Open OnDemand Lawrencium HPC Training

March 10, 2021

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Introduction

Slides and sample codes can be found on github https://github.com/lbnl-science-it/Training-OpenOnDemand

Video will be posted

There will be a hands-on session at the end of this training

Send your questions to chatroom

Fill out training survey

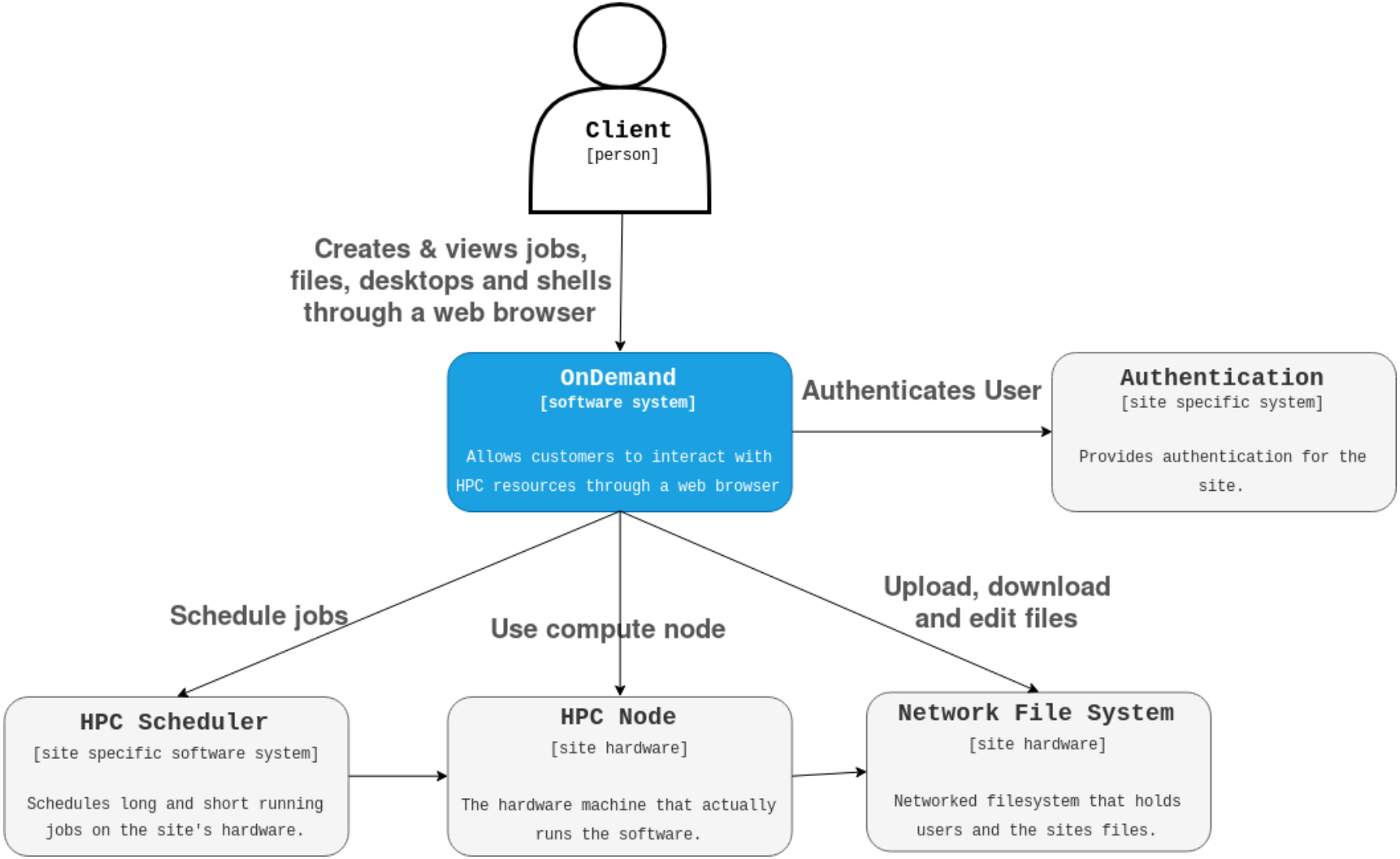
Outline

- What is Open OnDemand on Lawrencium
- How to access OOD
- Features
  - *File management*
  - *Cluster shell access*
  - *Job submission and monitoring*
  - *Interactive apps*
- Hands-on exercises

What is Lawrencium Open OnDemand

- Lawrencium OOD portal is based on an open source web platform https://openondemand.org/
- The project is designed by Ohio Supercomputer Center
- Users can access HPC cluster resources and services via a web browser
- Provide an intuitive interface and allows new users to be instantly productive at using the HPC resources for their research
- An alternative convenient way for experienced users to access the HPC resources.
- Flexible and extensible design that makes it easy to deploy new services as needed.

OOD at the System Level



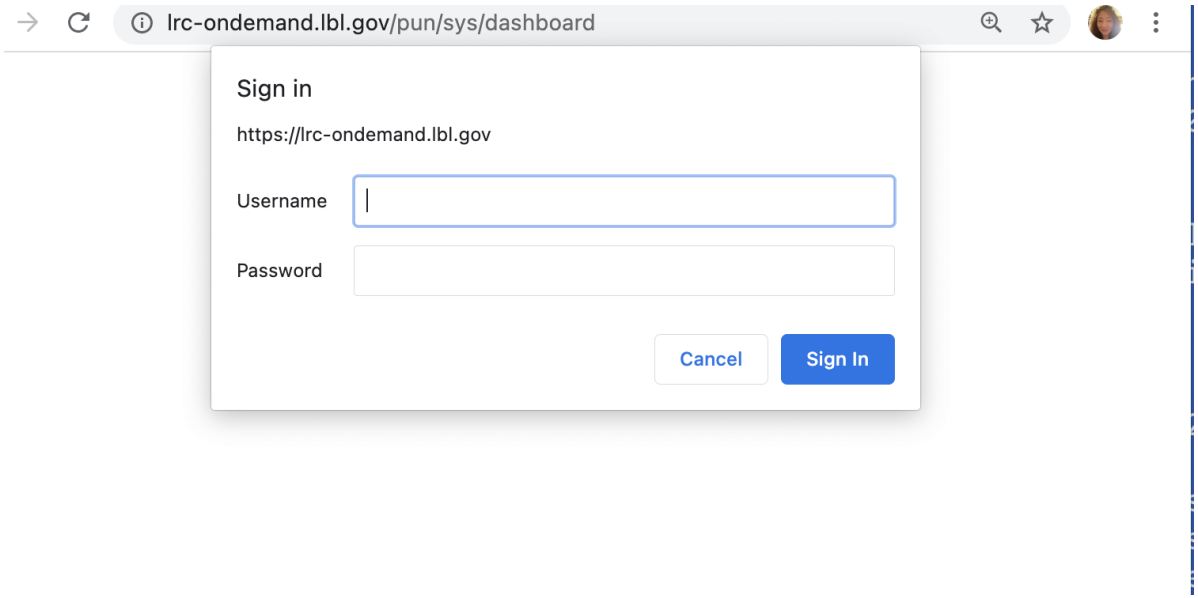
Services Provided

- Easy file transfer and management
- Command-line shell access
- Job submission and monitoring
- Interactive apps, graphic desktop environment
  - *Juyter Notebook*
  - *RStudio*
  - *MatLab*
  - *VMD*
- More apps will be added

