

# ARCATS Training Workshop

High Performance Computing and AI/ML

30 April 2025



TEXAS A&M UNIVERSITY  
SAN ANTONIO



High Performance  
Research Computing  
DIVISION OF RESEARCH

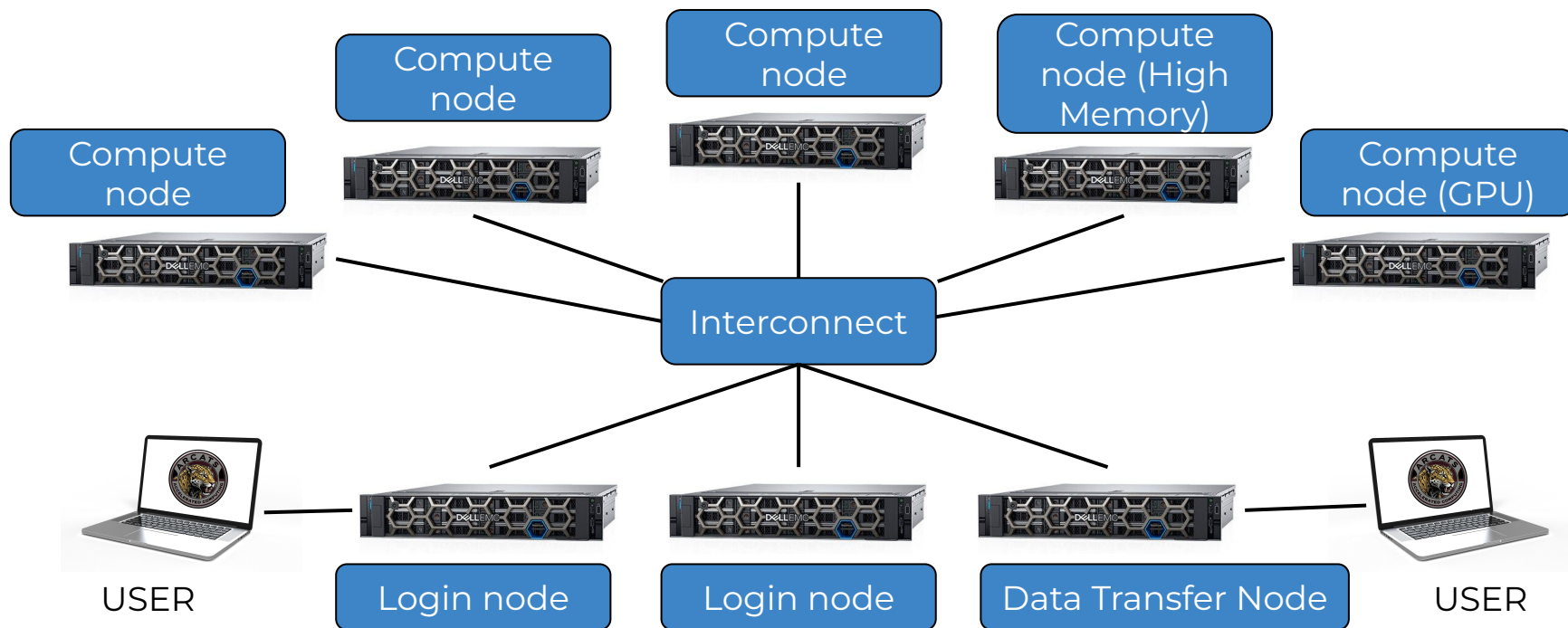


ARCATS Training Workshop | NSF Awards #2430335 and #2232895

# Workshop Outline

- High Performance Computing (HPC) Architecture
- Getting on Launch
- Overview of Launch Open OnDemand Portal
- Working in JupyterLab
- Coding in Python
- Introduction to AI/ML
- Deploying Deep Learning Models on HPC

