Intro Open OnDemand

Introduction: Open OnDemand is a NSF Funded Open Source HPC Project to provide a web-based portal and interface that enables the access and use of High Performance Computing (HPC) systems. ARCC uses Open OnDemand to enable access to Medicine Bow in a user-friendly manner. Discussed in this workshop is each feature of Open OnDemand including the Dashboard, Available Applications, File and Job Management, and Cluster status. There will be some overlap from other modules, but the intent here is to have a one-stop shop for all things Open OnDemand.

Course Goals:

How to navigate the Dashboa	rc
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- □ What applications are available and how to use them
- □ Starting HPC jobs on Open OnDemand

This workshop assumes that participants have already have an understanding of text editors and job scheduling

Sections:

- 1. Open OnDemand Dashboard
- 2. Applications in Open OnDemand
- 3. <u>Job Composer</u>
- 4. Interactive Applications

Open OnDemand Dashboard

Discussed in this section of the workshop is getting started with the Open OnDemand interface for MedicineBow, including logging and navigating the dashboard. This is more of an overview of the application and later sections will be the use of the available options found on the Dashboard.

- □ <u>Logging In</u>
- Overview of the Dashboard
- □ Message of the Day
- Pinned Applications
- □ Top Menu Left Side
- □ Top Menu Right Side
- □ Next Steps

Logging In

To login to the MedicineBow Open On Demand instance, you will first need to open a web browser (ARCC recommends using Google Chrome over other browsers to limit performance issues) and navigate to https://medicinebow.arcc.uwyo.edu.

- ☐ You will then be required to enter your ARCC username and password.
- You will also be required to enter your two-factor authentication

Overview of the Dashboard

On the dashboard, you may notice several things:

The message of the day, that provides ARCC announcements
A link to the ARCC help pages
Pinned applications
A top menu with options for the applications available on Open On Demand
Information about your login username and an option to log out

Message of the Day

The message of the day contains important information of users. There are static and some dynamic information. First it tells you what system you are on. Then some policy information about appropriate usage.

Occasionally, there will be an announcement about systems maintenance, or other news that can be important for users to know.

ARCC advises everyone to read the message of the day before diving in to running jobs.

Message of the Day

Welcome

Welcome to the University of Wyoming Medicine Bow Compute Cluster, hosted by the Advanced Research Computing Center (ARCC). This system is for authorized users only.

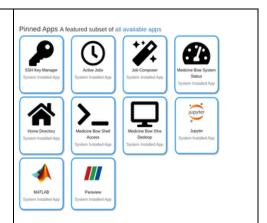
- Accounts are for single users only. Do NOT share your account with others.
- Users do not have "sudo" privileges and never will
- Please avoid building and installing your own MPI as you will miss key features of the job scheduler and interconnect for the cluster.

Pinned Applications

The Pinned applications are some of the most commonly used applications, with the basic functions of Open OnDemand of:

- □ ssh key managment
- ☐ Job managment
- □ System status
- □ Files
- □ Shell Access
- ☐ Interactive Desktop

Along with other interactive applications that ARCC has available



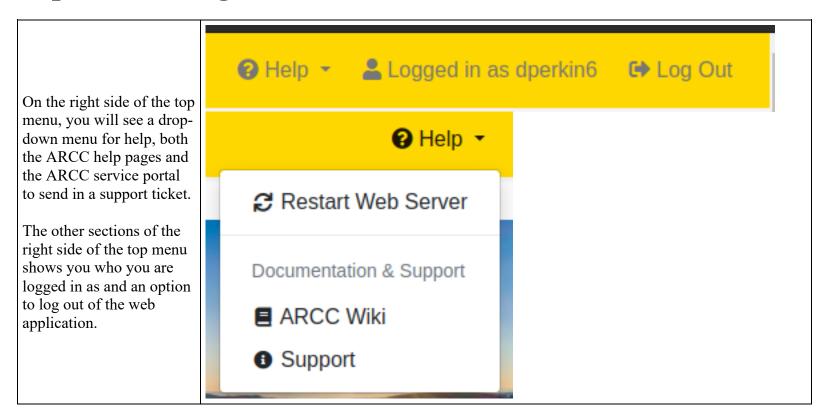
Top Menu - Left Side

On the left side of the top menu, you will see drop-down menus for all options available in MedicineBow Open OnDemand beyond what is pinned on the home page.