How to Access

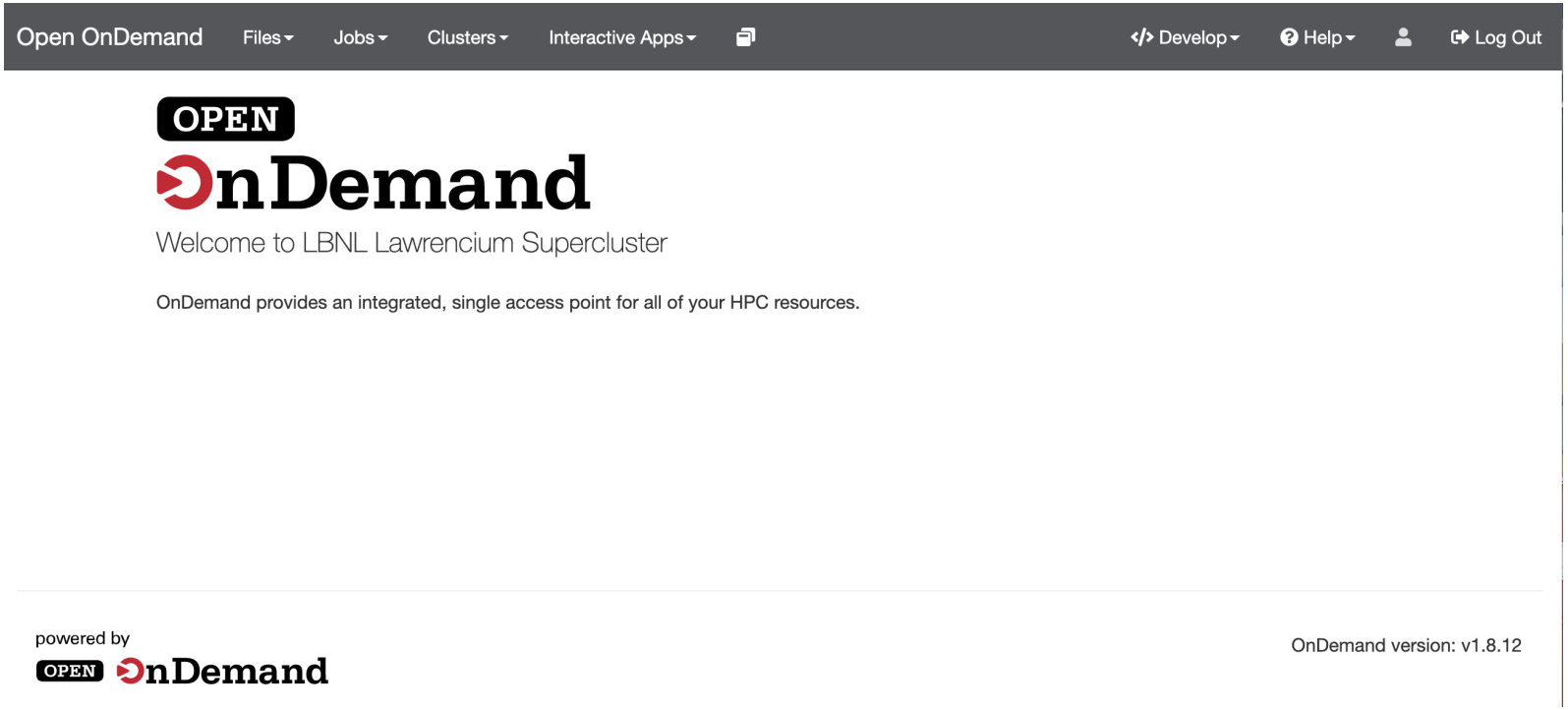
https://lrc-ondemand.lbl.gov/

Authetication

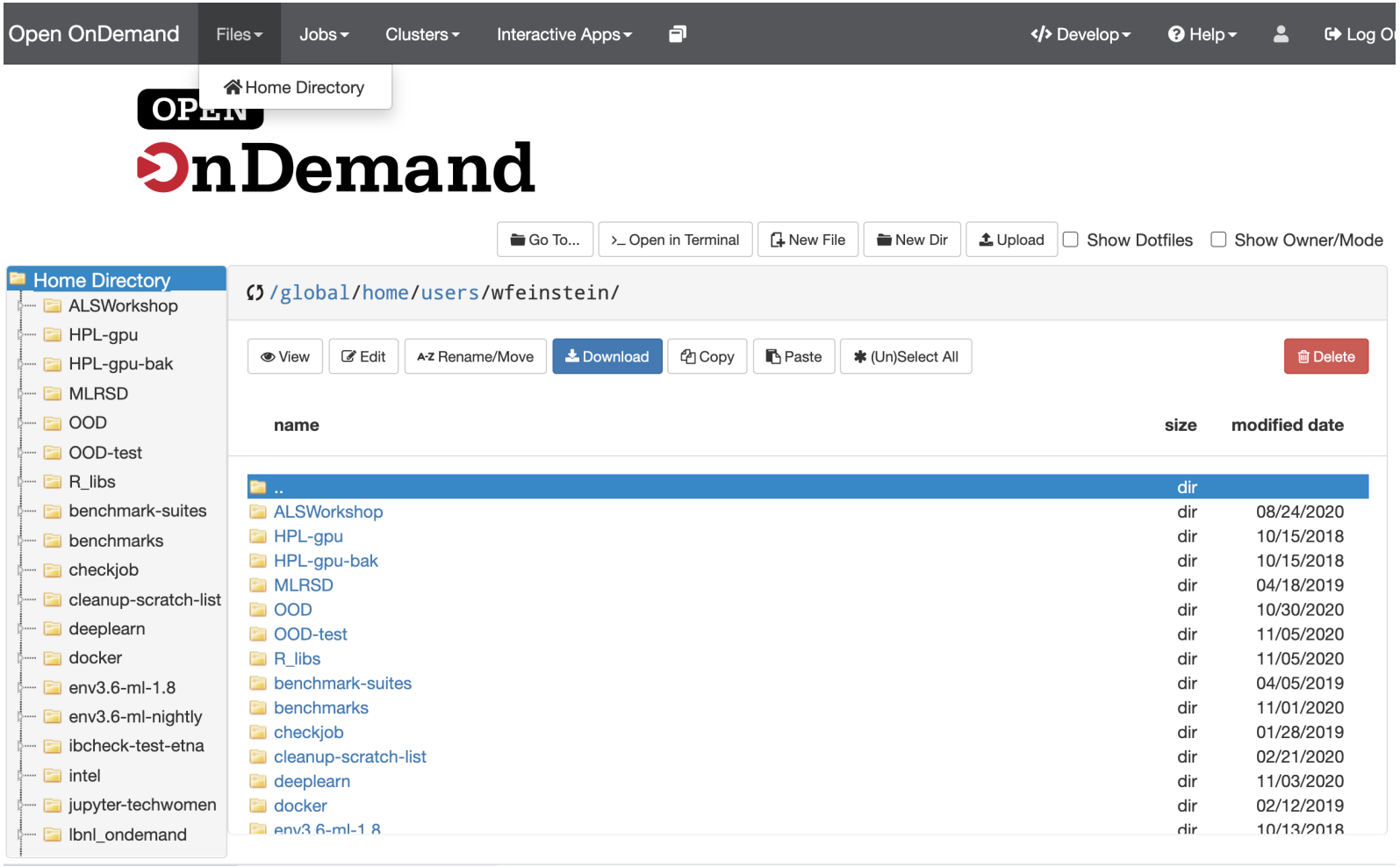


- Username: Lawrencium username
- Password: pin + OTP

Dashboard


Open OnDemand
Files
Jobs
Clusters
Interactive Apps
Develop
Help
Log Out
OPEN
OnDemand
Welcome to LBNL Lawrencium Supercluster
OnDemand provides an integrated, single access point for all of your HPC resources.
powered by
OPEN
OnDemand
OnDemand version: v1.8.12

Files

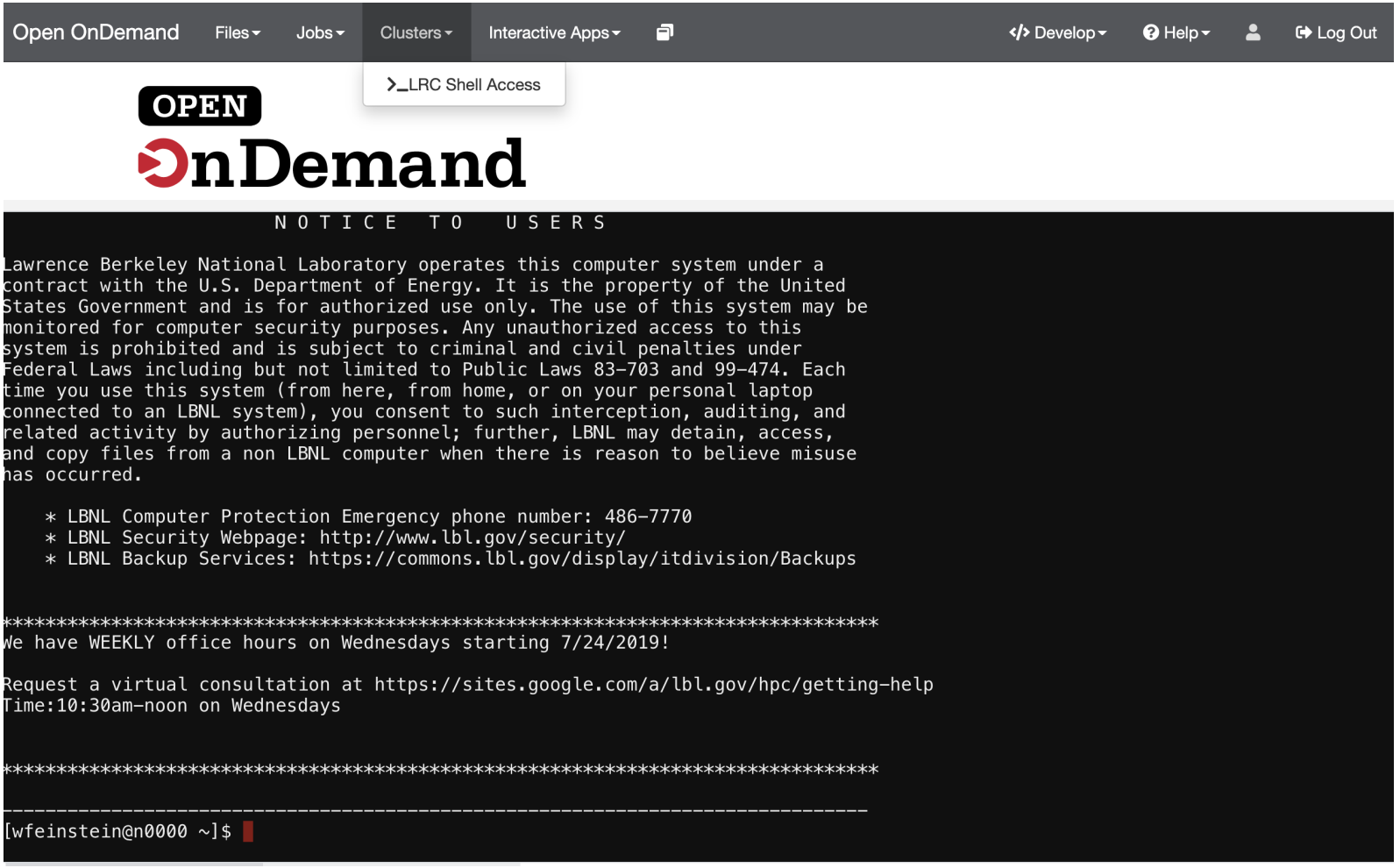

Open OnDemand
Files
Jobs
Clusters
Interactive Apps
Develop
Help
Log O
Home Directory
OPEN
OnDemand
Go To...
Open in Terminal
New File
New Dir
Upload
Show Dotfiles
Show Owner/Mode
Home Directory
ALSWorkshop
HPL-gpu
HPL-gpu-bak
MLRSD
OOD
OOD-test
R_libs
benchmark-suites
benchmarks
checkjob
cleanup-scratch-list
deeplearn
docker
env3.6-ml-1.8
env3.6-ml-nightly
ibcheck-test-etna
intel
jupyter-techwomen
lbnl_ondemand
/global/home/users/wfeinstein/
View
Edit
Rename/Move
Download
Copy
Paste
(Un)Select All
Delete
name
size
modified date
..
dir
ALSWorkshop dir 08/24/2020
HPL-gpu dir 10/15/2018
HPL-gpu-bak dir 10/15/2018
MLRSD dir 04/18/2019
OOD dir 10/30/2020
OOD-test dir 11/05/2020
R_libs dir 11/05/2020
benchmark-suites dir 04/05/2019
benchmarks dir 11/01/2020
checkjob dir 01/28/2019
cleanup-scratch-list dir 02/21/2020
deeplearn dir 11/03/2020
docker dir 02/12/2019