# HPC Architecture



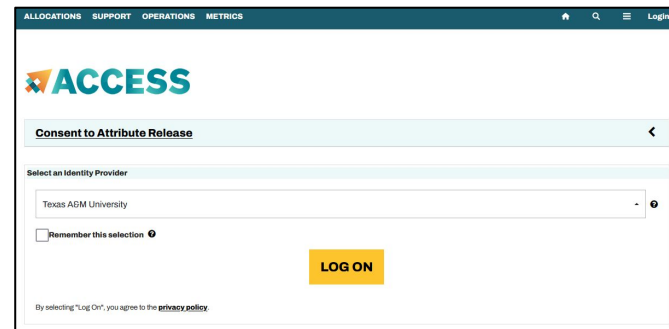
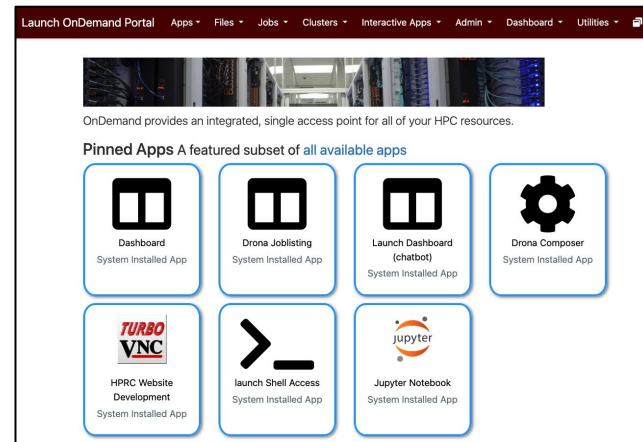
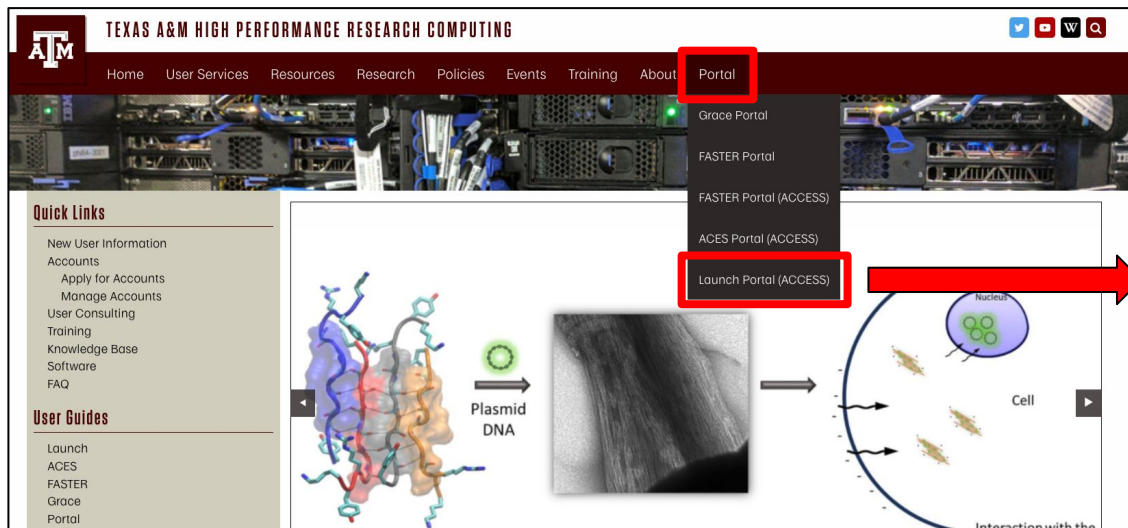
# Coordinating multiple users

- HPC systems can have thousands of users, many running analyses or scripts simultaneously.
- HPC usage is coordinated by job orchestration software (Slurm).
- Large jobs must be submitted to or run interactively on compute nodes.
- Login nodes are for small jobs (job script creation, data management).
- Interactive GUI applications are automatically launched on compute nodes.




# Getting on Launch

- Go to <https://hprc.tamu.edu>
- Hover over the “Portal” drop down menu
- Select “Launch Portal (ACCESS)”
- Log in via ACCESS
- Open On Demand Portal




# Launch Open OnDemand Portal

[Launch OnDemand Portal](#) [Apps](#) [Files](#) [Jobs](#) [Clusters](#) [Interactive Apps](#) [Admin](#) [Dashboard](#) [Utilities](#) [My Interactive Sessions](#) [Develop](#) [Help](#)