- ☐ ARCC Icon Back to the dashboard
- □ Apps Gives access to some of the options found in pinned apps.
- ☐ Files Access MedicineBow files
- □ Jobs Shows your active jobs and lets you create new jobs
- □ Clusters shows status of cluster and nodes as well as lets you open a web based terminal
- ☐ Interactive Apps
- □ My Interactive Sessions



Top Menu - Right Side



Applications in Open OnDemand

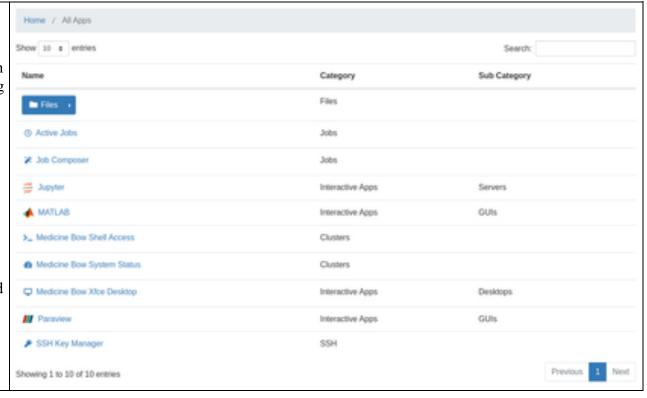
Open OnDemand makes it easy to access your favorite apps for data visualization, simulations, modeling, and more. Discussed in this module is where to find the available applications on MedicineBow Open OnDemand and what the purpose of each is. Some apps are covered more extensively in other tutorials and will be referenced where appropriate.

- □ All Applications
- ☐ The Files Category and App
- ☐ The Jobs Category
- □ Clusters Category
- ☐ Interactive Apps Category
- □ Next Steps

All Applications

In the drop down menu for "Apps" you can find all available tools you can use within the Open OnDemand interface, by selecting the "All Apps" option. When on this page, you will see icons and names for all available applications, the category they fall under and the subcategory such as:

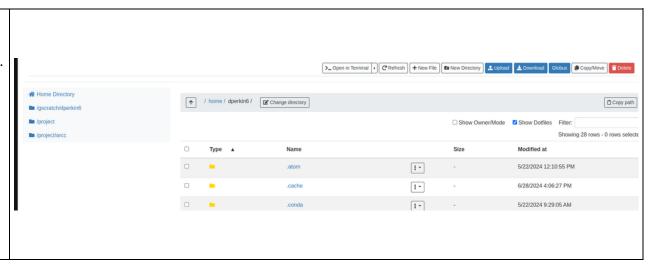
- □ Files
- Jobs
- ☐ Interactive Apps
 - Servers, GUIs, and Desktops
- □ Clusters
- \Box SSH



The Files Category and App

The files app allows users to view, upload, download, and edit files on the MedicineBow system. When clicking this app, notice that it opens a new browser tab that allows you to close the tab when done without closing the whole application.

The <u>Intro to Data Transfer</u> workshop provides more details on how to use this application to move data around.



The Jobs Category

Under Jobs there are two different applications. Active Jobs and the Job Composer. The Active Jobs app shows the status of jobs and many of the details. You can see all jobs on the system or just yours.

The job composer app will be covered more extensively in a later module of this tutorial.



Clusters Category

This category opens up a terminal in your web browser and enables users the ability to use it just as if they had a native application on their computer.