File/Directory Management

- Conventional command-line approach
  - *Linux file editing, vi, nano, emacs*
  - *File transfer: rsync, scp*
  - *Globus still an option of file transfer*
- New avenue to manage files/dirs
  - *Viewing files*
  - *Text editing*
  - *Copy/Paste*
  - *Renaming files*
  - *Creating files*
  - *Creating directories*
  - *Deleting files*
  - *File upload/download*

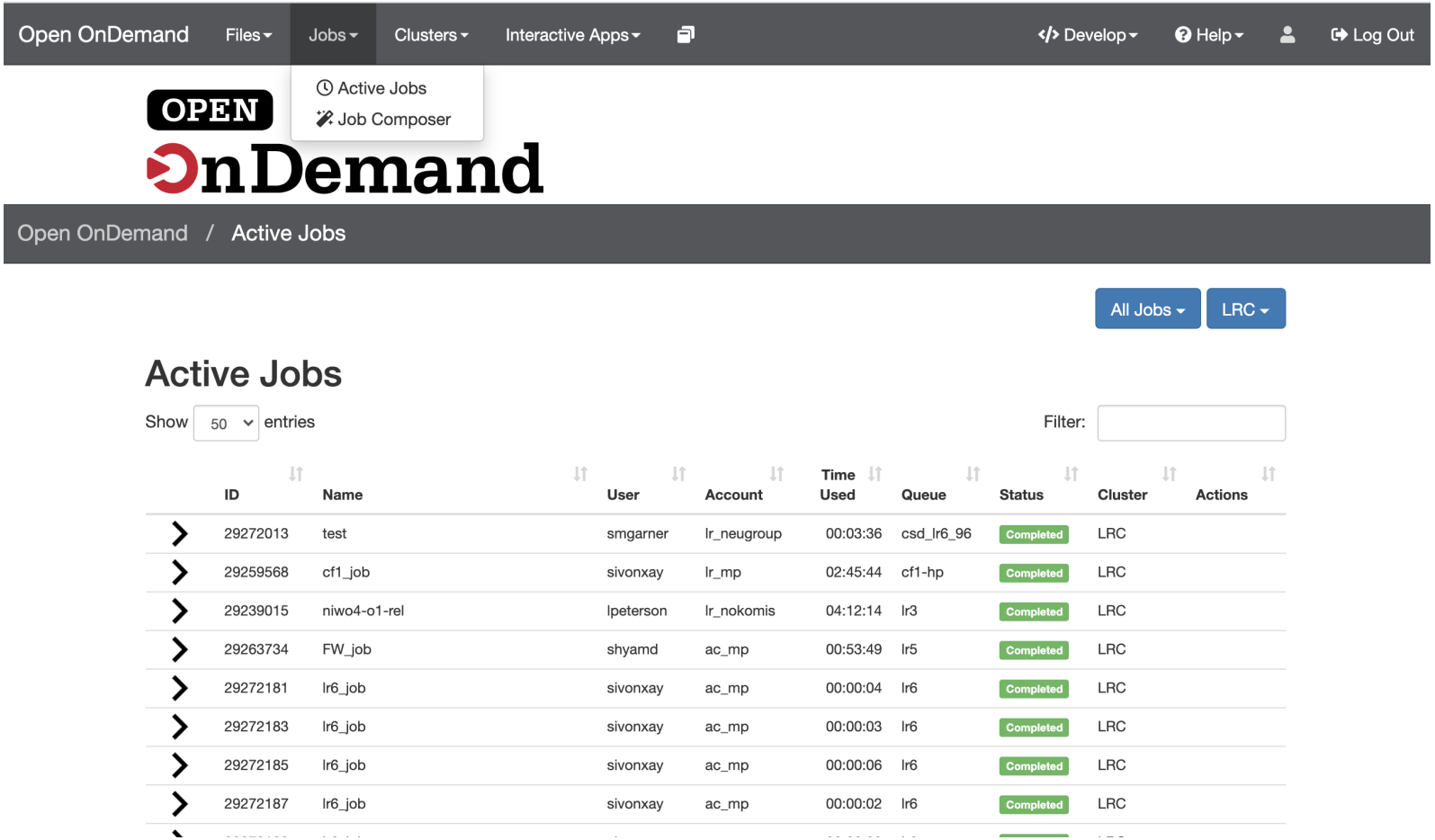
Cluster Shell Access

Provide the conventional cluster access: command-line/terminal



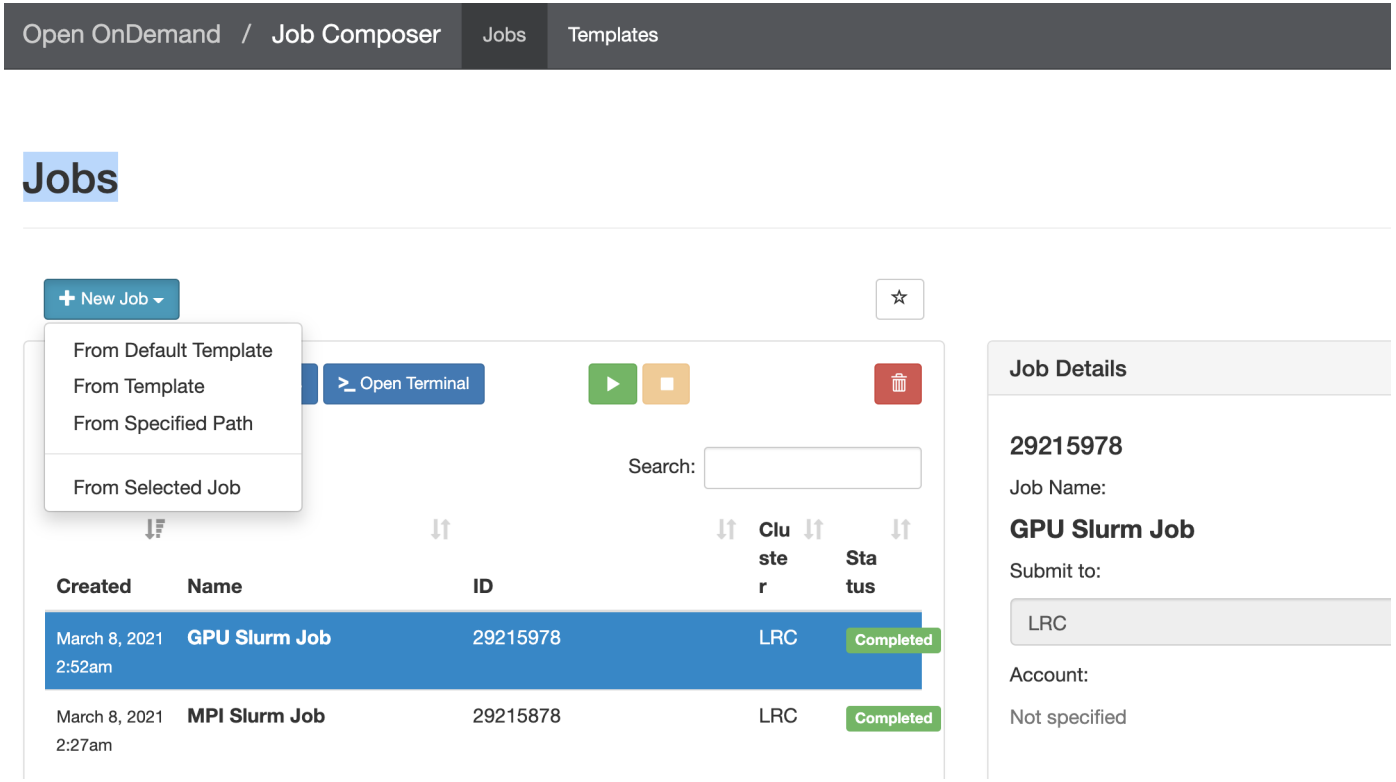
Job Management

Job monitoring, composing and submission



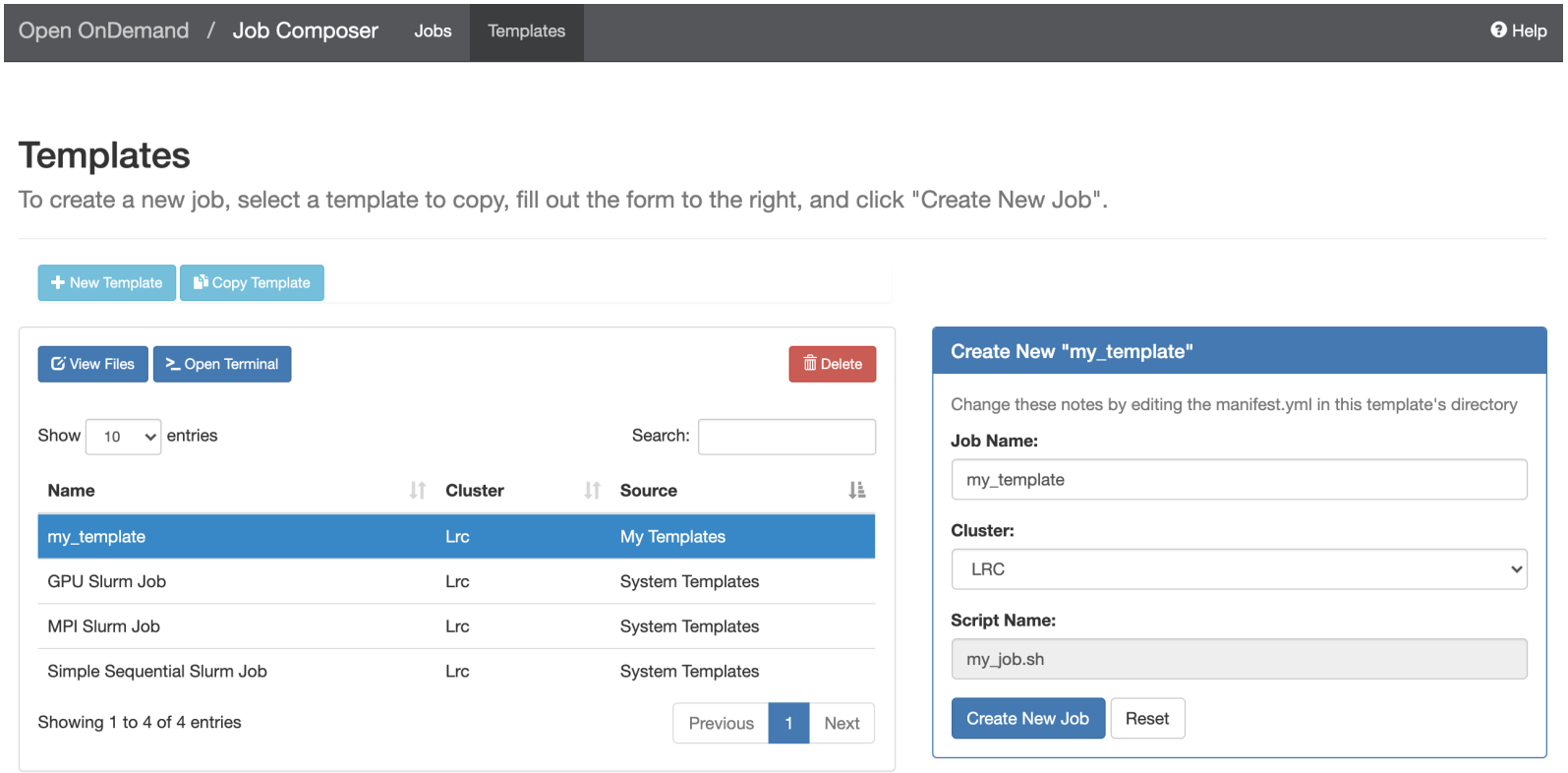
Job Composer

- From templates
- From specific path
- From selected job

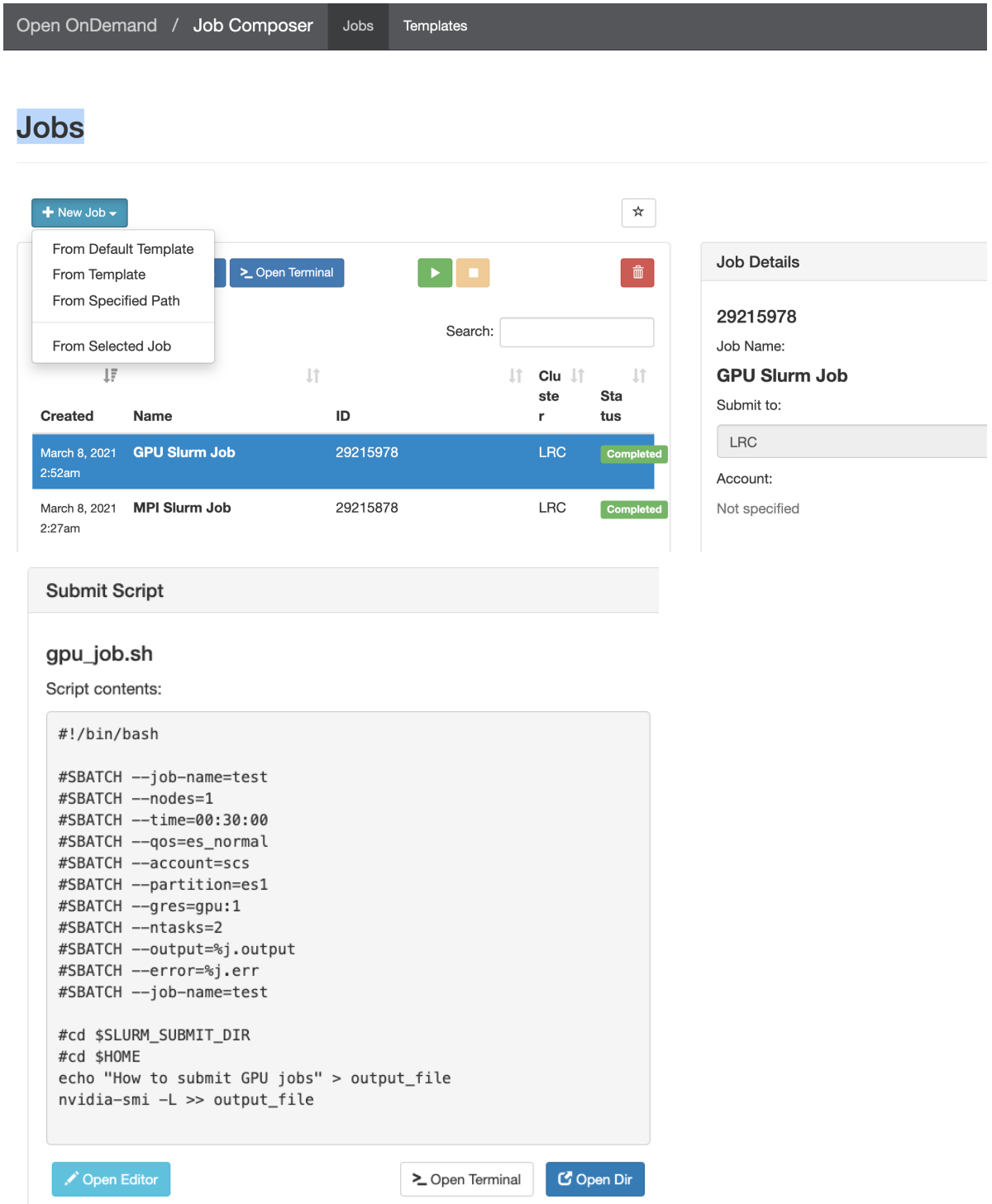


Job Templates

- Provided by system admins
- Defined by users



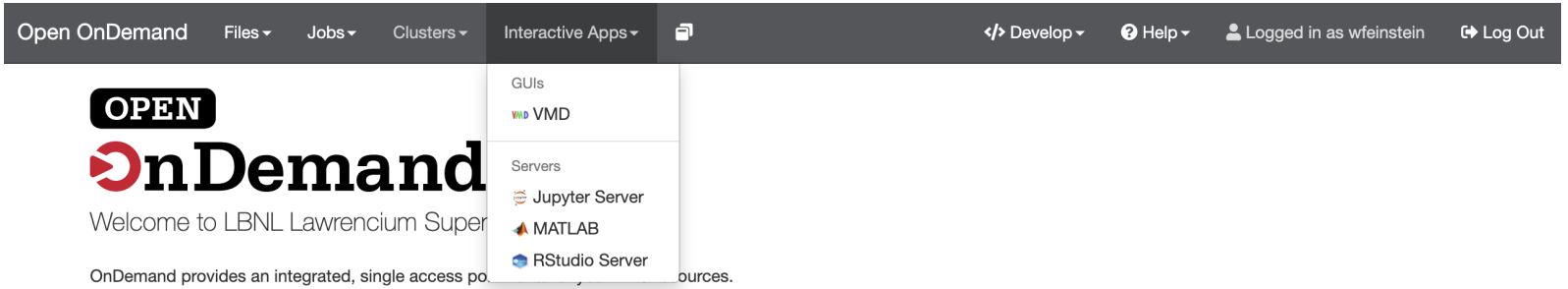
