

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

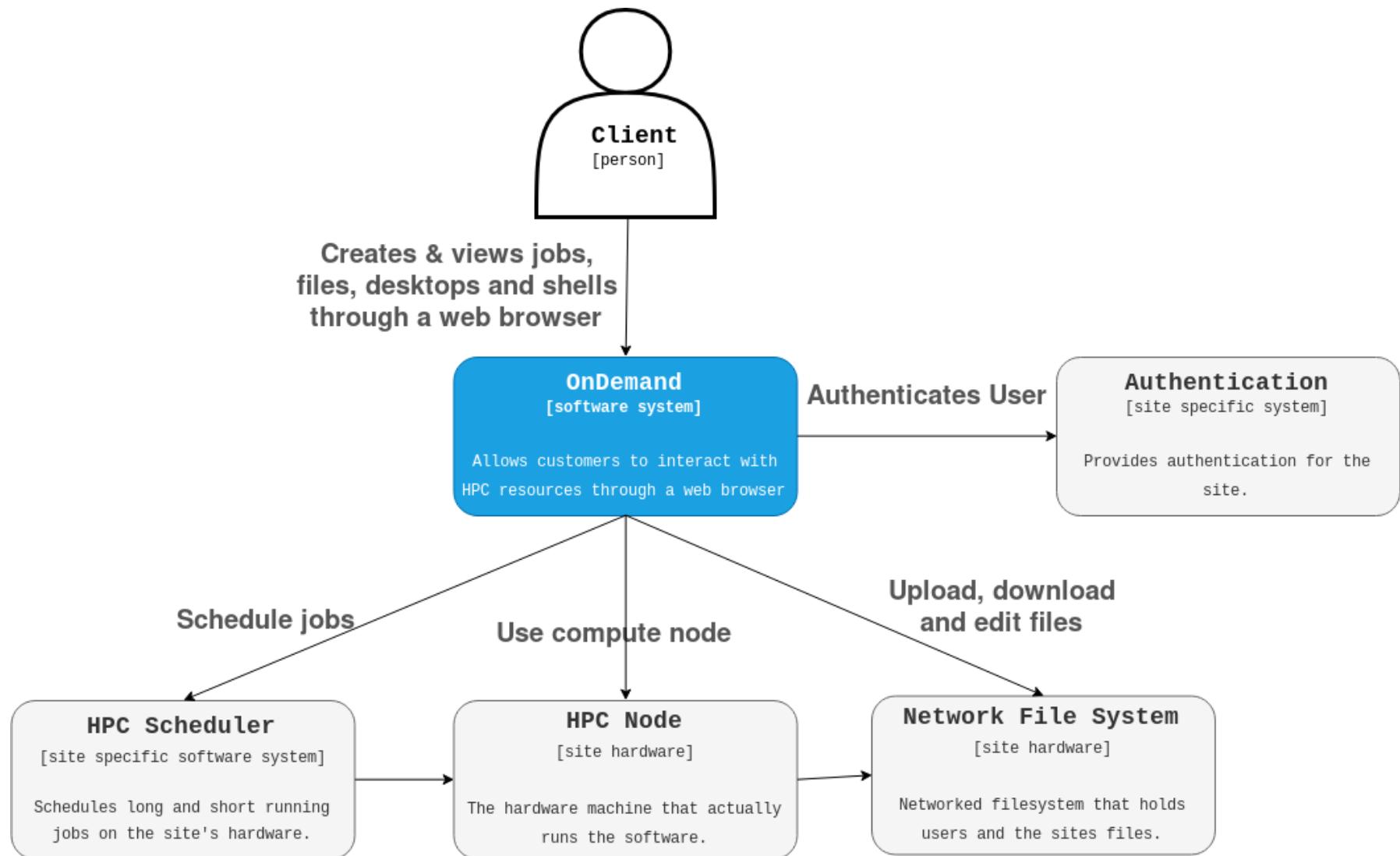
- Features
 - *File management*
 - *Cluster shell access*
 - *Job submission and monitoring*
 - *Interactive apps*

