# **Using Open OnDemand on Wulver**

## Hui (Julia) Zhao NJIT High Performance Computing



## Outline

Introduction and Dashboard

Overview and benefits

## File Management and Jobs

File Manager Features

Job Management

Jobs Menu, Active Jobs, Job Composer

## Interactive Apps Configuration

Configuring Interactive Apps on Open OnDemand

Additional Tools and Support



## **Introduction to Open OnDemand**

## What is Open OnDemand?

Open OnDemand is an open-source web portal offering browserbased access to HPC clusters.

## **Simplified HPC Access**

The platform eliminates the need for SSH or third-party tools, streamlining the process of connecting to HPC resources.

### **Intuitive User Interface**

It features a graphical user interface, making high-performance computing straightforward for researchers and scientists.

### **Designed for All Users**

Open OnDemand is suitable for both beginners and advanced HPC users, improving accessibility and productivity across research teams.



## **How Open OnDemand Works**

### **Access Portal**

### Authenticate & Launch

Users open a web browser and navigate to the institution's Open OnDemand portal, eliminating the need for SSH or specialized software. Users log in using institutional credentials. The portal authenticates access and provides dashboard for managing resources.

### **Select HPC Resources**

Through the graphical interface, users choose applications, submit jobs, or interact with HPC clusters.

### **Monitor & Retrieve Results**

Users can track job progress, view logs, and download results directly through the portal, making the HPC workflow seamless.

Portal Login	User Authentication	Job Submission Forms	Job Monitoring Tools
Access from Browser	Personalized Dashboard	Graphical Application Launchers	Log Access
No SSH Required		Resource Selection	File Download Options

## **Traditional HPC vs. Open OnDemand**

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## **Traditional HPC Access Challenges**

- Requires SSH access to connect to HPC clusters
- Relies on Linux terminal command-line interface
- No graphical user interface (GUI) available
- Steep learning curve for new users unfamiliar with commands

## **Open OnDemand Benefits**

- Simplifies file management with an intuitive GUI
- Provides web-based command-line shell access
- Allows creation, viewing, and management of jobs via graphical tools
- Enables running interactive desktop and applications like MATLAB, RStudio, Jupyter Notebook



# Accessing Open OnDemand at NJIT



### Webauth Authentication Service

A service requiring authentication has referred you here. For details about the Webauth Authentication Service visit http://ist.njit.edu/webauth.

UCID	
g07396	
Password	
••••••	
Login	

## **Open OnDemand Portal URL**

Visit: https://ondemand.njit.edu to access the NJIT Open OnDemand platform.

## **Login Credentials Required**

Log in using your UCID and password to ensure secure access to resources.

## **VPN Requirement for Off-Campus Access**

Use VPN if connecting from off-campus to maintain secure and authorized entry to the platform.



## **Open On Demand Dashboard**

	Files	Quick access to common directories allowing easy file browsing and management within the HPC environment.
::	Jobs Menu	Manage Slurm jobs efficiently, including submitting new jobs and monitoring current job statuses.
Ģ	Cluster Access	Interact directly with cluster resources to utilize computing power effectively for HPC tasks.
	Interactive Applications	Launch supported interactive applications such as MATLAB, RStudio, and Jupyter Notebook from the dashboard.
<u>+</u> †+	My Interactive Sessions	View and manage your running interactive sessions to monitor resource usage and control session lifecycle.



## File Manager in Open OnDemand

#### **Accessing File Manager Navigating Directories Viewing Directory Contents** Access File Manager via the 'Files' Navigate through home, project, and View directory contents with a clear ben OnDemand Files -Jobs 🔻 Clusters scratch spaces to locate needed dropdown on the Open OnDemand and organized interface showing files directories and files. dashboard. and folders. **Home Directory** Project Directory /project Scratch Directory /scratcl OnDema ▶\_

#### **Toolbar Functions**

Use the toolbar to change directories quickly, open a terminal session for command-line operations, and create or upload new files.