Job Submission Script

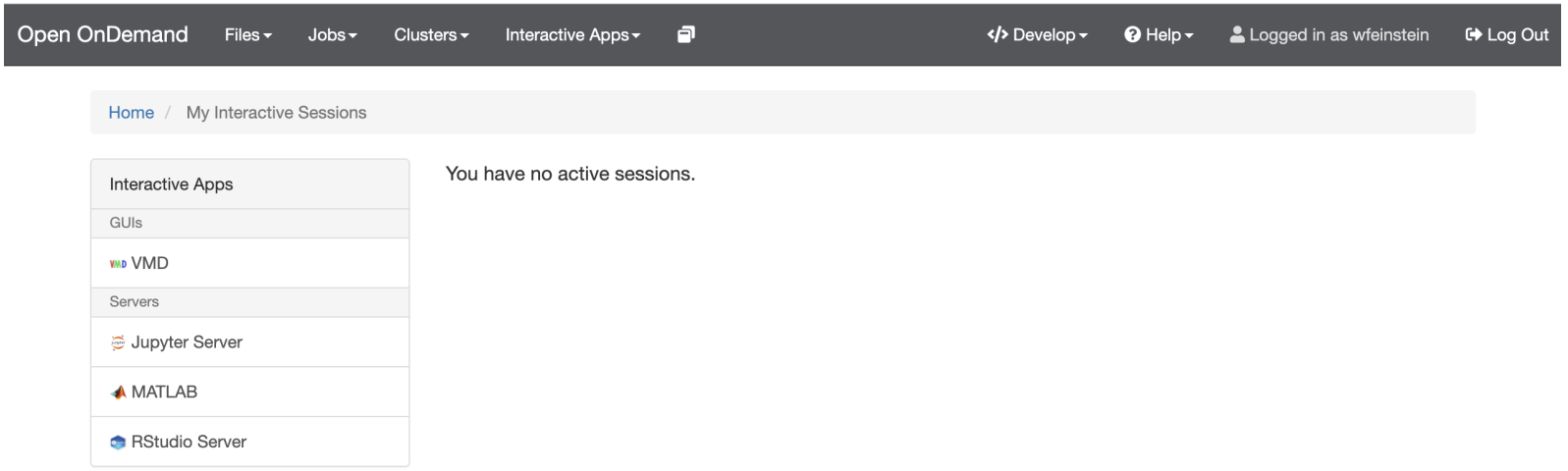


Job Submission Directory

- Two ways to cope with the default directory created by the job composer.
  - *The default directory as the working directory of your job.*
  - `/global/home/users/wfeinstein/ondemand/data/sys/myjobs/projects/default`
  - *You need to upload all input files to that directory before you can click the submit button.*
  - *This can be done by clicking 'Open Dir' right beneath the job script contents.*
  - *A file explorer will open the job directory in a new tab where you can do file transfers.*
  - *Have the input files stored somewhere in the cluster and don't want to move them around*
  - *Prefer to have an organized directories by yourself, such as home or scratch…*
  - *Add one command line in your job script*
  - `cd /path/to/job_working_dir`