- 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



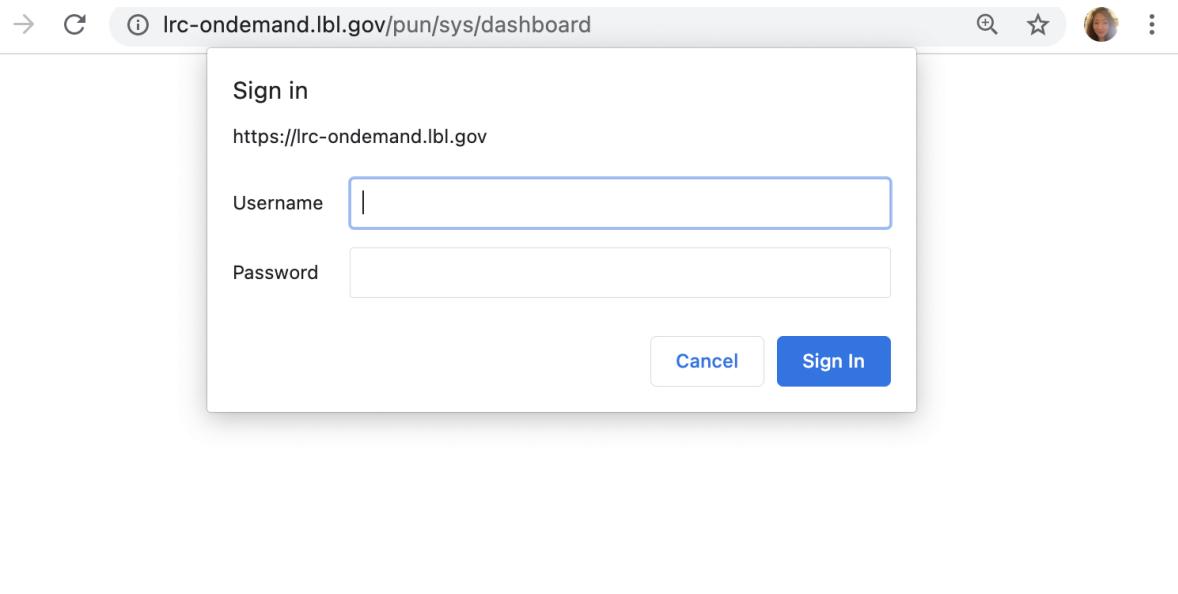
Services Provided

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

How to Access

<https://lrc-on-demand.lbl.gov/>

Authentication



- Username: Lawrencium username
- Password: pin + OTP

Dashboard

[Open OnDemand](#)[Files](#) ▾[Jobs](#) ▾[Clusters](#) ▾[Interactive Apps](#) ▾[Develop](#) ▾[Help](#) ▾[Log Out](#)**OPEN**

Welcome to LBNL Lawrencium Supercluster

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

powered by



OnDemand version: v1.8.12

Files

Open OnDemand Files ▾ Jobs ▾ Clusters ▾ Interactive Apps ▾ 

Develop ▾ Help ▾  Log Out

 Home Directory
OPEN

OnDemand

Go To... Open in Terminal New File New Dir Upload Show Dotfiles Show Owner/Mode

Home Directory

/global/home/users/wfeinstein/

View Edit A-z Rename/Move Download Copy Paste * (Un)Select All Delete

name	size	modified date
..	dir	08/24/2020
ALSWorkshop	dir	10/15/2018
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
env3.6-ml-1.8	dir	10/13/2018
env3.6-ml-nightly		
ibcheck-test-etna		
intel		
jupyter-techwomen		
lbnl_ondemand		

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

The screenshot shows the OnDemand web interface. At the top, there is a navigation bar with links for Open OnDemand, Files, Jobs, Clusters, Interactive Apps, a search icon, Develop, Help, and Log Out. Below the navigation bar, there is a large "OPEN" button and the OnDemand logo. A sub-menu titled "LRC Shell Access" is open. The main content area has a dark background and contains the following text:

N O T I C E T O U S E R S

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* LBNL Backup Services: <https://commons.lbl.gov/display/itdivision/Backups>

We have WEEKLY office hours on Wednesdays starting 7/24/2019!