### **Key Toolbar Features**

Toolbar features include directory navigation buttons, terminal launch, file creation, and upload options for efficient file handling.

#### **User-Friendly Operations**

The File Manager simplifies file operations without requiring command-line expertise



## **Jobs Menu and Active Jobs**

### Jobs Menu

Provides shortcuts to widgets for creating new Slurm jobs as well as viewing the status of your current ones.

## **Active Jobs**

The Active Jobs window opens in a new tab which shows the list of all the active jobs in the cluster.

## **Job Monitoring**

Users can monitor job status, view job details, and track progress conveniently within the Open OnDemand portal.

Open OnDemand	Files 🝷	Jobs 👻	Clusters -
		() Activ	ve Jobs
		🎇 Job (	Composer



## **Active Jobs**

• The Active Jobs window opens in a new tab which shows the list of all the active jobs in the cluster.

Open	OnDemand	Files - Jobs -	Clusters 👻 Intera	ctive Apps 🝷	Tools 🔻	My Interactive Sessions					🕄 Help 👻 💄 Lo	gged in as g07396	🕞 Log Out
												All Jobs	- Wulver -
Acti	50  entries											Filter:	
		A Name				å User	Account	🚖 Time Used 着	Queue	≜ Status	A Cluster	Actio	ins 🔺
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/	437433	COAMINE				1170	ZHIWEI	00.00.00	Digitietti	Queded	Walver		
>	497438	cox.h.pans2				hf78	zhiwei	00:00:00	bigmem	Queued	Wulver		
>	497437	cox.h.pans				hf78	zhiwei	00:00:00	bigmem	Queued	Wulver		
>	497427	cox.h.bl				hf78	zhiwei	00:00:00	bigmem	Queued	Wulver		
>	491773	clfaslazy				zd4	zd4	68:54:47	bigmem	Running	Wulver		
>	502579	prehp				hf78	zhiwei	00:08:02	bigmem	Running	Wulver		
>	502096	sa6b500cl160				sm3557	samaneh	00:00:00	general	Queued	Wulver		
>	502095	sa6b500cl160				sm3557	samaneh	00:00:00	general	Queued	Wulver		
>	502094	sa6b500cl160				sm3557	samaneh	00:00:00	general	Queued	Wulver		
>	502093	sa6b500cl160				sm3557	samaneh	00:00:00	general	Queued	Wulver		
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## **Job Composer: Creating New Jobs**

### From Default Template

- Create a new job with the system's default template
- Best for standard job submissions
- Navigate: Job Composer > New Job > From Default Template

### **From Template**

- Choose from predefined templates for various applications
- Navigate: Job Composer > New Job > From Template
- Select the desired template from the list

## From Specified Path

- Copy files from a chosen directory to create a job
- Ideal for using existing scripts or data
- Navigate to Job Composer > New Job
   > From Specified Path
- Configure job options as needed

## **From Selected Job**

- Duplicate existing jobs to modify or rerun quickly
- In Job Composer, select a job, then click New Job > From Selected Job
- Reuse configurations and scripts to save time



## **Login Shell**

## **Under Clusters -> Shell Access**

## **Under Files**



>_ Open in Terminal	C Refresh	+ New File	New Directory	🏦 Upload	🛓 Download



## **Interactive** Apps

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### **Interactive Apps Purpose**

## **Command-line Elimination**

Interactive Apps let users start and connect to batch jobs easily.

No command-line needed to start interactive apps.

**Common Applications** 

Supported interactive apps include:

Compute Desktop, Jupyter, MATLAB, RStudio, etc

## **Resource Configuration**

When launching, users select allocation (CPU vs. GPU), partition, resources (memory, CPUs), and walltime to tailor their interactive app sessions.





Desktops

Linux Desktop

## **Interactive Apps**

MISYS ANSYS

GUIs

- 🚵 Abaqus
- Altair
- 🕱 Avogadro2
- COMSOL Multiphysics
- GaussView
- 📣 MATLAB
- 👲 Spyder
- 🝯 Tecplot
- 🚴 VESTA

😹 VMD

Servers

👼 Jupyter

RStudio

• Select allocation (CPU vs. GPU) based on your computational needs.