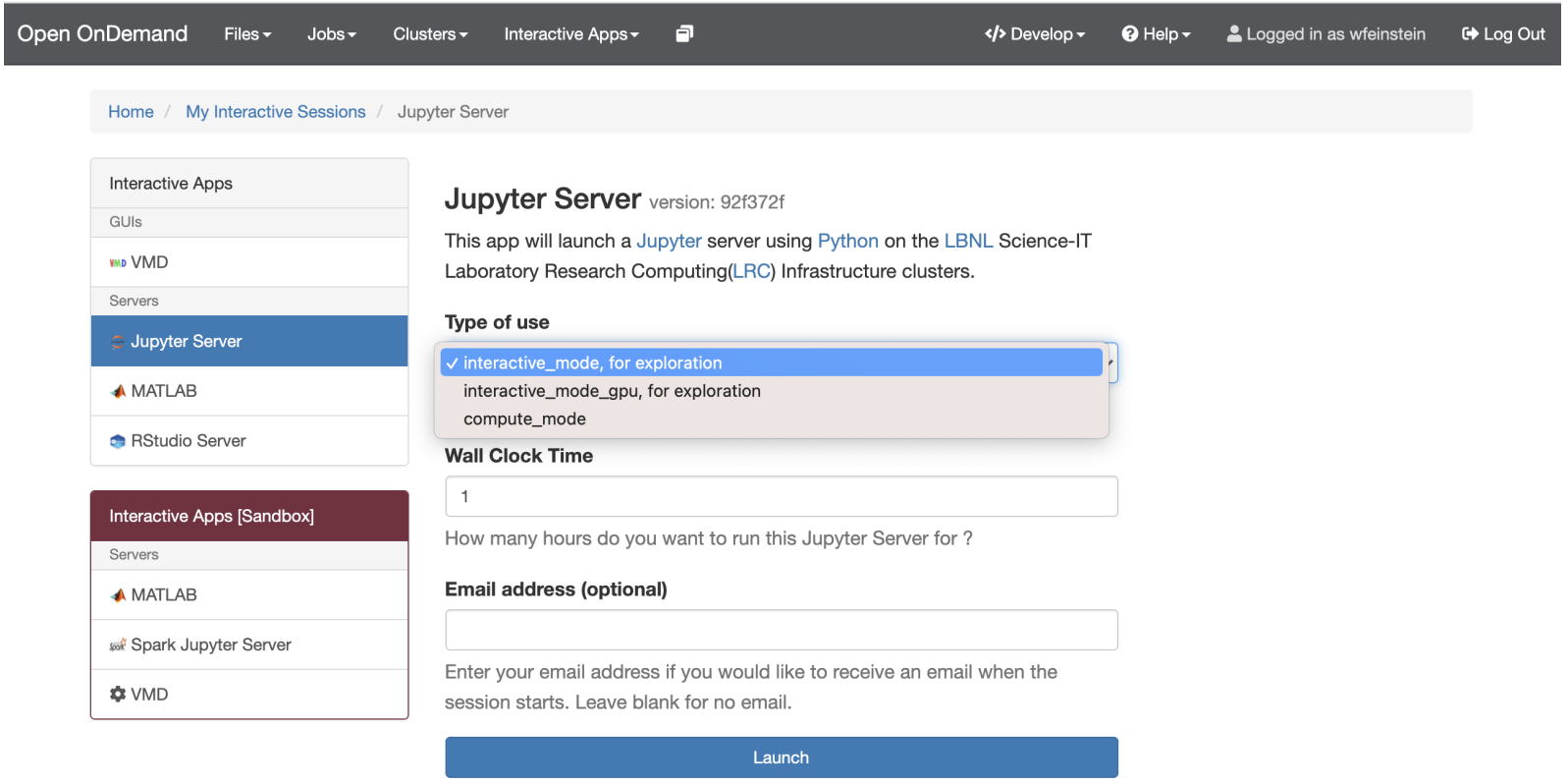
Interactive Apps





Jupyter Notebook App

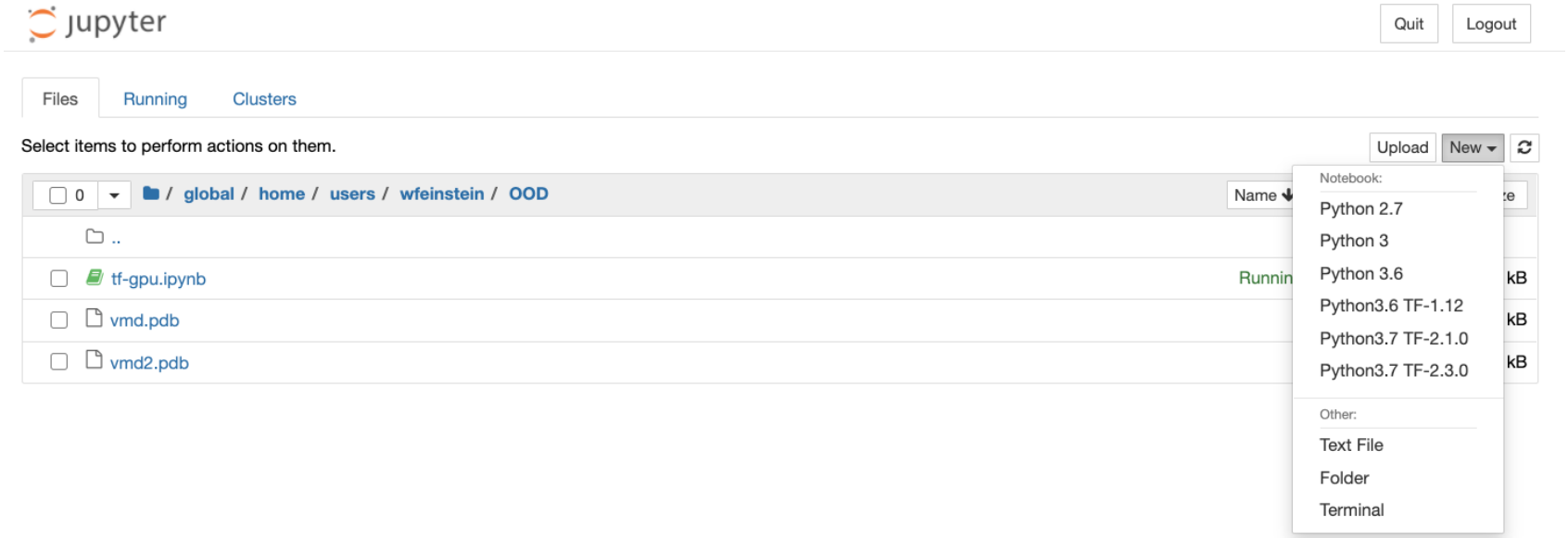
- Three types of use:
  - *Interactive-mode, for exploration*
  - *Interactive-mode-gpu, for exploration*
  - *Compute mode: standarded Lawrencium partitions (e.g.: lr5,lr6,es1…)*