Request a virtual consultation at <https://sites.google.com/a/lbl.gov/hpc/getting-help>
Time: 10:30am-noon on Wednesdays

[wfeinstein@n0000 ~]\$

Job Management

Job monitoring, composing and submission

Open OnDemand Files ▾ Jobs ▾ Clusters ▾ Interactive Apps ▾ 

◀ Develop ▾ ? Help ▾  Log Out

OPEN  Active Jobs
 Job Composer

OnDemand

Open OnDemand / Active Jobs

All Jobs ▾ LRC ▾

Active Jobs

Show entries Filter:

ID	Name	User	Account	Time Used	Queue	Status	Cluster	Actions
> 29272013	test	smgarner	lr_neugroup	00:03:36	csd_lr6_96	Completed	LRC	
> 29259568	cf1_job	sivonxay	lr_mp	02:45:44	cf1-hp	Completed	LRC	
> 29239015	niwo4-o1-rel	lpeterson	lr_nokomis	04:12:14	lr3	Completed	LRC	
> 29263734	FW_job	shyamd	ac_mp	00:53:49	lr5	Completed	LRC	
> 29272181	lr6_job	sivonxay	ac_mp	00:00:04	lr6	Completed	LRC	
> 29272183	lr6_job	sivonxay	ac_mp	00:00:03	lr6	Completed	LRC	
> 29272185	lr6_job	sivonxay	ac_mp	00:00:06	lr6	Completed	LRC	
> 29272187	lr6_job	sivonxay	ac_mp	00:00:02	lr6	Completed	LRC	

Job Composer

- From templates
- From specific path
- From selected job



Jobs

The interface shows a list of jobs. The first job listed is a "GPU Slurm Job" created on March 8, 2021, at 2:52am. It has the ID 29215978 and is associated with the cluster LRC, with a status of "Completed". The second job listed is an "MPI Slurm Job" created on March 8, 2021, at 2:27am. It has the ID 29215878 and is also associated with the cluster LRC, with a status of "Completed".

On the left, there is a sidebar with a "New Job" dropdown menu containing options: "From Default Template", "From Template", "From Specified Path", and "From Selected Job". There is also an "Open Terminal" button.

On the right, a "Job Details" panel is open for the first job. It displays the job ID (29215978), the job name ("GPU Slurm Job"), and the submit information ("Submit to: LRC"). It also indicates the account is "Not specified".

Created	Name	ID	Cluster	Status
March 8, 2021 2:52am	GPU Slurm Job	29215978	LRC	Completed
March 8, 2021 2:27am	MPI Slurm Job	29215878	LRC	Completed

Job Templates

- Provided by system admins
- Defined by users



Templates

To create a new job, select a template to copy, fill out the form to the right, and click "Create New Job".

The screenshot shows two panels. On the left is a table listing job templates. On the right is a modal dialog for creating a new template.

Left Panel: Job Templates List

- Buttons: **New Template**, **Copy Template**
- Buttons: **View Files**, **Open Terminal**
- Search:
- Table Headers: **Name**, **Cluster**, **Source**
- Table Data:

Name	Cluster	Source
my_template	Lrc	My Templates
GPU Slurm Job	Lrc	System Templates
MPI Slurm Job	Lrc	System Templates
Simple Sequential Slurm Job	Lrc	System Templates
- Show: **10** entries
- Search:
- Buttons: **Previous**, **1**, **Next**

Right Panel: Create New "my_template"

Change these notes by editing the manifest.yml in this template's directory

Job Name: my_template

Cluster: LRC

Script Name: my_job.sh

Create New Job, **Reset**

Job Submission Script

Open OnDemand / Job Composer Jobs Templates

Jobs

+ New Job ▾

- From Default Template
- From Template
- From Specified Path
- From Selected Job

