quantum materials.

05-20-2024  
RCC Spotlight: Carly Sweeney  
Carly Sweeney is a High-Performance Computing intern for the FSU Research Computing Center.

Pinned Apps A featured subset of all available apps

Interactive Apps

RCC Desktop System Installed App

Jupyter Notebook System Installed App

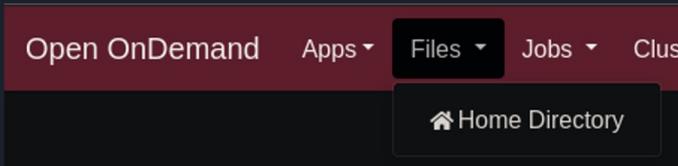
MATLAB System Installed App

RStudio 2023 System Installed App

## Landing Page

- Apps
- File Browser
- Active Jobs
- HPC Cluster Shell Access
- My Interactive Sessions

# Open OnDemand File Manager



- Browse files on the HPC
- View files
- Edit files
- Delete and move files
- Upload small files (code or small datasets < 10 GB)
- Download small files (code or small datasets < 10 GB)
- [Data Transfer Docs](#)

A screenshot of the Open OnDemand File Manager interface. The top navigation bar is dark red with white text, including 'Open OnDemand', 'Apps', 'Files', 'Jobs', 'Clusters', 'Interactive Apps', 'My Interactive Sessions', and 'All Apps'. The main content area is white and shows a file browser for the 'Home Directory'. The current path is '/ gpfs / home / sat10c /'. There are buttons for 'Open in Terminal', 'Refresh', 'New File', 'New Directory', 'Upload', 'Download', 'Copy/Move', and 'Delete'. A table of files is displayed with columns for 'Type', 'Name', 'Size', and 'Modified at'. The table shows 11 files, including folders like '00-sat10c\_staffdir', 'ado', 'cryosparc\_test', 'cryosparc\_tutorial', 'Desktop', 'Dissertation', 'Documents', 'Downloads', and 'jupyterenv'.

Type	Name	Size	Modified at
Folder	00-sat10c_staffdir	-	5/17/2024 2:48:20 PM
Folder	ado	-	6/18/2024 12:49:48 PM
Folder	cryosparc_test	-	8/6/2024 3:55:47 PM
Folder	cryosparc_tutorial	-	6/24/2024 1:19:02 PM
Folder	Desktop	-	5/22/2024 11:05:40 AM
Folder	Dissertation	-	11/4/2022 9:11:29 AM
Folder	Documents	-	8/9/2024 12:43:24 PM
Folder	Downloads	-	6/11/2024 6:32:18 PM
Folder	jupyterenv	-	8/23/2024 12:47:00 PM

# Resource Allocation (OOD)

SLURM Account

Also called Queue or Partition

Number of hours

Maximum amount of time that your job needs to run. Check your max runtime of your slurm account

Amount of memory requested

Include the byte measurement unit (e.g. 2G, 10G, etc). This is the total amount of memory per node

Number of nodes

Usually this will be one, but if you know that your job supports distributed computing, specify the number here.

Number of cores

This is the total amount of cores allocated to this job

GPUs



## SLURM Account

- The set of computers you want to use
- If you leave this blank, it will default to the **genacc\_q** SLURM Account.

# Resource Allocation (OOD)

SLURM Account

Also called Queue or Partition

Number of hours

Maximum amount of time that your job needs to run. Check your max runtime of your slurm account

Amount of memory requested

Include the byte measurement unit (e.g. 2G, 10G, etc). This is the total amount of memory per node

Number of nodes

Usually this will be one, but if you know that your job supports distributed computing, specify the number here.

Number of cores

This is the total amount of cores allocated to this job

GPUs



## Number of Hours

- Maximum amount of time you expect to need for your work
- Maximum runtime for each Slurm Account

# Resource Allocation (OOD)

SLURM Account

Also called Queue or Partition

Number of hours

Maximum amount of time that your job needs to run. Check your max runtime of your slurm account

Amount of memory requested

Include the byte measurement unit (e.g. 2G, 10G, etc). This is the total amount of memory per node

Number of nodes

Usually this will be one, but if you know that your job supports distributed computing, specify the number here.

Number of cores

This is the total amount of cores allocated to this job

GPUs

## Amount of Memory Requested

- The total amount of memory you expect to need per node for your job



# Resource Allocation (OOD)

SLURM Account

Also called Queue or Partition

Number of hours

Maximum amount of time that your job needs to run. Check your max runtime of your slurm account

Amount of memory requested

Include the byte measurement unit (e.g. 2G, 10G, etc). This is the total amount of memory per node

Number of nodes

Usually this will be one, but if you know that your job supports distributed computing, specify the number here.

Number of cores

This is the total amount of cores allocated to this job

GPUs

## Number of Nodes

- The number of individual computer machines you want to use.
- Not all OOD apps will have this option available



# Resource Allocation (OOD)

SLURM Account

Also called **Queue** or **Partition**

Number of hours

Maximum amount of time that your job needs to run. Check your max runtime of your slurm account

Amount of memory requested

Include the byte measurement unit (e.g. 2G, 10G, etc). This is the total amount of memory per node

Number of nodes

Usually this will be one, but if you know that your job supports distributed computing, specify the number here.