Slurm Account, Partition, QOS from an Access Shell

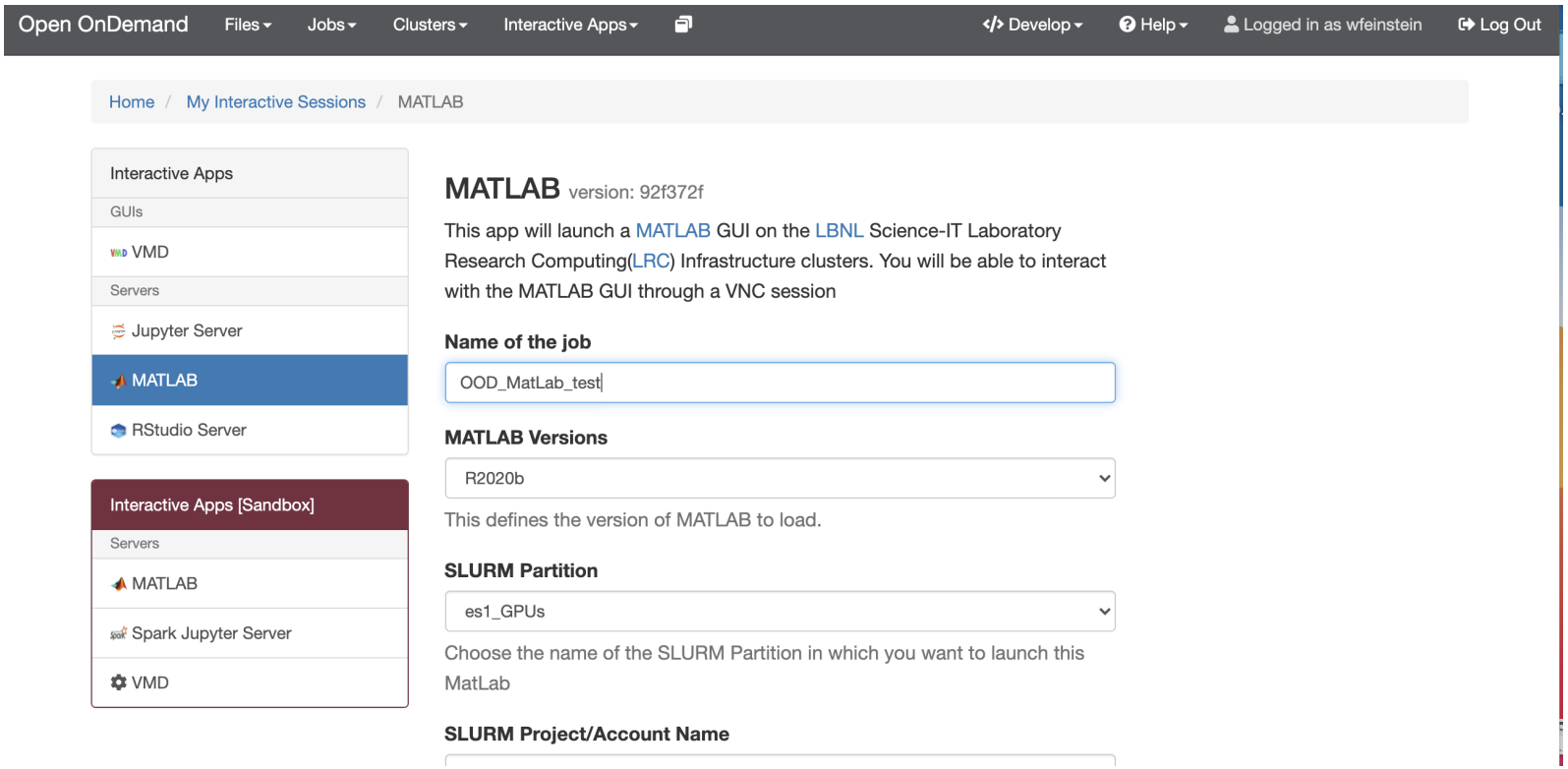
```
sacctmgr show association user=wfeinstein -p

Cluster|Account|User|Partition|Share|Priority|GrpJobs|GrpTRES|GrpSubmit|GrpWall|GrpTRESMins|MaxJobs|MaxTRES|MaxTRESPerNode|MaxSubmit|MaxWall|Max
 QOS|GrpTRESRunMins|
perceus-00|pc_scs|wfeinstein|lr6|1|||||||||||lr_debug,lr_lowprio,lr_normal|||
perceus-00|ac_test|wfeinstein|lr5|1|||||||||||lr_debug,lr_lowprio,lr_normal|||
perceus-00|pc_test|wfeinstein|lr4|1|||||||||||lr_debug,lr_lowprio,lr_normal|||
perceus-00|pc_test|wfeinstein|lr_bigmem|1|||||||||||lr_debug,lr_lowprio,lr_normal|||
perceus-00|lr_test|wfeinstein|lr3|1|||||||||||condo_test|||
perceus-00|scs|wfeinstein|es1|1|||||||||||es_debug,es_lowprio,es_normal|||
...
```