- Choose the partition appropriate for your job.
- Configure memory, number of CPUs, and GPUs if applicable.
- Set wall time to define session duration.
- Specify account and load necessary modules for your environment.



## **Open OnDemand Linux Desktop**

- The first step is to select the Interactive apps and then click the Desktop in the Open OnDemand dashboard.
- Fill in the form to launch the interactive desktop on the compute nodes.

### Linux Desktop

This app will launch an interactive desktop on a compute node. You will be have full access to the resources defined below. This is analogous to an interactive batch job.

How many resources do you need for this desktop?

4 Cores

 $\odot$  8 Cores

 $\odot$  16 Cores

 $\bigcirc$  32 Cores

○ 16 Cores, 1 GPU

 $\odot$  32 Cores, 1 GPU

How many hours do you need the resources for?

1				
Account				
walsh		~		
QoS				
standard		~		
Partition				
general		~		
Launch				



## Launching the Interactive Session



plications :			J
Filesystem root	research	proc	
boot	sys	mmfs1	
shared	tmp		
pts	var		
shm	File System		
local	Home		
	Filesystem root boot boot shared pts shm iocal	Filesystem root boot sys boot shared tmp var ishm File System iocal Home	Filesystem research proc boot sys mmfs1 boot sys mmfs1 boot tmp pts var File System local Home

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## Jupyter Notebook in Open OnDemand

## What is Jupyter Notebook?

A web-based interactive computing environment for creating and sharing documents that contain live code, equations, visualizations, and narrative text.

### Launching Jupyter Notebook

From the Open OnDemand dashboard, go to Interactive Apps > Jupyter Notebook. ίΞ

### **Requirements for Use**

- Your environment must have Jupyter Notebook installed. (conda install -c condaforge jupyter notebook)
- You need jupyter to run the Notebook environment, and ipykernel to execute Python code within it.



## Jupyter Notebook

### Jupyter

This app will launch a Jupyter server

Mode

 $\bigcirc$  Jupyter Lab

Jupyter Notebook

#### Type of Environment

#### Conda environment

- Select the type of environment in which you want to use Jupyter.
- Choose Conda environemnt if you have created Conda environment with Jupyter Notebook and other Python packages installed
- If you select Python module, it will load System Installed JupyterLab or JupyterNotebook. Please note you may not have additional packages to run the Python script
- System installed Jupyter has **NumPy**, **Matplotlib**, **SciPy** and you don't have permission to install the additional packages.
- Refer to the Conda Documentation for instructions on creating a Conda environment and installing packages within it.

#### Conda Environment to be Activated

#### tensorflow

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- Select the name of environment to be activated. This field is mandatory if you choose Conda environemnt.
- Your environment must have **Jupyter Notebook**. Check Jupyter Documentation for details.

#### Enter the full path of the case directory

#### /project/hpcadmins/g07396/

#### Account

walsh

#### Partition

general		/

 $\sim$ 

NJIT

QOS

debug

#### Number of hours (max 72)

Maximum wall time requested

Number of cores (max 64)

Number of cores on node

Number of GPUs (max 4)

#### Total GB memory (max 480)

4

1

- This field is optional. By default, 4 GB of memory per core will be used unless specified here.
- For SU calculation, the memory value will be divided by 4 GB, and the result will be used to determine SU usage.
- For example, if 4 cores and 128GB of memeory are requested, the SU will be calculated based on 128/4=32 cores.
- □ Get email notifications
  - Receive an email when the session starts, and ends.
  - Guest users will not receive any notifications.