Number of cores

This is the total amount of cores allocated to this job

GPUs



## Number of Cores

- The total number of cores you want to use for your job
- Maximum cores for each Slurm Account

# Resource Allocation (OOD)

SLURM Account

genacc\_q

Also called Queue or Partition

Number of hours

1

Maximum amount of time that your job needs to run. Check your max runtime of your slurm account

Amount of memory requested

16G

Include the byte measurement unit (e.g. 2G, 10G, etc). This is the total amount of memory per node

Number of nodes

1

Usually this will be one, but if you know that your job supports distributed computing, specify the number here.

Number of cores

16

This is the total amount of cores allocated to this job

GPUs

0



## GPUs

- The number of GPU cards you want to use for your job
- can leave at 0 if none needed



# Command-Line Batch Jobs - Translating the Job Script

```
#!/bin/bash
#SBATCH -J "MyJob"
#SBATCH -A backfill12
#SBATCH -t 4:00:00
#SBATCH --mem=16G
#SBATCH -n 16
#SBATCH -N 1
#SBATCH --gres=gpu:1

module load gnu openmpi
srun example.x
```

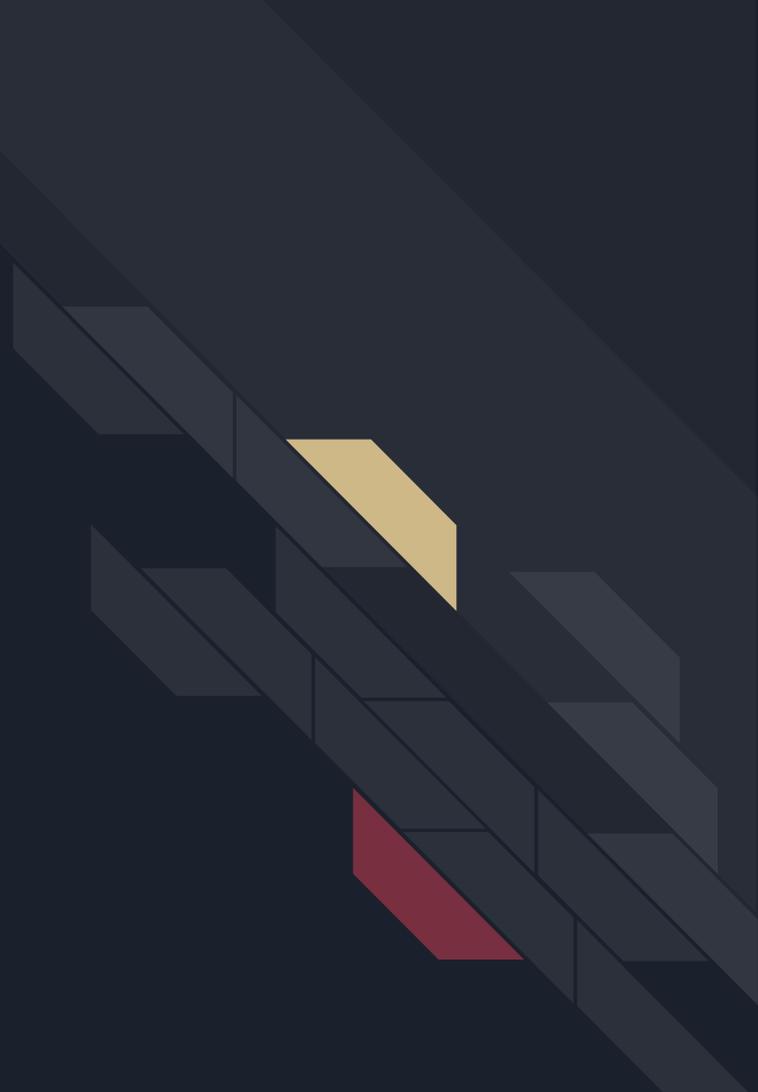
- Reference to “MyJob”
- backfill2 SLURM Account
- 4 hours max runtime
- 16 GB of memory per node
- 16 cores
- 16 cores on 1 physical computer node (don't spread the cores over multiple nodes)
- 1 GPU card of any type
- Need the OpenMPI built with the default GNU compilers
- Run my code called example.x



# How to submit a job? CLI

```
[paul@rumba ~]$
```

Support from RCC Team



# Register For an Account

## Faculty Requirements

- FSU ID and password

## Student Requirements

- FSU ID and password
- Faculty Sponsor

## Guest (non-FSU)

- Guest FSU ID
- Faculty Sponsor



The screenshot shows the login page for the FSU Research Computing Center. At the top, there is a navigation bar with 'FLORIDA STATE UNIVERSITY' on the left, the FSU logo in the center, and 'LOGIN OR SIGNUP' and 'STATUS 1' on the right. Below the navigation bar, the page title is 'FSU RESEARCH COMPUTING CENTER' with the subtitle 'INFORMATION TECHNOLOGY SERVICES'. A navigation menu includes 'HOME' and 'MANAGE'. The main content area is divided into three columns. The left column has a 'Manage' section with links for 'Account', 'Groups', and 'HPC Partitions', and a note: 'If you notice any issues or have suggestions, please let us know.' The middle column is for 'FSUID Login' and contains a text input field for 'FSUID', a text input field for 'FSUID Password', and a 'Login' button. A note below the password field states: '(this is the same account you use to login to Canvas or my.fsu.edu)'. A link for 'Reset system account password.' is also present. The right column is for users who 'Don't have an FSUID?' and contains a 'Signup as Guest --' button. A note explains: 'You need to have an FSUID in order to sign-up for a RCC account. Fortunately, getting a guest FSUID requires only a few steps.'