Jupyter Notebook

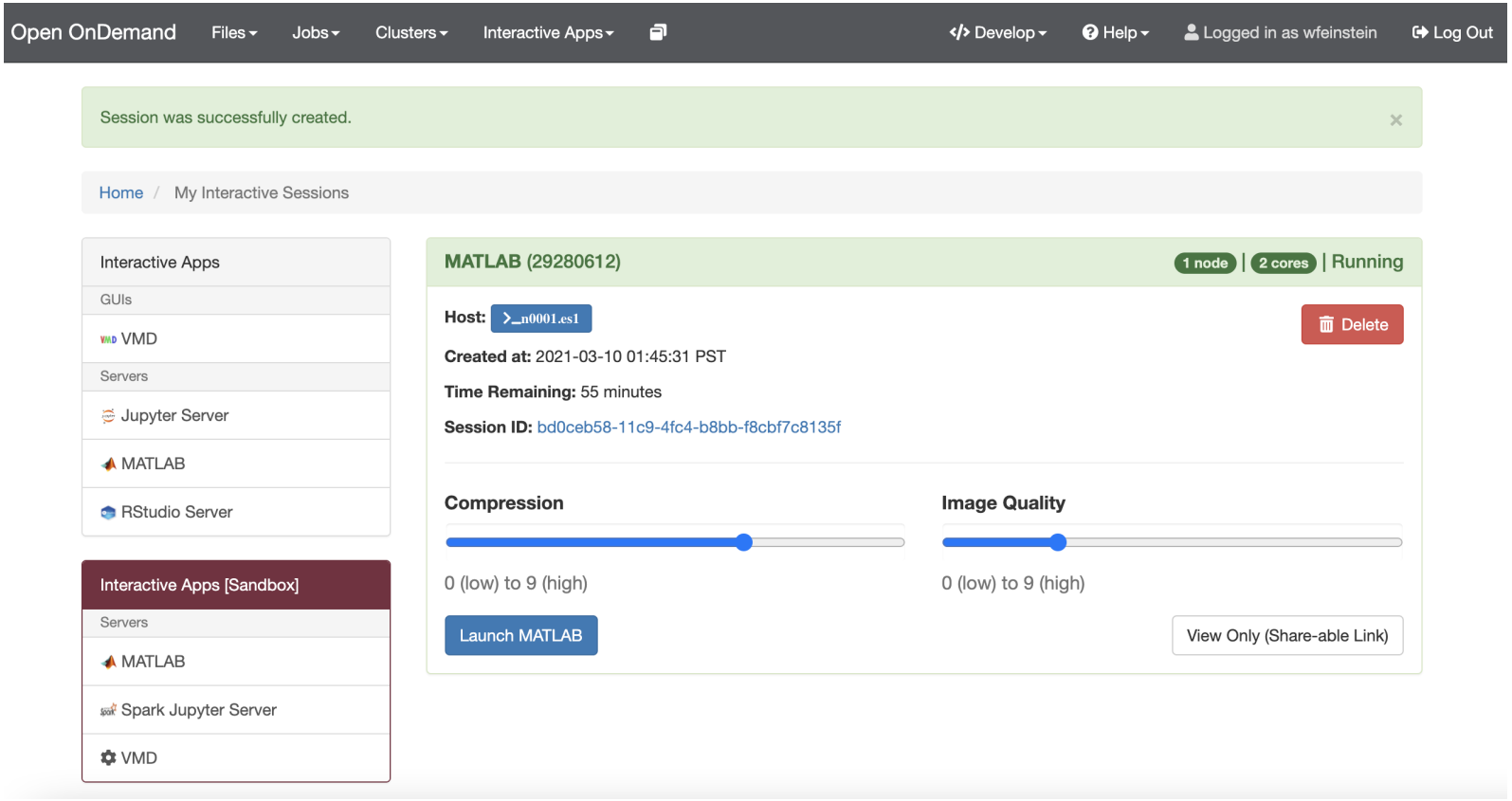


Matlab App

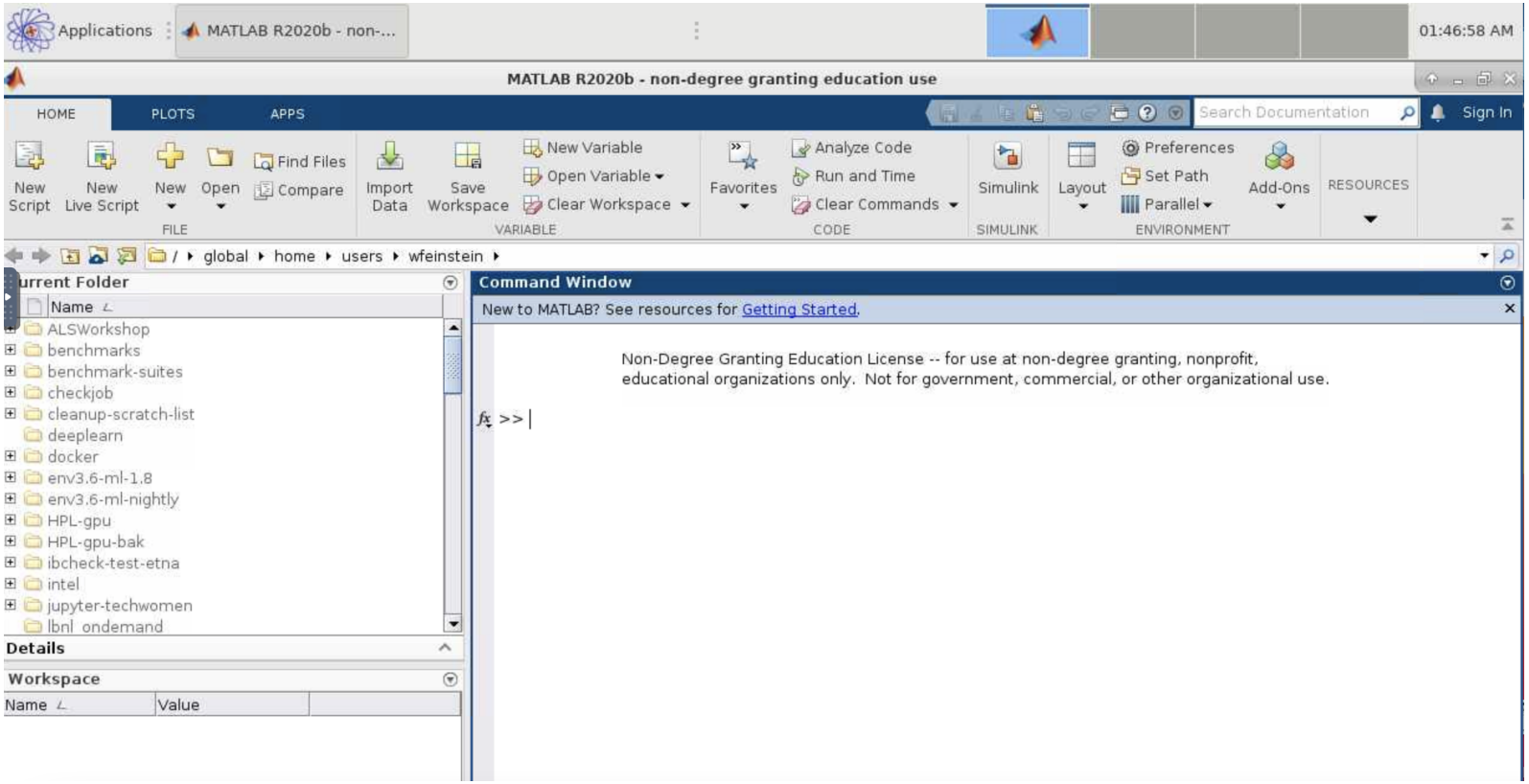
- Enabled on GPU and CPU nodes



Matlab App Launch

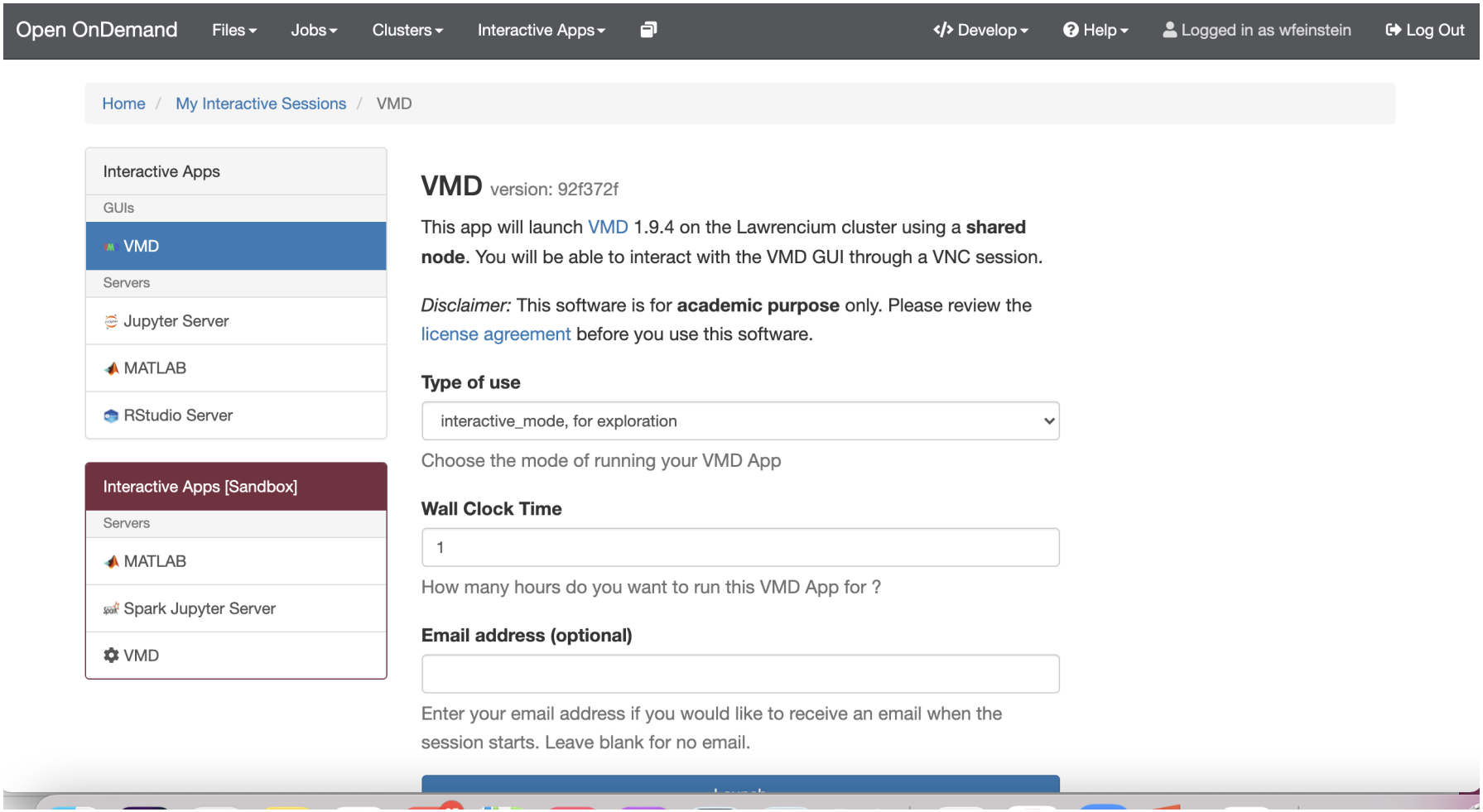


Matlab App GUI

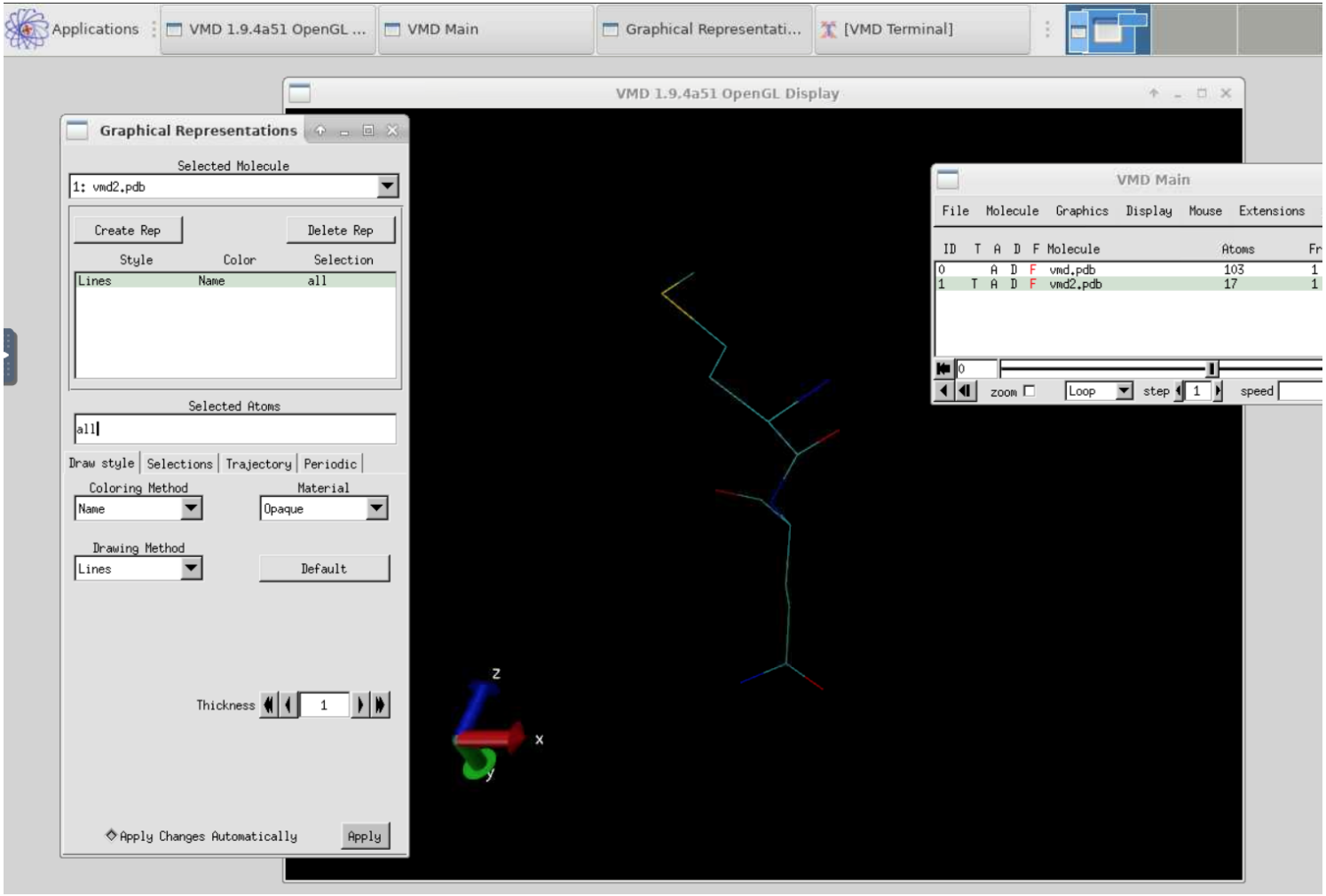


VMD App (Visual Molecular Dynamics)