## Jupyter Notebook

Your environment must have Jupyter Notebook installed. (conda install -c conda-forge jupyter notebook)

Home / My Interactive Sessions / Jupyter

### Failed to stage the template with the following error:

Jupyter is not installed on 'tensorflow'. Please check https://hpc.njit.edu/Software/programming/python/jupyter on how to install Jupyt

The jupyter metapackage, installed via conda install -c conda-forge jupyter, includes:

- **IPyKernel**: The Python kernel for executing code in Jupyter Notebooks.
- Notebook: The web server and interface for creating and interacting with Jupyter Notebooks.



## Jupyter Notebook

## Launch Jupyter Notebook session

**Check logs** 

Jupyter (506255)	1 node   2 cores   Running	dc	/ home / 0f34df-4644	g07396 / ondemand / data / sys / -4244-86bd-455931e9a244 /	dashboard / batch_co	onnect / sys / Jupyt	er / output /
					Show Owner/	Mode 🗆 Show Do	otfiles Filter:
Host: >_n0047	🙁 Delete						Showing 12 rows - 0 rows selected
			Туре	Name	*	Size 🍦	Modified at
Created at: 2025-04-30 15:43:19 EDT			•	assets	: -	-	3/31/2025 5:31:37 PM
Time Remaining: 57 minutes			lì.	after.sh	:-	308 Bytes	4/30/2025 3:43:19 PM
Session ID: dc0f34df-4644-4244-86bd-	-455931e9a244		li	before.sh	• •	1.43 KB	4/30/2025 3:43:19 PM
			li	config.py	•	428 Bytes	4/30/2025 3:43:24 PM
You can get log details about your job by o	clicking the Session ID link above and then		lì	connection.yml	•	99 Bytes	4/30/2025 3:43:33 PM
clicking and reviewing the output.log file.			li	job_script_content.sh	: -	6.66 KB	4/30/2025 3:43:21 PM
				job_script_options.json	: -	594 Bytes	4/30/2025 3:43:21 PM
Connect to Jupyter			li	output.log	•	34.4 KB	4/30/2025 3:45:04 PM
			<b>B</b>	script.sh	: -	890 Bytes	4/30/2025 3:43:21 PM



## **Using Jupyter Notebook Effectively**

Practical tips for running and managing Jupyter Notebook sessions on Open OnDemand

- Manage your notebooks within the session; remember to save your work frequently to prevent data loss.
- Allocate appropriate resources (CPU, memory, time) based on your task's requirements to ensure smooth performance.
- Shut down sessions when finished to free up system resources.
- Check "My Interactive Sessions" and click "Delete" to terminate active sessions.
- For custom environments, ensure the ipykernel package is installed to access different Python environments.



## **RStudio in Open OnDemand**

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## What is RStudio?

An integrated development environment (IDE) for R, providing tools for coding, history, connections, and more. Ideal for statistical computing, data visualization, and working with R packages.

### Launching RStudio in Open OnDemand

Access from the dashboard under Interactive Apps > RStudio Server. Choose between running on a shared node for low-intensity tasks or as a Slurm batch job for intensive tasks.

## **(**

## **Resource Configuration Options**

Select R version, account, partition, QOS, walltime, number of cores, and number of GPUs if using a GPU partition when launching your RStudio session.



## Rstudio

- The first step is to select the Interactive apps and then click the RStudio Server in the Open OnDemand dashboard.
- Then you will see a form which needs to be filled to launch the RStudio Server on the compute nodes.

### RStudio

- This app will launch RStudio on Wulver
- Works with R module or conda installed R

#### R version

4.4.1			`

This defines the version of R you want to load.

#### If choose "custom", enter commands below to load your custom R environment

 For example, to use a Conda nstalled R environment, you might enter: module load Miniforge3; conda activate my\_conda\_r\_env

#### Account

walsh	~
Partition	
general	~
QoS	
standard	~

Number of hours

1		
Maximum wall time requested		

#### Number of cores

1

Number of cores on node type (4 GB per core unless requesting whole node).