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


**Pinned Apps** A featured subset of [all available apps](#)




**Dashboard**  
System Installed App




**Drona Joblisting**  
System Installed App




**Launch Dashboard (chatbot)**  
System Installed App




**Drona Composer**  
System Installed App



**HPRC Website Development**  
System Installed App

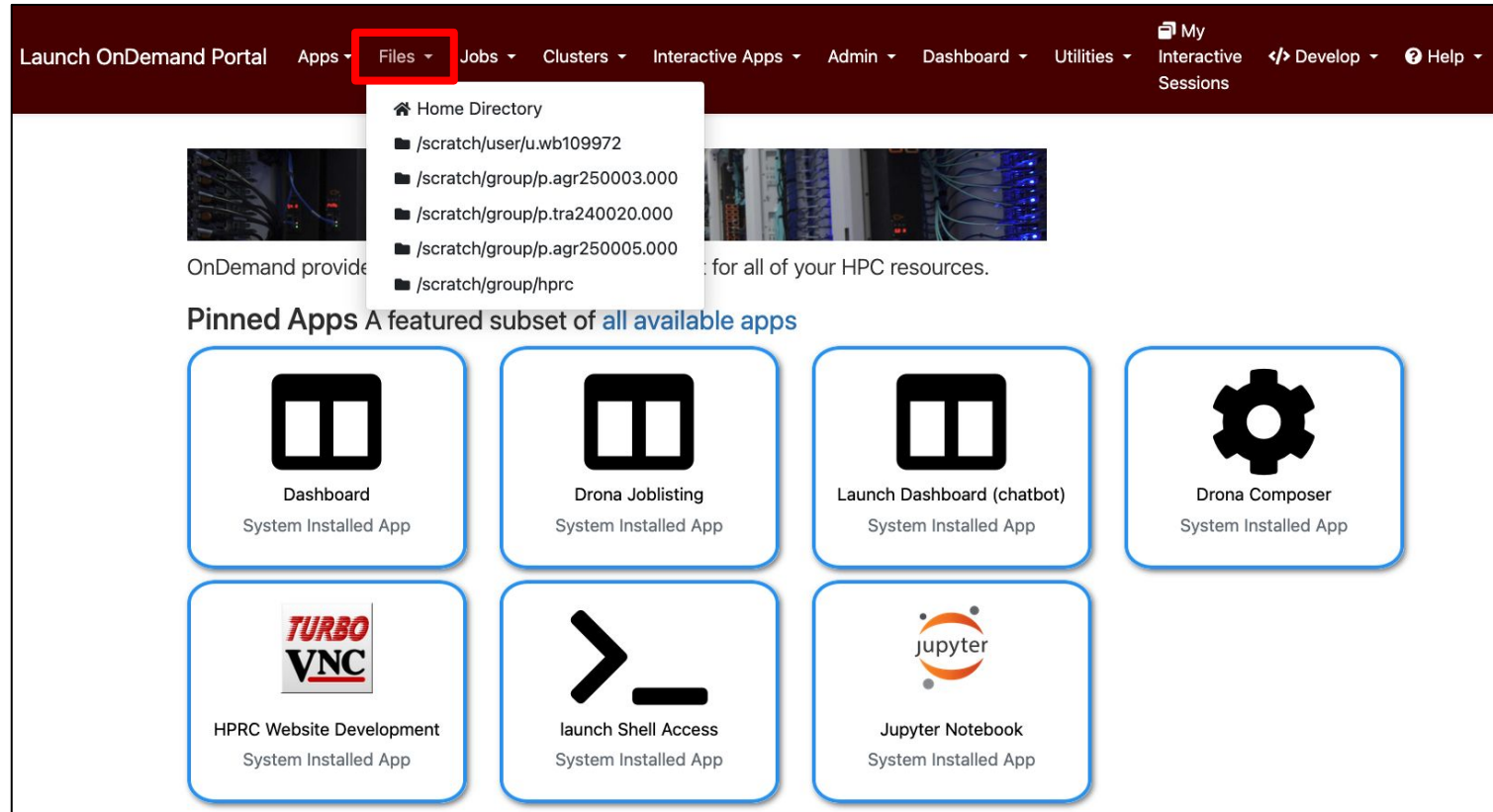


**launch Shell Access**  
System Installed App



**Jupyter Notebook**  
System Installed App

# Launch Open OnDemand Portal: File Browser



The screenshot displays the Open OnDemand Portal interface. The top navigation bar includes links for Launch OnDemand Portal, Apps, Files (highlighted with a red box), Jobs, Clusters, Interactive Apps, Admin, Dashboard, Utilities, My Interactive Sessions, Develop, and Help. A dropdown menu is open under the 'Files' link, showing a 'Home Directory' and a list of scratch directories: /scratch/user/u.wb109972, /scratch/group/p.agr250003.000, /scratch/group/p.tra240020.000, /scratch/group/p.agr250005.000, and /scratch/group/hprc. Below the navigation bar, there is a section for 'Pinned Apps' with a featured subset of all available apps. The pinned apps are arranged in two rows: Dashboard, Drona Joblisting, Launch Dashboard (chatbot), Drona Composer, HPRC Website Development, launch Shell Access, and Jupyter Notebook. Each app card includes an icon, the app name, and the text 'System Installed App'.

Launch OnDemand Portal Apps **Files** Jobs Clusters Interactive Apps Admin Dashboard Utilities My Interactive Sessions Develop Help

- Home Directory
  - /scratch/user/u.wb109972