[www.rcc.fsu.edu/manage](http://www.rcc.fsu.edu/manage)

# Infrastructure

## Physical Location

- Cluster held in the Sliger Data Center in Innovation Park.
- Tours available!

## Standard RCC accounts

- 1 Home directory per user
- 150GB of Parallel Storage
- Temporary Scratch Space (Space Limit is variable)
- Access to the General Access Queues
- Accessible via Open On Demand and CLI



# Infrastructure

Email [support@rcc.fsu.edu](mailto:support@rcc.fsu.edu)  
for more information

## Additional Paid Features for RCC Accounts

- Access to highly scalable Parallel and Archival storage systems
- Priority access to dedicated computing resources in your own queue
- Custom and specialized hardware and infrastructure (as available)
- [docs.rcc.fsu.edu](https://docs.rcc.fsu.edu)





# Support Services

Email [support@rcc.fsu.edu](mailto:support@rcc.fsu.edu)  
with any HPC  
questions or concerns

## Basic Software Support

- Basic Software installation, configuration, and maintenance
- Technical support for installed applications and software
- Workflow process support and improvement assistance
- Assistance with HPC commands and utilities

## Additional Paid Support ([more Information](#))

- Software Development Consulting
- Complex or Highly Customized Software Installations
- In-depth HPC and software focused consulting for research projects