Open Terminal

Search:

Created	Name	ID	Cluster	Status
March 8, 2021 2:52am	GPU Slurm Job	29215978	LRC	Completed
March 8, 2021 2:27am	MPI Slurm Job	29215878	LRC	Completed

Job Details

29215978

Job Name: **GPU Slurm Job**

Submit to: **LRC**

Account: Not specified

Submit Script

gpu_job.sh

Script contents:

```
#!/bin/bash

#SBATCH --job-name=test
#SBATCH --nodes=1
#SBATCH --time=00:30:00
#SBATCH --qos=es_normal
#SBATCH --account=scs
#SBATCH --partition=es1
#SBATCH --gres=gpu:1
#SBATCH --ntasks=2
#SBATCH --output=%j.output
#SBATCH --error=%j.err
#SBATCH --job-name=test

#cd $SLURM_SUBMIT_DIR
#cd $HOME
echo "How to submit GPU jobs" > output_file
nvidia-smi -L >> output_file
```

Open Editor

Open Terminal

Open Dir

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

Open OnDemand Files ▾ Jobs ▾ Clusters ▾ Interactive Apps ▾  Develop ▾ Help ▾ Logged in as wfeinstein Log Out

OPEN

Welcome to LBNL Lawrencium Super
OnDemand provides an integrated, single access po...
ources.

GUIs
 VMD

Servers
 Jupyter Server
 MATLAB
 RStudio Server

Open OnDemand Files ▾ Jobs ▾ Clusters ▾ Interactive Apps ▾  Develop ▾ Help ▾ Logged in as wfeinstein Log Out

[Home](#) / My Interactive Sessions

Interactive Apps

GUIs

 VMD

Servers

 Jupyter Server

 MATLAB

 RStudio Server

You have no active sessions.

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 ...)*

The screenshot shows the 'Interactive Apps' section of the Jupyter Notebook App. On the left, there's a sidebar with 'Interactive Apps' and 'Interactive Apps [Sandbox]' sections. The 'Interactive Apps' section contains 'GUIs' (VMD), 'Servers' (Jupyter Server, selected), MATLAB, and RStudio Server. The 'Interactive Apps [Sandbox]' section contains MATLAB, Spark Jupyter Server, and VMD. The main area displays the 'Jupyter Server' configuration page. It shows the version (92f372f) and a description: 'This app will launch a Jupyter server using Python on the LBNL Science-IT Laboratory Research Computing(LRC) Infrastructure clusters.' A dropdown menu for 'Type of use' has 'interactive_mode, for exploration' selected. Below it are 'interactive_mode_gpu, for exploration' and 'compute_mode'. A 'Wall Clock Time' input field contains '1'. A note asks, 'How many hours do you want to run this Jupyter Server for ?'. An 'Email address (optional)' input field is present, with a note: 'Enter your email address if you would like to receive an email when the session starts. Leave blank for no email.' A large blue 'Launch' button is at the bottom.

Open OnDemand Files ▾ Jobs ▾ Clusters ▾ Interactive Apps ▾ 📁

Developer Mode Help ▾ Logged in as wfeinstein Log Out

Home / My Interactive Sessions / Jupyter Server

Interactive Apps

GUIs

VMD

Servers

Jupyter Server

MATLAB

RStudio Server

Interactive Apps [Sandbox]

Servers

MATLAB

Spark Jupyter Server

VMD

Jupyter Server version: 92f372f

This app will launch a [Jupyter](#) server using [Python](#) on the [LBNL](#) Science-IT Laboratory Research Computing([LRC](#)) Infrastructure clusters.

Type of use

- interactive_mode, for exploration
- interactive_mode_gpu, for exploration
- compute_mode

Wall Clock Time

1

How many hours do you want to run this Jupyter 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

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

[Quit](#)[Logout](#)[Files](#) [Running](#) [Clusters](#)

Select items to perform actions on them.