  - /scratch/group/p.agr250003.000
  - /scratch/group/p.tra240020.000
  - /scratch/group/p.agr250005.000
  - /scratch/group/hprc

OnDemand provide for all of your HPC resources.

**Pinned Apps** A featured subset of [all available apps](#)

- Dashboard**  
System Installed App
- Drona Joblisting**  
System Installed App
- Launch Dashboard (chatbot)**  
System Installed App
- Drona Composer**  
System Installed App
- HPRC Website Development**  
System Installed App
- launch Shell Access**  
System Installed App
- Jupyter Notebook**  
System Installed App

# Launch Open OnDemand Portal: File Browser

Launch OnDemand Portal | Apps | Files | Jobs | Clusters | Interactive Apps | Admin | Dashboard | Utilities | My Interactive Sessions | Develop | Help | Logged in as u.wb109972 | Log Out

Open in Terminal | Refresh | New File | New Directory | Upload | Download | Copy/Move | Delete

Home Directory

- /scratch/user/u.wb109972
- /scratch/group/p.agr250003.000
- /scratch/group/p.tr240020.000
- /scratch/group/p.agr250005.000
- /scratch/group/hprc

/ home / u.wb109972 / | Change directory | Copy path

Show Owner/Mode | Show Dotfiles | Filter: | Showing 7 of 36 rows - 0 rows selected

Type	Name	Size	Modified at
File	ollama-linux-amd64.tgz	1.83 GB	11/8/2024 3:10:36 PM
File	XDMoD_DataPull.R	2.36 kB	11/6/2024 11:42:17 AM
Folder	bin		11/6/2024 10:14:48 AM
Folder	Desktop		
Folder	Downloads		3/19/2025 2:50:20 PM
Folder	iib		11/6/2024 9:36:22 AM


View | Edit | Rename | Download | Delete

Navigate to home or scratch space here.

This drop down menu provides access to edit, rename, or download files.