<https://rcc.fsu.edu/software>

# Software

## Scientific

Armadillo (C++)  
BOOST  
FFTW  
OpenCV

## Data Science

NiftyReg  
HDF5  
Apache Spark  
R

## Chemistry

ABINIT  
NWChem  
GROMACS  
Wannier90

## Bioinformatics

Trimmomatic  
MIGRATE  
MAUVE  
MAFFT

## Parallel

OpenMPI  
MVAPICH2  
CUDA  
TotalView



# RCC Service Metrics

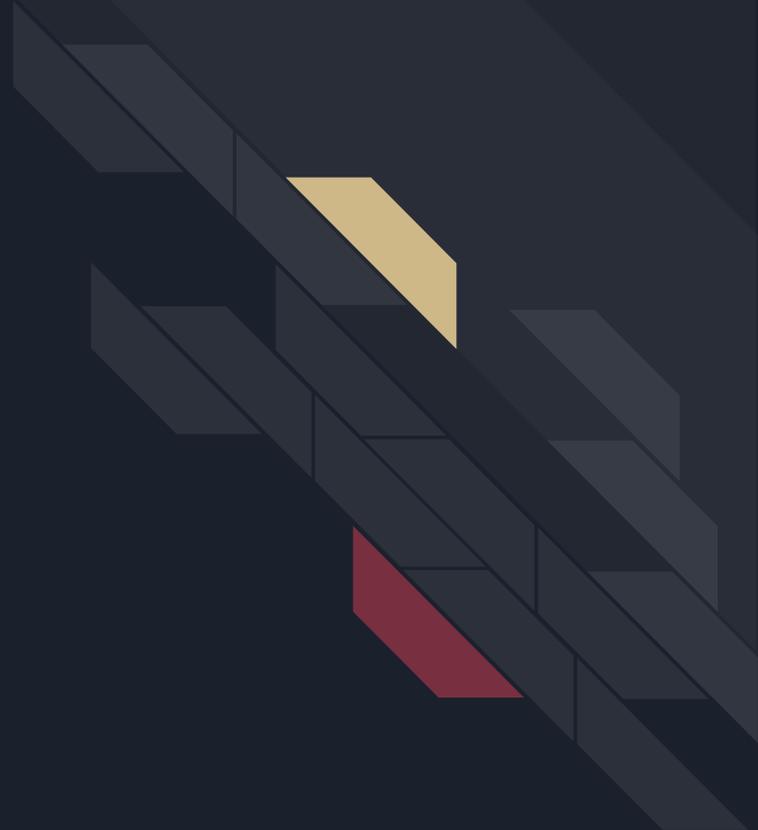
**2 Million**

Average Jobs  
per Year

**2,200**

Support Cases  
Serviced since  
2022

# Research Computing Center Services and Updates





# RCC Services and Updates

## Hardware Innovation

- Water cooled servers, third chiller
- CEPH archival storage

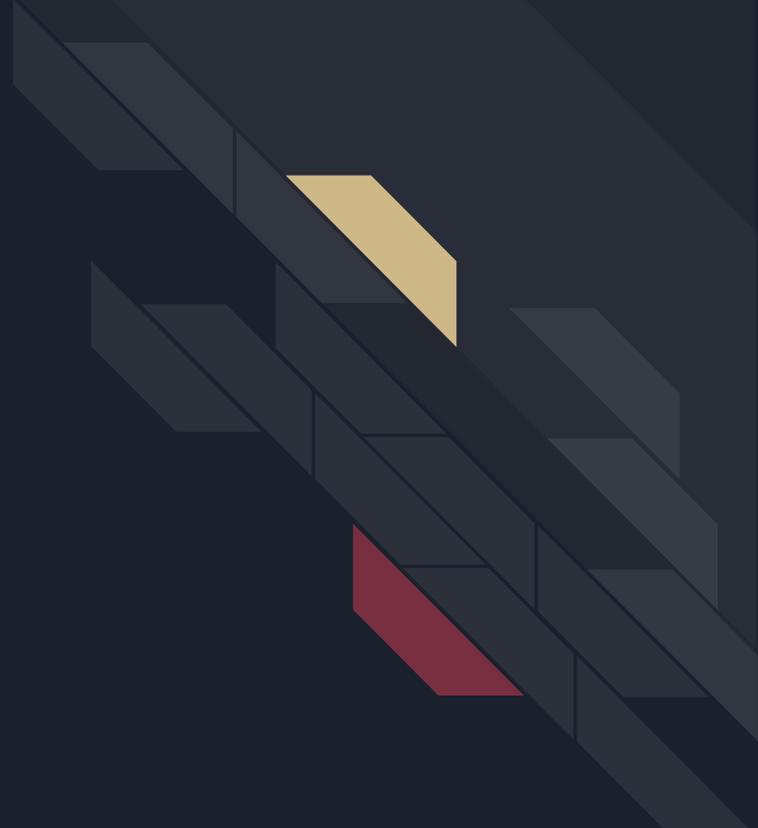
## Interdisciplinary Data Humanities Initiative (IDHI)

- Since Fall 2022
- Support for researchers in the Humanities, Social Sciences, and Arts

## Health Research Initiatives

- REDCap
- Lunch, Learn, and Collaborate (Summer)

More High Performance  
Computing Resources





# Workshops

In Class workshops and  
classroom accounts available  
upon request

## Spring 2025

- Introduction to HPC
- Python Bootcamp
- Intermediate Python
- Intermediate SQL

## Other Past Workshops

- Introduction to Linux
- Introduction to SQL
- Introduction to Digital Humanities
- Parallel Matlab