0 / global / home / users / wfeinstein / OOD

Name ↴

Upload New ↴

Name	Type	Size
..	Folder	1 kB
tf-gpu.ipynb	Notebook	Python 2.7 Python 3 Python 3.6 Python3.6 TF-1.12 Python3.7 TF-2.1.0 Python3.7 TF-2.3.0
vmd.pdb	Text File	1 kB
vmd2.pdb	Text File	1 kB

Running

Other:

- Text File
- Folder
- Terminal

Matlab App

- Enabled on GPU and CPU nodes

The screenshot shows the Open OnDemand web interface for launching interactive sessions. The top navigation bar includes links for Open OnDemand, Files, Jobs, Clusters, Interactive Apps, Develop, Help, and Log Out. The user is logged in as wfeinstein.

The main content area displays the "Interactive Apps" section. Under "Interactive Apps", the "MATLAB" option is selected and highlighted in blue. Other options include GUIs, VMD, Servers, Jupyter Server, and RStudio Server. A sidebar titled "Interactive Apps [Sandbox]" lists Servers, MATLAB, Spark Jupyter Server, and VMD.

The central panel shows the configuration for launching a MATLAB session:

- MATLAB** version: 92f372f
- Description: This app will launch a MATLAB GUI on the LBNL Science-IT Laboratory Research Computing(LRC) Infrastructure clusters. You will be able to interact with the MATLAB GUI through a VNC session.
- Name of the job**: OOD_MatLab_test
- MATLAB Versions**: R2020b
- SLURM Partition**: es1_GPUs
- SLURM Project/Account Name**: (empty input field)

Matlab App Launch

Open OnDemand Files ▾ Jobs ▾ Clusters ▾ Interactive Apps ▾

Develop ▾ Help ▾ Logged in as wfeinstein Log Out

Session was successfully created.

Home / My Interactive Sessions

Interactive Apps

GUIs

VMD VMD

Servers

Jupyter Server

MATLAB

RStudio Server

Interactive Apps [Sandbox]

Servers

MATLAB

Spark Jupyter Server

VMD

MATLAB (29280612)

1 node | 2 cores | Running

Host: >_n0001.es1

Delete

Created at: 2021-03-10 01:45:31 PST

Time Remaining: 55 minutes

Session ID: bd0ceb58-11c9-4fc4-b8bb-f8cbf7c8135f

Compression



0 (low) to 9 (high)