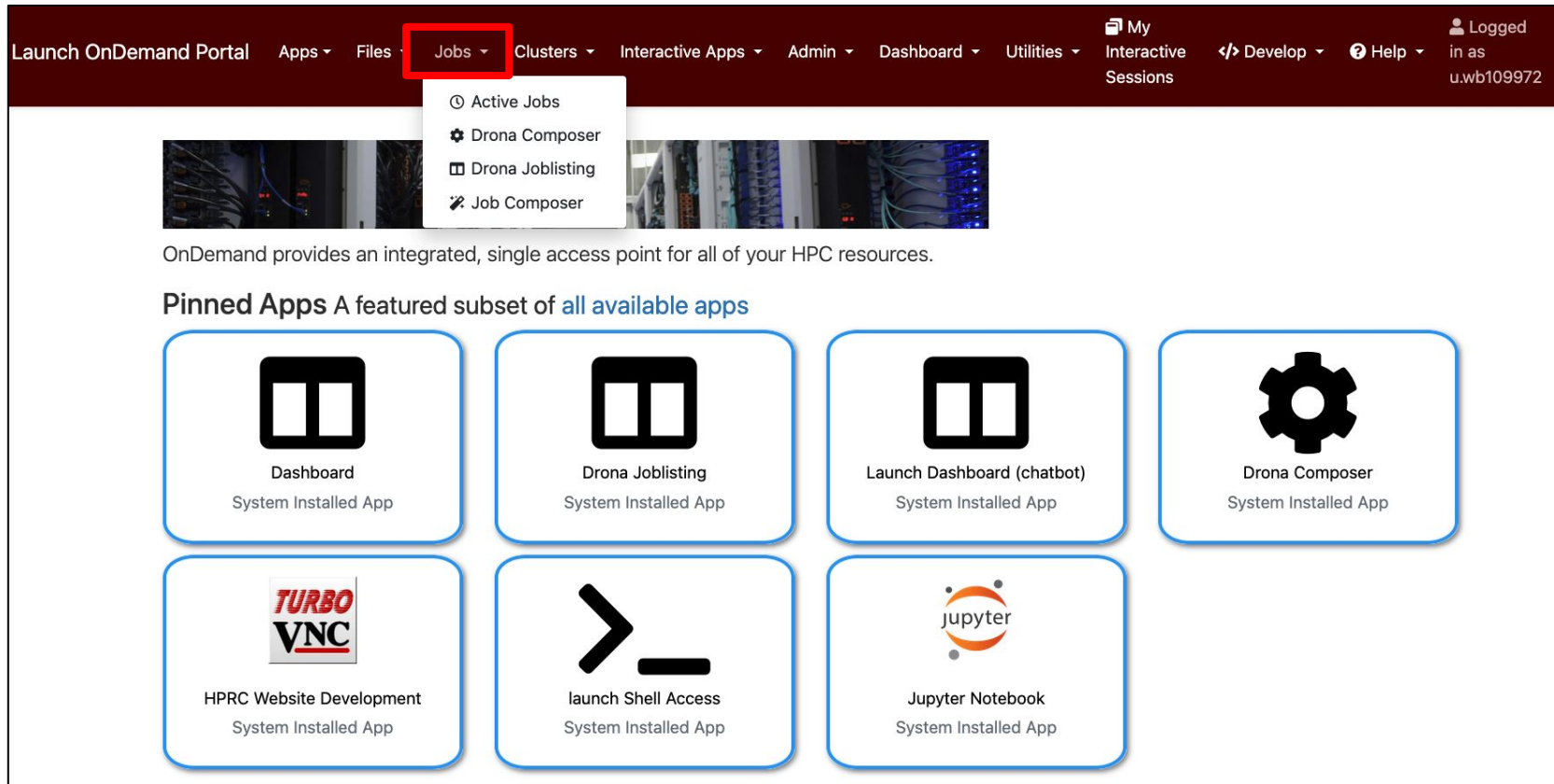
# Launch Open OnDemand Portal: File Browser



The screenshot displays the Open OnDemand File Browser interface. At the top, there is a navigation bar with a 'Save' button, the current file path '/home/u.wb109972/XDMod\_DataPull.R', and settings for 'Key Bindings' (Default), 'Font Size' (12px), 'Mode' (Text), and 'Theme' (Solarized Light). The main area is a code editor with a light yellow background, showing an R script. The script includes comments and code for setting up the environment, connecting to the XDMoD data warehouse, and creating a pie chart of user data by parent science.

```
1 ##### Before running:
2 # Get api key from XDMod
3 # add api key to .Renviron
4 # XDMod_API_TOKEN=<my secret xdmod api token>
5
6 # Load the required packages and set up the environment
7 suppressPackageStartupMessages(library(tidyverse))
8 suppressPackageStartupMessages(library(plotly))
9 suppressPackageStartupMessages(library(reticulate))
10 use_condaenv("xdmod-notebooks")
11 suppressPackageStartupMessages(library(rxdmmod))
12 suppressPackageStartupMessages(library(ggthemes))
13
14 # Get XDMod connection
15 dw <- xdmod_get_datawarehouse('https://xdmod.access-ci.org')
16
17 # Get data
18 xdmod_df = xdmod_get_raw_data(dw,
19   duration = c('2024-10-01', '2024-10-31'),
20   realm = 'Jobs',
21   filter=list(Resource=c("Texas A&M U FASTER"))
22 )
23
24
25 # Pie Chart of Number of Users by Parent Science
26 unique_user = xdmod_df[!duplicated(xdmod_df$User),]
27
28 to_pie = as.data.frame(table(unique_user$`Parent Science`))
29 colnames(to_pie)[1] = paste("Parent Science")
30
31 ggplot(to_pie, aes(x="", y=Freq, fill=`Parent Science`)) +
32   geom_bar(stat="identity", width=1, color = "white") +
33   coord_polar("y", start=0) +
34   scale_fill_manual(values=c("#8B1E3F", "#3C153B", "#89BD9E",
35     "#F0C987", "#DB4C40", "#2081C3",
36     "#60E1E0", "#B88E8D", "#34435E")) +
37   theme_void()
38
```