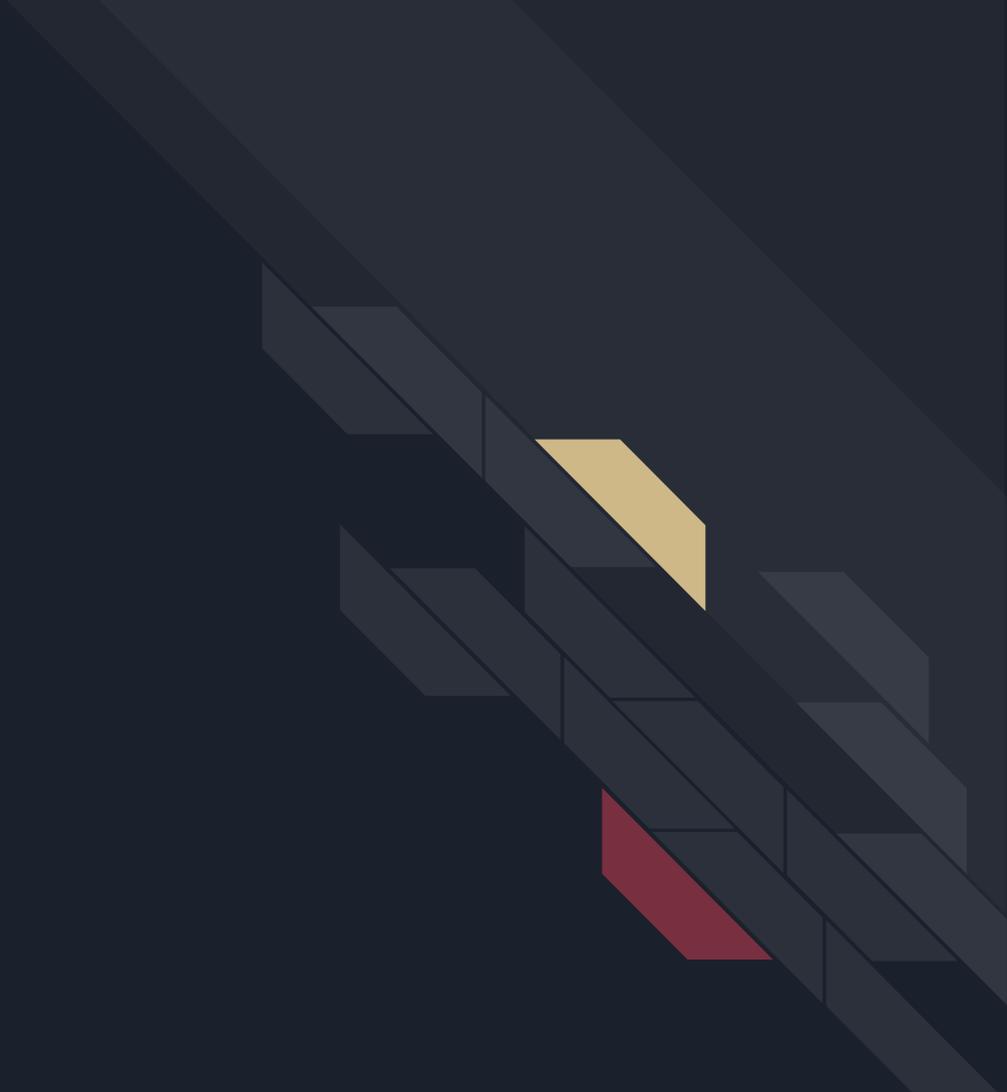


# Software Team Services

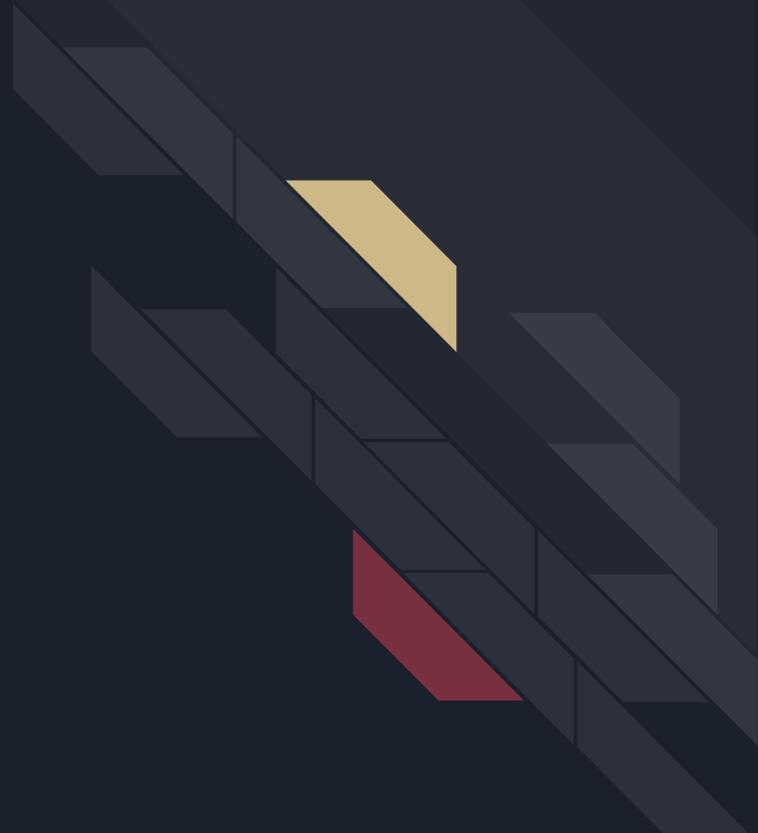
Email us at [support@rcc.fsu.edu](mailto:support@rcc.fsu.edu)  
for any questions or concerns

- Regular Office Hours 9AM - 5PM Monday through Friday
  - We work a hybrid schedule and are available by Zoom or email
  - Dirac Science Library 151
- [HPC Drivers Ed](#) - Introductory HPC materials
- [docs.rcc.fsu.edu](https://docs.rcc.fsu.edu) - RCC Official Documentation
- [BYU's Job Scheduling Video](#) - Job Scheduling Animation

Questions?



# Exercise



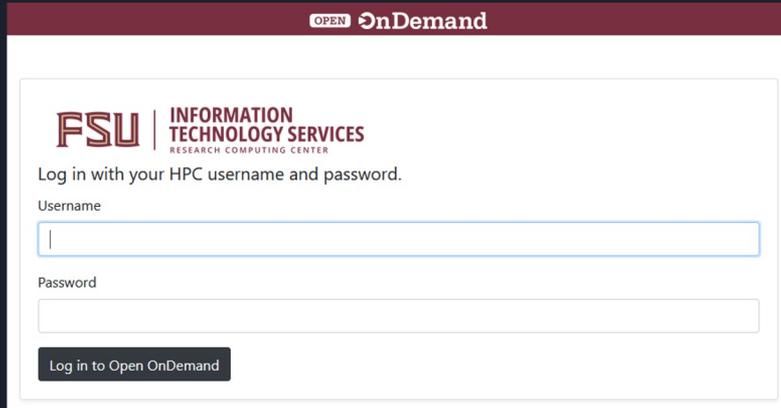


## Exercise A:

1. Navigate to <https://ondemand.rcc.fsu.edu>
2. Log in with your RCC Credentials
3. Navigate to the MATLAB Interactive App
4. Set up a MATLAB Job with the following resources:
  - a. *4 Hours*
  - b. *Using the **workshop** SLURM Account*
  - c. *4 Cores*
  - d. *16 GB of Memory*
  - e. *No GPUs*
  - f. *MATLAB 2022b Version*
  - g. *Leave everything else default*
5. Launch the job
6. Open the MATLAB window in OOD and look around a bit!