#### Number of GPUs

0

Number of GPU or Cuda devices



Launch

## Launch Rstudio

### RStudio (503799)

Host: >\_n0056

Created at: 2025-04-27 21:34:03 EDT

Time Remaining: 27 minutes

Session ID: bf251d48-9fe3-4038-b334-b51dabad08ff

R Connect to RStudio Server

D	File Edit	Code	View	Plots	Session	Build	Debug	Profile	Tools	Help
I	•••	👉 -   🔓			Go to file	function/		- Addins	; <b>-</b>	
Console	Terminal >	Back	ground	Jobs ×						
💿 R 4.	4.1 · /mmfs	1/home/g	07396/							

R version 4.4.1 (2024-06-14) -- "Race for Your Life" Copyright (C) 2024 The R Foundation for Statistical Computing Platform: x86\_64-pc-linux-gnu

R is free software and comes with ABSOLUTELY NO WARRANTY. You are welcome to redistribute it under certain conditions. Type 'license()' or 'licence()' for distribution details.

Natural language support but running in an English locale

R is a collaborative project with many contributors. Type 'contributors()' for more information and 'citation()' on how to cite R or R packages in publications.

Type 'demo()' for some demos, 'help()' for on-line help, or 'help.start()' for an HTML browser interface to help. Type 'q()' to quit R.

>



### Interactive Apps

#### Desktops

Linux Desktop

-			
G		le.	
	v	13	

Misys ANSYS

🚵 Abaqus

- Altair

🕱 Avogadro2

COM	SOL M	ultiphy	sics
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📣 MATLAB

🗯 Spyder

🝯 Tecplot

🚴 VESTA

😹 VMD

Servers

👼 Jupyter

💿 RStudio

## **Other Interactive Apps**

- Interactive Apps include ANSYS, Abaqua, COMSOL, GaussView, Spyder, Tecplot, BESTA, VMD, Matlab, and more.
- These applications offer flexibility and ease of use for complex HPC tasks without requiring command-line expertise.



## Tools



## Joblist

The Joblist tool provides information about your past jobs run in the specified period and the service Units(SU) consumed.

## **Quota Info**

Quotainfo is a tool to check disk usage quotas, helping users keep track of their allocated storage space on HPC clusters.



## **Additional Tools Available**

## Checkload

The checkload tool provides real-time information about the current load on the HPC cluster, assisting users in monitoring the CPU load, state across all compute nodes

### Homespace

Homespace tool offers details about the home directory space usage, enabling users to manage their files and storage efficiently within their personal workspace.

## qoslist

Displaying All QOS Entries for a User Across All Associated Accounts



## **Key Features Recap**

## open In Demand

### **File Management**

Upload, download, view, and edit files easily via the webbased file manager. Navigate home, project, and scratch spaces with directory browsing and file operations.

### Web-based Shell Access

Access a command-line shell through the browser without needing SSH. Execute commands directly on the HPC cluster with terminal access integrated within the portal.

### Launching GUI Applications

Run interactive graphical applications such as Jupyter Notebook, RStudio, MATLAB, and more through the Interactive Apps feature, simplifying usage without command-line commands.

### Job Submission and Monitoring

Submit, manage, and monitor batch jobs using the Job Composer and Jobs Menu. View active jobs in the Active Jobs window and download job output files easily.

### **Graphical Desktop Sessions**

Access full graphical Linux desktop environments via browser-based sessions, allowing users to work in a familiar desktop interface remotely on HPC resources.



## **Getting Help & Support for NJIT HPC**

NJIT HPC Documentation Open OnDemand Documentation

**HPC Support Email** 

T

**Research** Computing Facilitator

**Office Hour** 

Date: Every Monday and Wednesday Location: GITC 2404 Time: 2:00 PM - 4:00 PM

Please visit: NJIT HPC website Explore official Open at https://hpc.njit.edu.

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detailed instructions and troubleshooting at https://openondemand.org.

Consult with the Research Open a ticket using email: OnDemand documentation for hpc@njit.edu to request help Computing Facilitator and or report problems with HPC help with HPC user/course services. assistance.

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