# Launch Open OnDemand Portal: Jobs



The screenshot displays the Launch OnDemand Portal interface. The top navigation bar includes links for Launch OnDemand Portal, Apps, Files, Jobs, Clusters, Interactive Apps, Admin, Dashboard, Utilities, My Interactive Sessions, Develop, Help, and a user status indicator (Logged in as u.wb109972). The Jobs menu is highlighted with a red box, and its dropdown menu is visible, listing Active Jobs, Drona Composer, Drona Joblisting, and Job Composer. Below the navigation bar, a banner image shows server racks. The main content area features a heading "OnDemand provides an integrated, single access point for all of your HPC resources." followed by a section titled "Pinned Apps A featured subset of all available apps". This section contains seven app tiles, each with an icon, name, and status "System Installed App".

Launch OnDemand Portal Apps Files **Jobs** Clusters Interactive Apps Admin Dashboard Utilities My Interactive Sessions Develop Help ? Help Logged in as u.wb109972

- Active Jobs
- Drona Composer
- Drona Joblisting
- Job Composer

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

**Pinned Apps** A featured subset of [all available apps](#)

Icon	App Name	Status
	Dashboard	System Installed App
	Drona Joblisting	System Installed App
	Launch Dashboard (chatbot)	System Installed App
	Drona Composer	System Installed App
	HPRC Website Development	System Installed App
	launch Shell Access	System Installed App
	Jupyter Notebook	System Installed App

# Launch Open OnDemand Portal: Jobs

Launch OnDemand Portal Apps Files Jobs Clusters Interactive Apps Admin Dashboard Utilities My Interactive Sessions </> Develop ? Help Logged in as u.wb109972

Active Jobs Drona Composer Drona Joblisting Job Composer

Launch OnDemand Portal Apps Files Jobs Clusters Interactive Apps Admin Dashboard Utilities My Interactive Sessions </> Develop ? Help Logged in as u.wb109972 Log Out

Your Jobs All Clusters

## Active Jobs

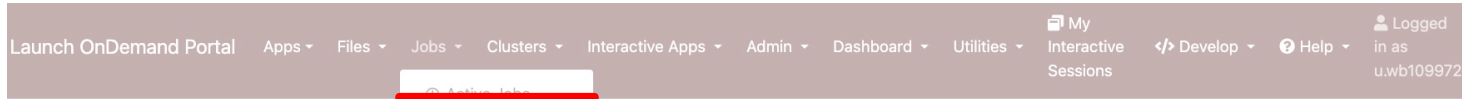
Show 50 entries Filter:

ID	Name	User	Account	Time Used	Queue	Status	Cluster	Actions
> 27243	sys/dashboard/sys/vnc	u.wb109972	friendly	00:01:56	gpu	Running	launch	