# Solution

1. Open OOD in a Browser  
<https://ood.rcc.fsu.edu>



OPEN OnDemand

**FSU** | INFORMATION TECHNOLOGY SERVICES  
RESEARCH COMPUTING CENTER

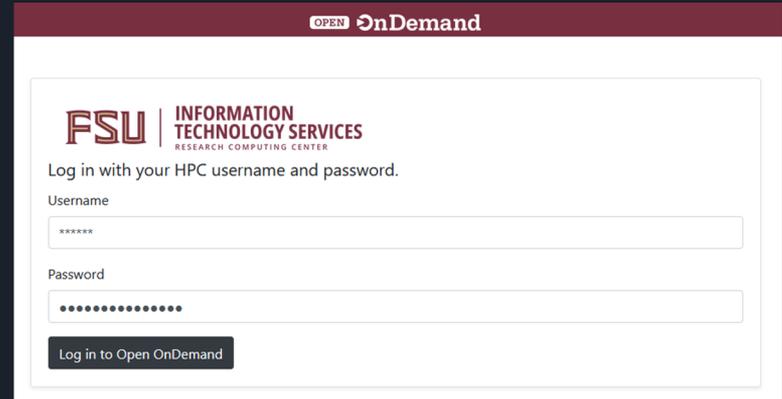
Log in with your HPC username and password.

Username

Password

Log in to Open OnDemand

2. Log in with Your RCC Credentials



OPEN OnDemand

**FSU** | INFORMATION TECHNOLOGY SERVICES  
RESEARCH COMPUTING CENTER

Log in with your HPC username and password.

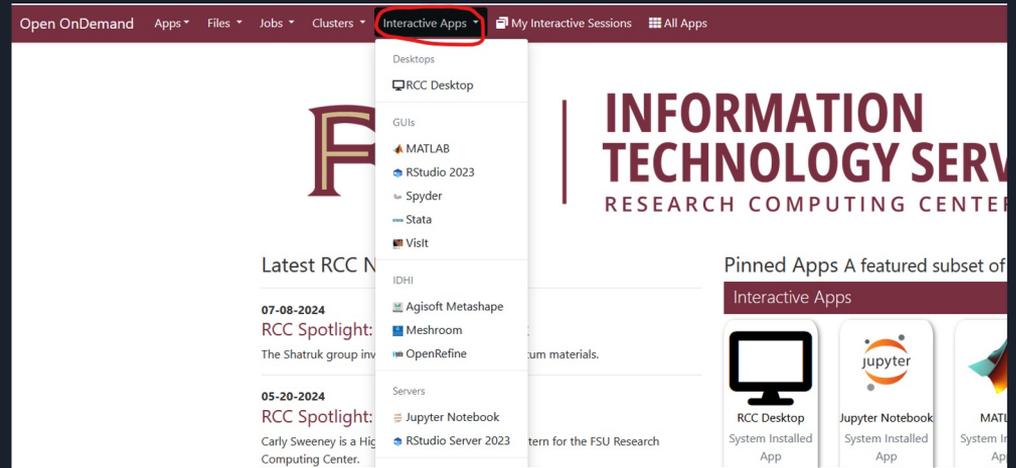
Username

Password

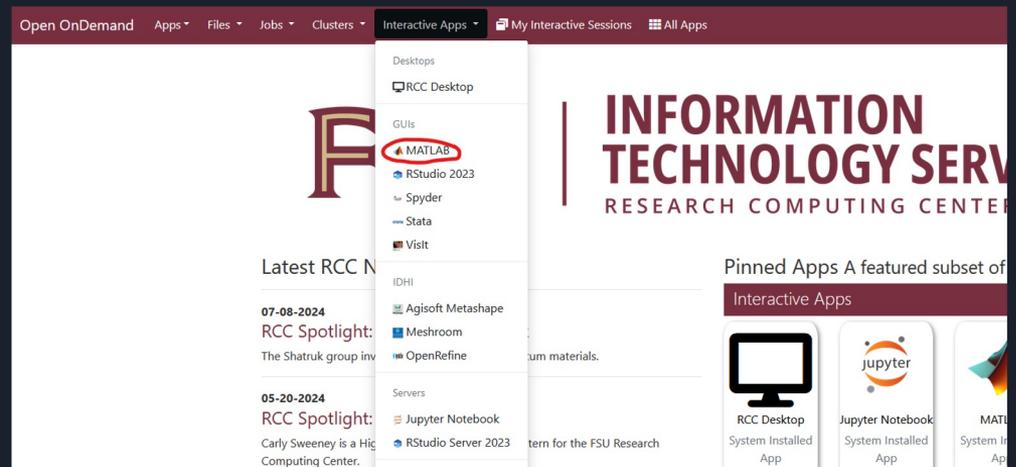
Log in to Open OnDemand

# Solution

## 3. Navigate to the MATLAB Interactive App



This screenshot shows the Open OnDemand web interface. The top navigation bar includes 'Open OnDemand', 'Apps', 'Files', 'Jobs', 'Clusters', 'Interactive Apps', 'My Interactive Sessions', and 'All Apps'. The 'Interactive Apps' dropdown menu is open, displaying categories: Desktops (RCC Desktop), GUIs (MATLAB, RStudio 2023, Spyder, Stata, Visit), IDHI (Agisoft Metashape, Meshroom, OpenRefine), and Servers (Jupyter Notebook, RStudio Server 2023). The main content area features a large 'F' logo, 'Latest RCC News' with two spotlight items, and a 'Pinned Apps' section with 'Interactive Apps' highlighted. Below this, three app tiles are visible: 'RCC Desktop', 'Jupyter Notebook', and 'MATLAB'.