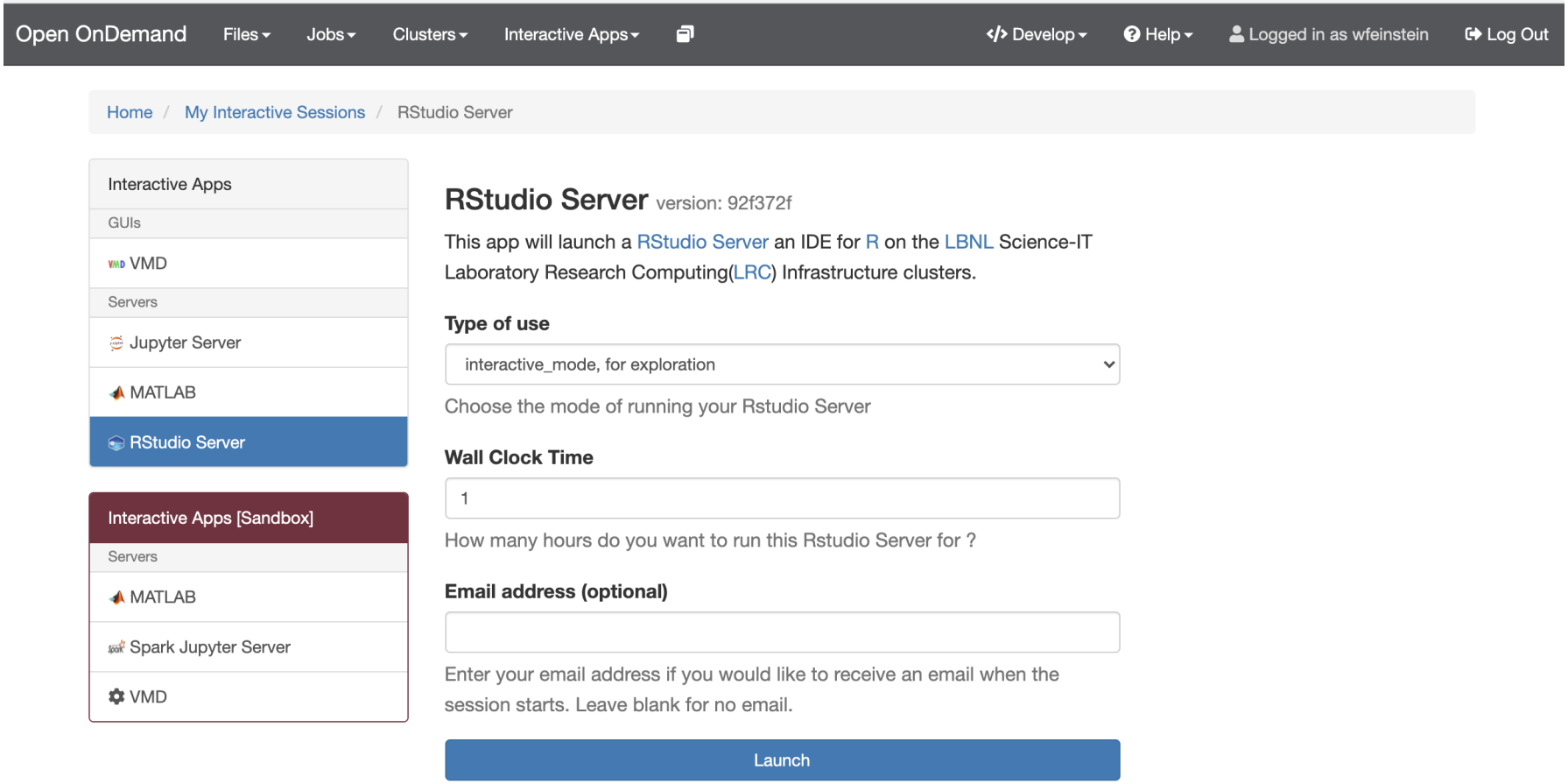
A molecular visualization program for displaying, animating, and analyzing large biomolecular systems using 3-D graphics and built-in scripting.



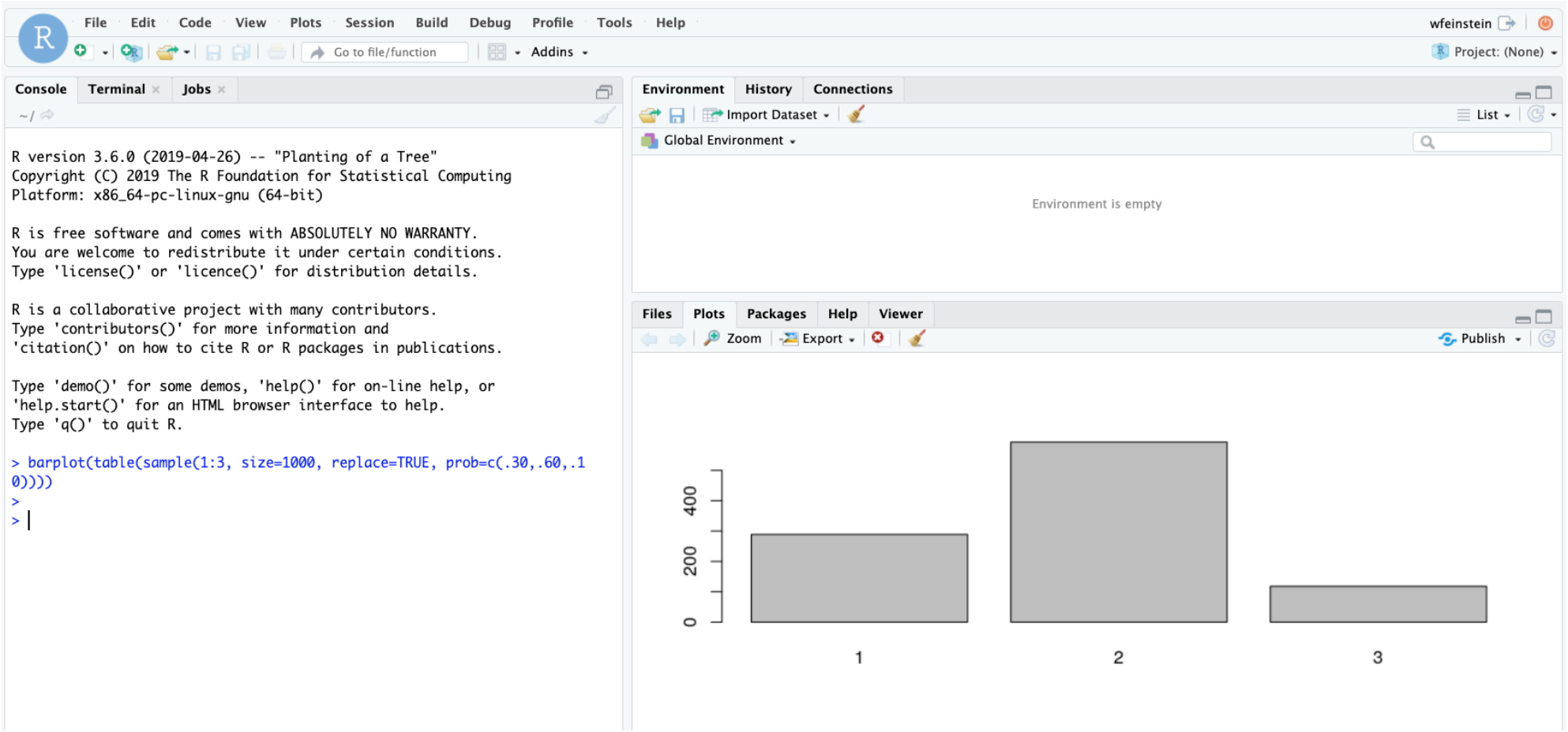
VMD Example


Applications
VMD 1.9.4a51 OpenGL ...
VMD Main
Graphical Representati...
[VMD Terminal]
VMD 1.9.4a51 OpenGL Display
Graphical Representations
Selected Molecule
1: vmd2.pdb
Create Rep
Delete Rep
Style
Color
Selection
Lines
Name
all
Selected Atoms
all
Draw style
Selections
Trajectory
Periodic
Coloring Method
Name
Material
Opaque
Drawing Method
Lines
Default
Thickness
1
Apply Changes Automatically
Apply
VMD Main
File
Molecule
Graphics
Display
Mouse
Extensions
ID T A D F Molecule Atoms Fr
0 A D F vmd.pdb 103 1
1 T A D F vmd2.pdb 17 1
zoom
Loop
step
1
speed
z
x
y

RStudio App


Open OnDemand
Files
Jobs
Clusters
Interactive Apps
Develop
Help
Logged in as wfeinstein
Log Out
Home / My Interactive Sessions / RStudio Server
Interactive Apps
GUIs
VMD
Servers
Jupyter Server
MATLAB
RStudio Server
Interactive Apps [Sandbox]
Servers
MATLAB
Spark Jupyter Server
VMD
RStudio Server version: 92f372f
This app will launch a RStudio Server an IDE for R on the LBNL Science-IT Laboratory Research Computing(LRC) Infrastructure clusters.
Type of use
interactive_mode, for exploration
Choose the mode of running your Rstudio Server
Wall Clock Time
1
How many hours do you want to run this Rstudio Server for ?
Email address (optional)
Enter your email address if you would like to receive an email when the session starts. Leave blank for no email.
Launch

RStudio GUI


File Edit Code View Plots Session Build Debug Profile Tools Help
wfeinstein
Go to file/function
Addins
Project: (None)
Console Terminal Jobs
~/
R version 3.6.0 (2019-04-26) -- "Planting of a Tree"
Copyright (C) 2019 The R Foundation for Statistical Computing
Platform: x86_64-pc-linux-gnu (64-bit)
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.
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.
> barplot(table(sample(1:3, size=1000, replace=TRUE, prob=c(.30,.60,.10))))
>
>
Environment History Connections
Import Dataset
List
Global Environment
Environment is empty
Files Plots Packages Help Viewer
Zoom
Export
Publish
0
200
400
1
2
3

Log out and Cleanup

- Log out the portal properly
  - *Clicking 'Log out' from the top navigation bar;*
- Cleanup
  - *The portal stores temporary files for interactive apps in $HOME/ondemand/data/sys/dashboard/.*
  - *It is a good habit to clean this directory periodically.*
  - `rm -rf $HOME/ondemand/data/sys/dashboard/batch_connect/sys/*`

Getting help

- Virtual Office Hours:
  - *Time: 10:30am - noon (Wednesdays)*
  - *Online request*
- Sending us tickets at hpcshelp@lbl.gov
- More information, documents, tips of how to use LBNL Supercluster http://scs.lbl.gov/

To improve our HPC training and services, please fill out Training Survey

Hands-on Exercise

Open Ondemand Navigation

https://lrc-ondemand.lbl.gov/