Launch MATLAB

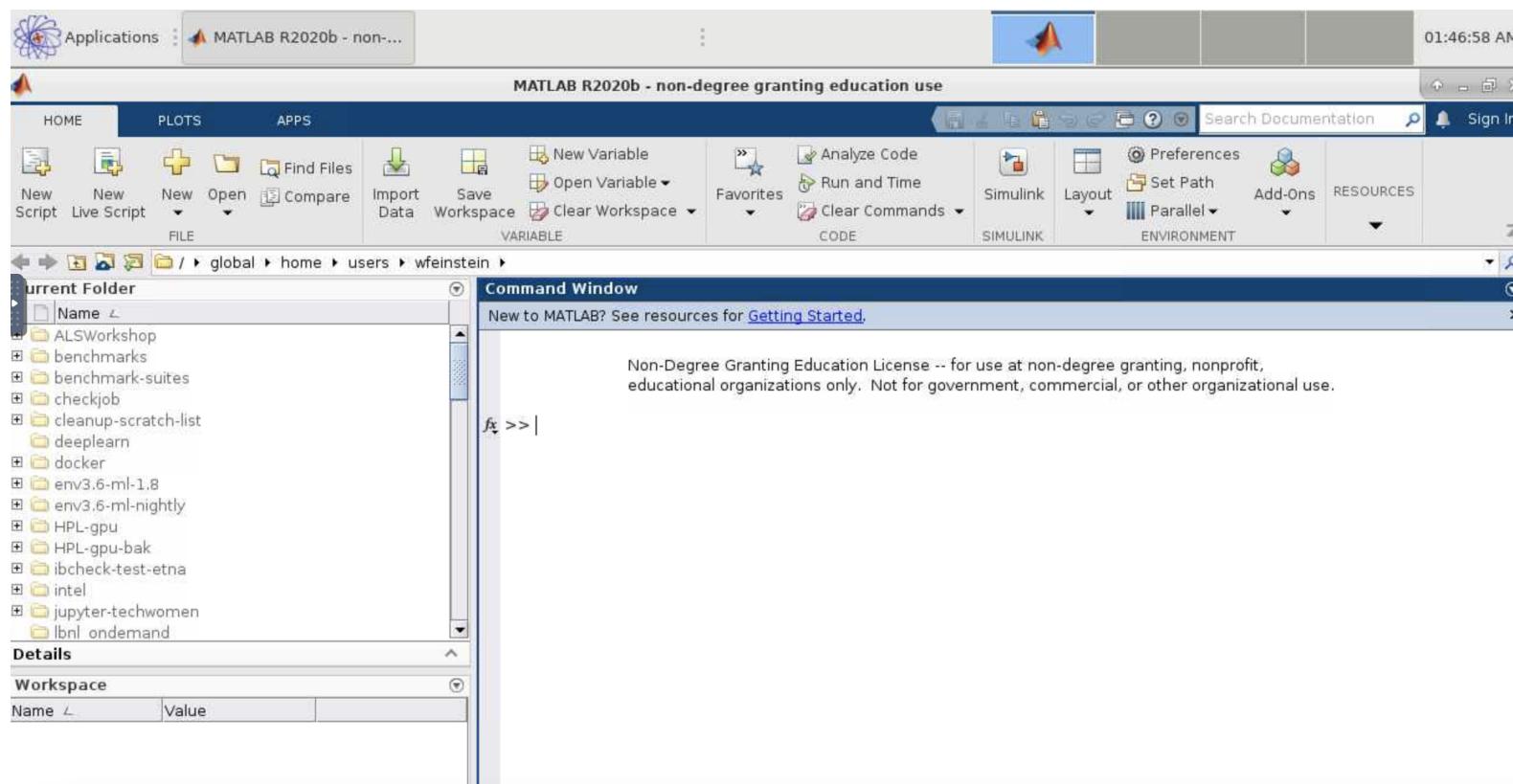
Image Quality



0 (low) to 9 (high)

View Only (Share-able Link)

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.

Open OnDemand Files ▾ Jobs ▾ Clusters ▾ Interactive Apps ▾ 

Develop ▾ Help ▾ Logged in as wfeinstein Log Out

Home / My Interactive Sessions / VMD

Interactive Apps

GUIs

VMD

Servers

Jupyter Server

MATLAB

RStudio Server

VMD version: 92f372f

This app will launch **VMD** 1.9.4 on the Lawrencium cluster using a **shared node**. You will be able to interact with the VMD GUI through a VNC session.

Disclaimer: This software is for **academic purpose** only. Please review the [license agreement](#) before you use this software.