This screenshot is identical to the one above, but with a red circle highlighting the 'MATLAB' option in the 'GUIs' section of the 'Interactive Apps' dropdown menu.

# Solution

## 4. Set up a MATLAB Job with the following resources:

- *4 Hours*
- *Using the workshop SLURM Account*
- *4 Cores*
- *16 GB of Memory*
- *No GPUs*
- *MATLAB 2022b Version*
- *Leave everything else default*

MATLAB version: f464f49

This app will launch a MATLAB GUI on the HPC. You will be able to interact with the MATLAB GUI through a VNC session.

SLURM Account

Also called Queue or Partition

Number of hours

Maximum amount of time that your job needs to run. Check your max runtime of your slurm account

Amount of Memory

Include the byte measurement unit (e.g. 2G, 10G, etc). This is the total amount of memory per node

Number of cores

This is the total amount of cores allocated to this job. You are limited to 1 node.

GPUs

Increase this number above 0 if you need GPUs. Maximum is 4. Note that most GPU nodes only have 2 GPUs so you may get an error on some SLURM accounts/partitions if you select above 2.

**WARNING!** Requesting GPUs can dramatically increase the wait time for your job to start.

MATLAB version

Select the version of MATLAB you would like to use

Extra module (optional)

Select an extra module to use. For example, if you need to use a specific MATLAB version, you can select the corresponding module.

# Solution

## 5. Launch the job

- *Click the blue Launch button at the bottom of the Open OnDemand job setup screen.*

MATLAB version

2022b

Select the version of MATLAB you would like to use

Extra module (optional)

GNU 8.3.1

Select an extra module version only if you have add-ons or MEX files that require a specific compiler

I would like to receive an email when the session starts

Resolution

width 1152 px height 720 px

Reset Resolution

Launch

\* The MATLAB session data for this session can be accessed under the [data root directory](#).

# Solution

## 6. Open the MATLAB window

- *A Queuing Screen*
- *The job will appear in BLUE while it waits for resources*
- *When the job is ready, the box will turn green*
- *Click the blue “Launch MATLAB” button*

MATLAB (9958863) 1 node | 4 cores | Starting

**Created at:** 2024-09-17 11:56:34 EDT Delete

**Time Remaining:** 3 hours and 59 minutes

**Session ID:** c1246a9f-dd05-4f31-ad04-43afa961cf09

---

Your session is currently starting... Please be patient as this process can take a few minutes.

MATLAB (9958861) 1 node | 4 cores | Running

**Host:** >\_hpc-i35-2-1.local Delete

**Created at:** 2024-09-17 11:53:29 EDT

**Time Remaining:** 3 hours and 58 minutes

**Session ID:** 609bad0b-a849-4cc1-9fe0-b6c3580e49d3

noVNC Connection  Native Instructions

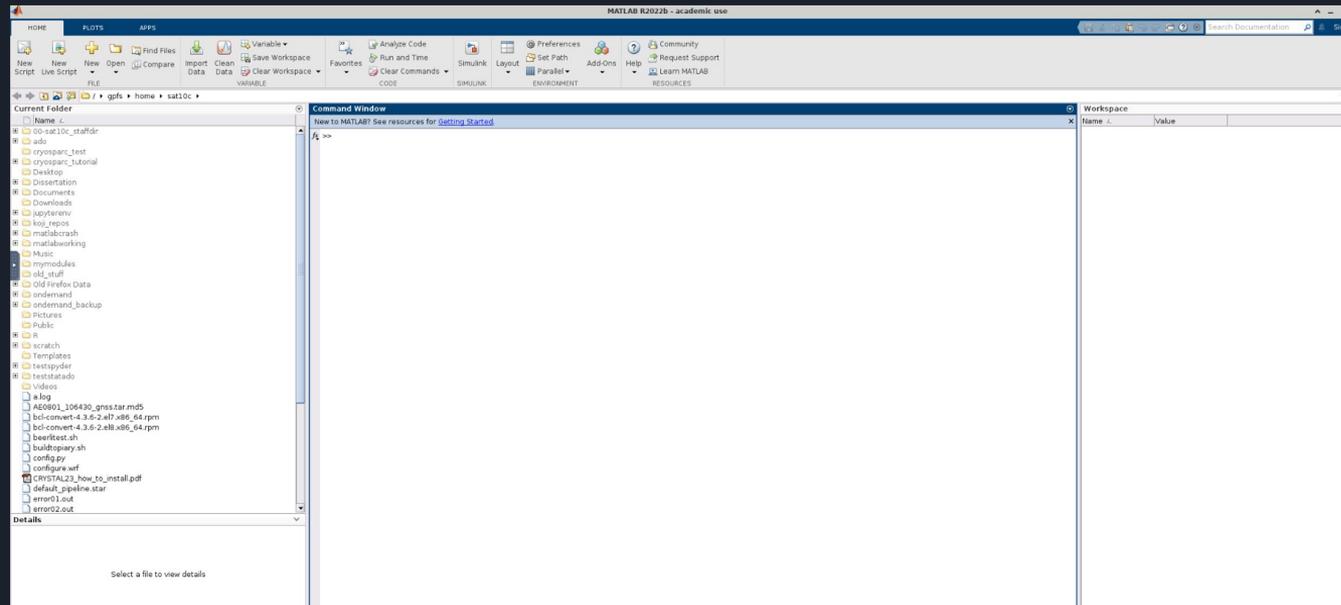
Compression 0 (low) to 9 (high) Image Quality 0 (low) to 9 (high)