Showing 1 to 1 of 1 entries

Previous 1 Next

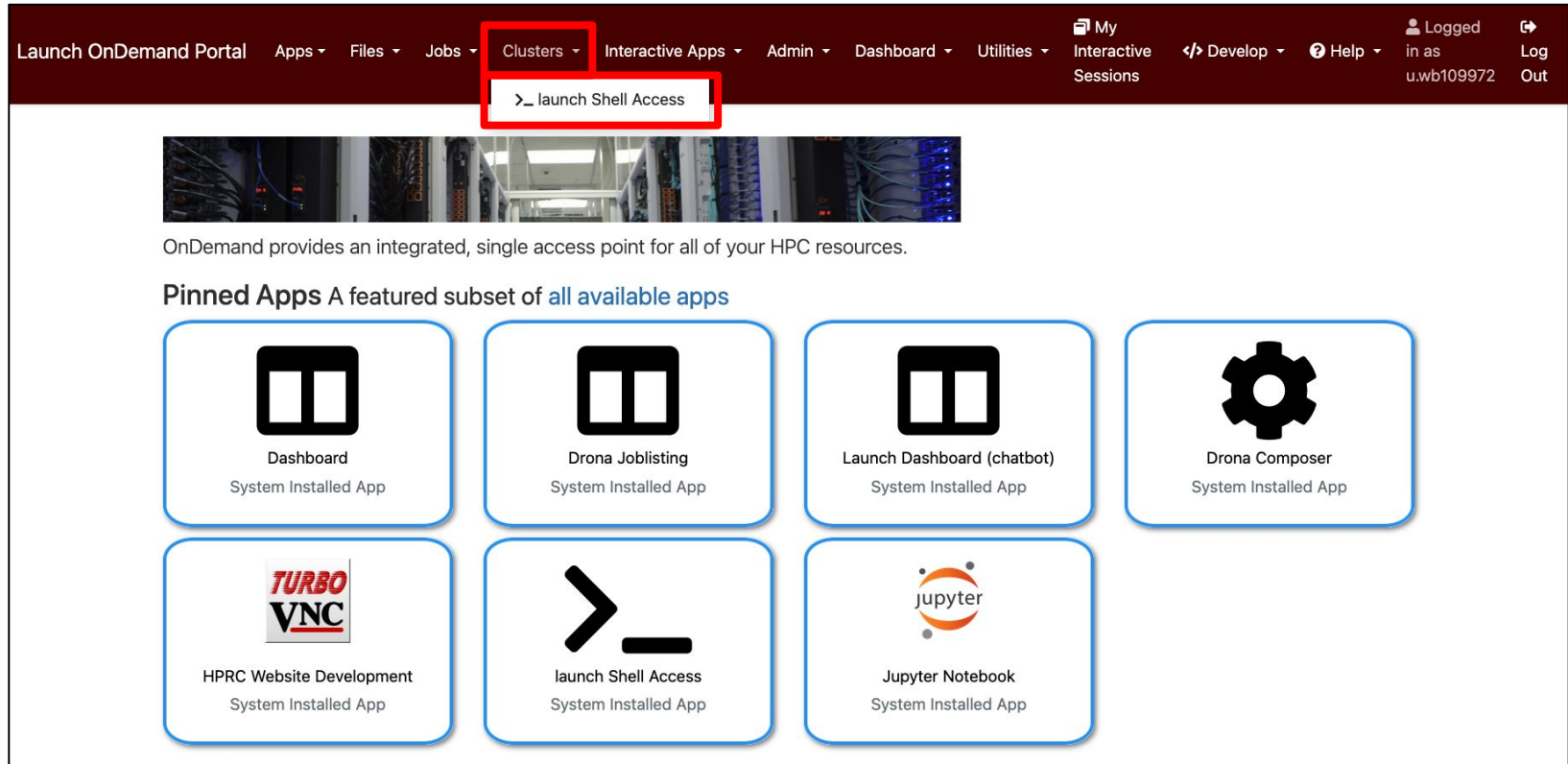
# Launch Open OnDemand Portal: Jobs



The 'Drona Composer (LAUNCH)' form is displayed. It features the ATM High Performance Research Computing logo and the title 'DRONA COMPOSER (LAUNCH)'. The form includes several input fields and buttons for configuring a job:

- Job Name:** A text input field.
- Location:** A text input field with a 'Change' button. The current value is '/scratch/user/u.wb109972/drona\_composer/runs'.
- Environments:** A dropdown menu showing 'Generic' with a '+' button to add more.
- Upload files:** A dropdown menu with 'Select an option' and an 'Add' button.
- Add modules:** A text input field with a 'Default (foss/2023b)' dropdown and an 'Add' button.
- Number of tasks:** A text input field with the value '1' and a spinner control.
- Advanced task options:** A checkbox.
- Use Accelerator:** A dropdown menu with the option '-- Choose an option --'.