It also has a section for system status





Interactive Apps Category

This category has three sub categories: ☐ Servers - refers to JupyterLab server covered extensively in another module Show 10 ¢ entries Search: Interacti GUIs - Graphical user interfaces Name Category **Sub Category** are applications that would Jupyter Interactive Apps Servers typically work on a desktop, but ▲ MATLAB Interactive Apps **GUIs** on MedicineBow Medicine Bow Xfce Desktop Desktops o MatLab Paraview GUIs Interactive Apps o Paraview ☐ Desktops - a desktop environment on the cluster

Open OnDemand Job Composer

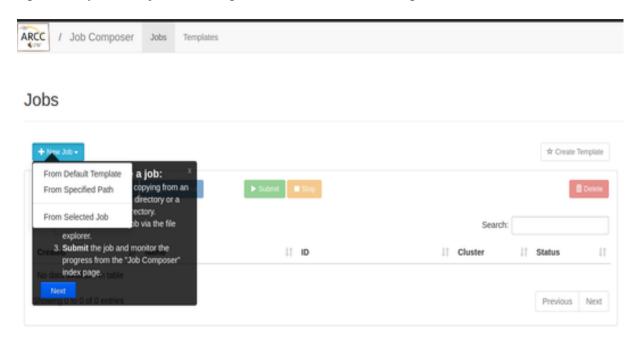
The Open OnDemand Job Composer enables users to create job scripts and submit them without ever using the command line. This is paricularly helpful for new users who have never opened a terminal or are unfamiliar with Linux command line behavior. However, some knowledge of Slurm and ARCC's required Slurm directives is needed to successfully submit jobs on MedicineBow. Discussed in this section of the workshop is the use of the Job Composer and common issues that arise with it.

- ☐ First Look at the Job Composer
- ☐ Create a Job With a Template

- □ Job Editor
- □ Job Options
- □ Job Submission
- □ In Conclusion
- ☐ Finally The End

First Look at the Job Composer

When opening the Job Composer for the first time, there are a few pop up prompts to follow to get started creating a job. There are also two items in the top menu 1) for Job management and 2) for job templates. Notice that the "New Job" button allows user to select a previously created job with the path, or from a Default Template as well as a new one if there is a job in the selections below.



Create a Job With a Template

	Julio Details
	Job hame: (default) Simple Sequential Job Submit to
If someone has never created a batch job in Slurm before, a template is a good place to get started into seeing how one would look like. In this example, we will create a Default Template and then edit it in the steps	Medicine Bow Account: Trust specified
below.	Solpt location:
After clicking the "New Job" Button and selecting the "Default Template" option, we are presented with a new box on the right of the first look. Notice the parameters already set:	/home/liperkint/undersond/dets/tys/tryjoto/projects/defself//S Solyt name: main_job.sh
 □ Job Name □ Account □ Along with script location and name 	Epider Contents: main, job.sh
☐ As well as a preview of what the job looks like	Submit Script
This default will not run on ARCC systems "as-is". Edits will be required.	main_job.sh bolyr contents:
	#1/bin/besh # JOB MEADONS MEME #Sho "Welle Morte"
	✓ Open Gallers (a) Open Gallers (b) Open Gallers (c) Open Gallers (c) Open Gallers (d) Open Gallers (e) Open Gall

Job Editor

When we click the light blue button on the bottom of the right box, we get a new window to pop up with a text editor-like appearance. If we then look at ARCC's documentation on <u>Required Inputs</u>, we know what to add to get a job to run by adding the account and time Slurm directives.

```
Save /home/dperkin6/ondemand/data/sys/myjobs/projects/default/1/main_job.sh

#!/bin/bash
# JOB HEADERS HERE

#SBATCH --account=arcc
#SBATCH --time=0-00:01:00
echo "Hello World"
```

If we click save and go back to the Job Composer page, we should see our changes in the preview.

```
#!/bin/bash
# JOB HEADERS HERE

#SBATCH --account=arcc
#SBATCH --time=0-00:01:00
echo "Hello World"
```

Job Options

Now that our job will run, we still might need to make some changes to the job options that will work best for us. If we Job Options click the "Job Options" Dob Options Hello world Template Cluster button on the left Medicine Bow box we get presented with a new view: Specify job script main_job.sh ☐ We can rename the job to Files larger than 65KB are omitted for the job script field "Hello world Template" that Account makes more sense for us to find arcd later Account is an optional field. If not set, the account may be auto-set by the submit filter. ☐ Leave cluster and job script fields Job array specification as the default because that is the 1-10 system we want and the file we Job arrays are optional, e.g. 1-10 iust editied Copy environment ☐ We can add account here instead Reset Back of in the script, but it's just a good practice to have it in the script