Launch MATLAB View Only (Share-able Link)

# Solution

## 7. Click the “Launch MATLAB” button

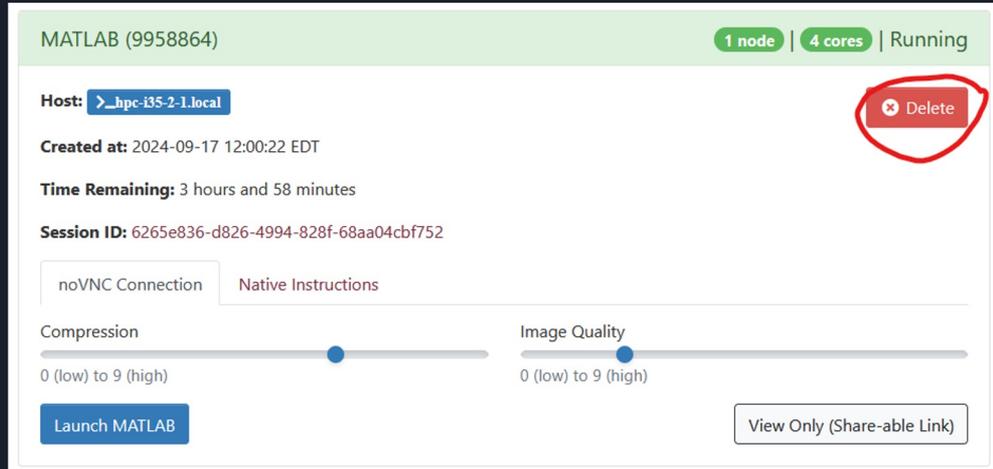
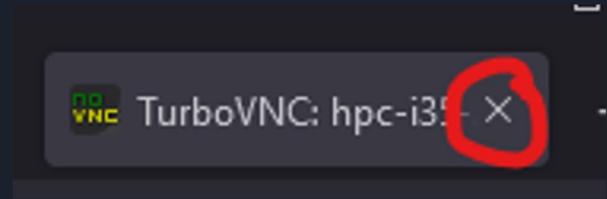
- *It may take 2-3 minutes for MATLAB to fully launch*



# Solution

## 8. Close the session:

- Close the tab your Open OnDemand session
- You will be back to the “My Interactive Sessions” tab
- Click the “Delete” button to end the job

A screenshot of the Open OnDemand session management interface. The session is titled "MATLAB (9958864)" and is in a "Running" state, using "1 node" and "4 cores". The host is identified as "hpc-i35-2-1.local". The session was created on "2024-09-17 12:00:22 EDT" and has "3 hours and 58 minutes" remaining. The session ID is "6265e836-d826-4994-828f-68aa04cbf752". There are two tabs: "noVNC Connection" and "Native Instructions". Below the tabs are two sliders: "Compression" (0 to 9, low to high) and "Image Quality" (0 to 9, low to high). A blue "Launch MATLAB" button is on the left, and a "View Only (Share-able Link)" button is on the right. A red circle highlights a "Delete" button with an 'X' icon in the top right corner.



# Exercise B: MPI Trapezoid Example Program

1. Open a terminal
2. Log in to your HPC Account
3. Prepare the code
  - Copy the code to your current working directory

```
cp /gpfs/research/software/examples/trap.c .
```

- (Note: If you are in-person, this will already be in your home directory)



# Exercise: MPI Trapezoid Example Program

## 4. Compile the code with the MPI Compiler

```
module load gnu openmpi  
mpicc trap.c -o example.x -lm
```

## 5. Write a short script which will submit this job and save the script in a file called **testjob.sh**:

- Slurm Account: workshop
- Time: 2 hours
- Cores: 16

# Exercise: MPI Trapezoid Example Program

(Note: If you are in-person, this will already be in your home directory)

```
#!/bin/bash
#SBATCH -J "testjob"
#SBATCH -A workshop
#SBATCH -t 2:00:00
#SBATCH -n 16

module load gnu openmpi
srun example.x
```

## Sample Script:

- *We don't need to specify memory since the defaults will be sufficient for us*
- *We don't need to specify nodes. Since this code uses MPI, it can run across multiple nodes. SLURM is free to allocate as many nodes as it needs*
- *We don't need any GPUs for this job, so we can leave out the `-gres=gpu` line*



# Exercise: MPI Trapezoid Example Program

## 6. Submit the job

```
sbatch testjob.sh
```

## 7. Outputs to screen a job ID number (number will change each job)

```
Submitted batch job 123456
```

## 8. Get output file

- *When the job is complete, a new file will be present called **Slurm-123456.out***
- *The results from your job will be in there*