# Launch Open OnDemand Portal: Shell Access



The screenshot displays the OnDemand Portal interface. The top navigation bar is dark red with white text. The 'Clusters' dropdown menu is open, showing a red-bordered box around the '>\_ launch Shell Access' option. Below the navigation bar, there is a banner image of server racks. The text 'OnDemand provides an integrated, single access point for all of your HPC resources.' is displayed. Below this, the section 'Pinned Apps A featured subset of all available apps' is shown. There are seven app tiles arranged in two rows. The first row contains four tiles: 'Dashboard', 'Drona Joblisting', 'Launch Dashboard (chatbot)', and 'Drona Composer'. The second row contains three tiles: 'HPRC Website Development', 'launch Shell Access', and 'Jupyter Notebook'. Each tile has an icon, a title, and the text 'System Installed App'.

Launch OnDemand Portal Apps Files Jobs Clusters Interactive Apps Admin Dashboard Utilities My Interactive Sessions Develop Help Logged in as u.wb109972 Log Out

>\_ launch Shell Access

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

**Pinned Apps** A featured subset of [all available apps](#)

**Dashboard**  
System Installed App

**Drona Joblisting**  
System Installed App

**Launch Dashboard (chatbot)**  
System Installed App

**Drona Composer**  
System Installed App

**HPRC Website Development**  
System Installed App

**launch Shell Access**  
System Installed App

**Jupyter Notebook**  
System Installed App

# Launch Open OnDemand Portal: Shell Access

```
*****  
This computer system and the data herein are available only for authorized  
purposes by authorized users. Use for any other purpose is prohibited and may  
result in disciplinary actions or criminal prosecution against the user. Usage  
may be subject to security testing and monitoring. There is no expectation of  
privacy on this system except as otherwise provided by applicable privacy laws.  
Refer to University SAP 29.01.03.M0.02 Acceptable Use for more information.  
*****  
Last login: Mon Apr  7 14:39:49 2025 from 10.74.0.6  
[u.wb109972@launch-login2 ~]$
```

# Access the training materials

Run the following commands in the Launch terminal:

```
# Navigate to your scratch directory
cd $SCRATCH

# Copy the materials
cp -r /scratch/training/arcats .
```

# Launch Open OnDemand Portal: Interactive Apps

Launch OnDemand Portal Apps Files Jobs Clusters **Interactive Apps** Admin Dashboard Utilities My Interactive Sessions Develop Help Logged in as u.wb109972

GUI


- MATLAB
- VNC


Servers


- CodeAI
- Jupyter Notebook
- JupyterLab
- JupyterLab (ARCATS)
- RStudio
- Stable Diffusion
- Text Generation


OnDemand provides an integrated, single access point to all your computing resources.


**Pinned Apps** A featured subset of all apps

 **Dashboard**  
System Installed App

 **Launch Dashboard (chatbot)**  
System Installed App

 **Drona Composer**  
System Installed App

 **TURBO VNC**

 **jupyter**



# JupyterLab

- Web-based IDE (Interactive Development Environment)
- Can be used for Python, Julia, and R
- Integrates text and code blocks
- Great for interactive coding and developing workflows



# Starting JupyterLab

The screenshot displays the OnDemand Portal interface. The top navigation bar includes links for Launch OnDemand Portal, Apps, Files, Jobs, Clusters, Interactive Apps (highlighted with a red box), Admin, Dashboard, Utilities, My Interactive Sessions, Develop, Help, and a user profile section indicating the user is logged in as u.wb109972.

The 'Interactive Apps' dropdown menu is open, showing a list of applications categorized under 'GUI' and 'Servers'. The 'JupyterLab (ARCATS)' option is highlighted with a red box.

The main content area features a section titled 'Pinned Apps A featured subset of all apps'. Below this, there are several app tiles, each with an icon and a label. The tiles include:

- Dashboard (System Installed App)
- Drone (System Installed App)
- Launch Dashboard (chatbot) (System Installed App)
- Drona Composer (System Installed App)
- TURBO VNC
- Jupyter

# Starting JupyterLab

## JupyterLab (ARCATS)

This app will launch a [JupyterLab](#) server on the LAUNCH cluster.

Module

Python/3.10.8

Environment to be activated

/sw/hprc/sw/Python/virtualenvs/Python/3.10.8/arcats-ai-env/bin/activate

Node type

CPU only

- Select a GPU node for software that supports GPU processing.

Number of hours (max 48)

4

Number of cores (max 192)

2

Total GB memory (max 371)

24

Account

This field is optional.

Email

This field is optional.

☐ I would like to receive an email when the session starts

Launch

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