Type of use

interactive_mode, for exploration

Choose the mode of running your VMD App

Wall Clock Time

1

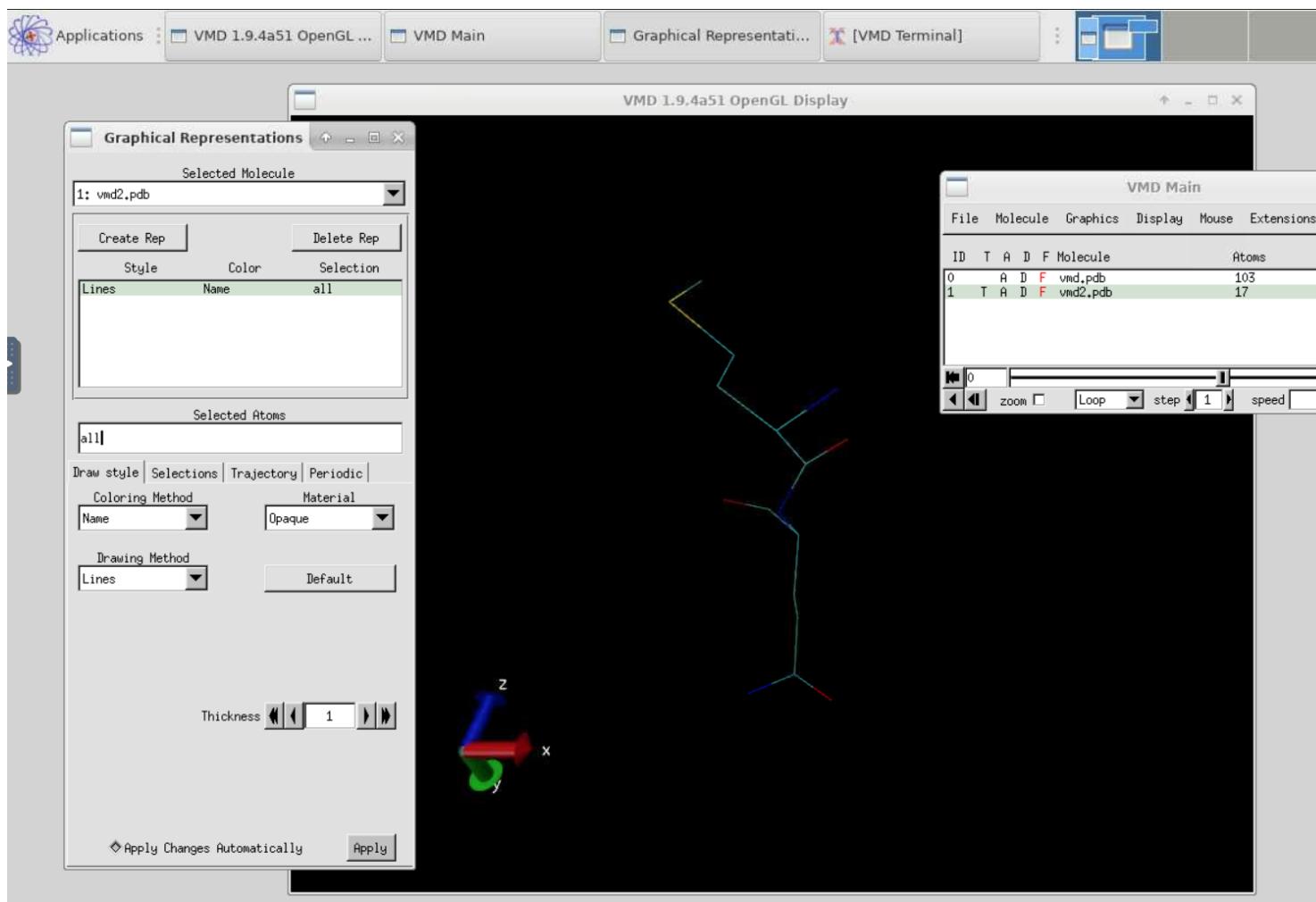
How many hours do you want to run this VMD App for ?

Email address (optional)

Enter your email address if you would like to receive an email when the session starts. Leave blank for no email.



VMD Example



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 VMD
- Servers
- Jupyter Server
- MATLAB
- RStudio Server**

Interactive Apps [Sandbox]

- Servers
- MATLAB
- Spark Jupyter Server
- VMD 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 · Project: (None) ·

R · Go to file/function · Addins ·

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 · Global Environment · List ·

Environment is empty

Files Plots Packages Help Viewer · Publish ·

Zoom Export ·

A bar plot with three bars. The x-axis is labeled with 1, 2, and 3. The y-axis has tick marks at 0 and 400. The first bar (labeled 1) reaches approximately 300 on the y-axis. The second bar (labeled 2) reaches approximately 600 on the y-axis. The third bar (labeled 3) reaches approximately 100 on the y-axis.

Category	Value
1	~300
2	~600
3	~100

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/>