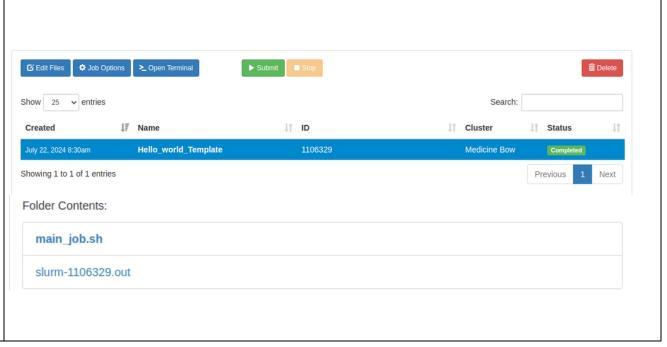
Job Submission

With all of the edits made, we can now submit the job to the cluster to run. The steps to do so are:

- 1. Make sure the Job is selected in the left box
- 2. Click the green "Submit" button



If we refresh the page, we see in the left box that this simple job has been completed and a file for our output was created on the right box



In Conclusion

This module was a simple tutorial for using the Job Composer in Open OnDemand. This tool helps to send jobs to the MedicineBow cluster without the need for using a terminal. That said, the concepts for job submission with Slurm still apply to this tool and it is important to understand what each are doing, but most importantly:

- ☐ ARCC's required inputs
- □ Other Slurm directives that are important to the success of the job
- ☐ How to use Lmod to load software
- Awareness of where the locations on the system where the script is created and output are placed

If used wisely, the Open OnDemand Job Composer can be an easy-to-use tool for creating jobs on MedicineBow and the other tutorials on Intro to Linux, Text Editors, Lmod, and Job Submission are extremely beneficial for the successful use of the tool.

Interactive Applications

In the applications module in this tutorial the interactive applications were mentioned as available, but there are some nuances to getting them started and working for your use case. On this module we will go over getting the interactive desktop, MATLAB, and Paraview interactive applications working. Jupyter Notebooks will be covered in another workshop.

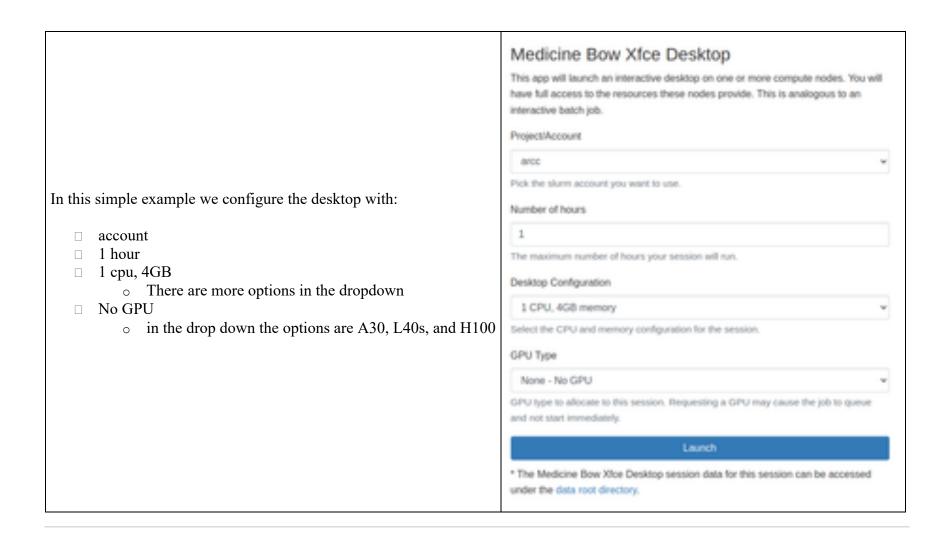
- □ <u>Interactive Desktop</u>
- □ Configuring the Desktop
- □ Launching the Desktop
- Exploring the Desktop
- □ MATLAB
- □ Parallel Computing in MATLAB
- □ ParaView
- □ <u>Using Paraview</u>
- □ Managing Interactive Sessions
- □ Next Steps

Interactive Desktop

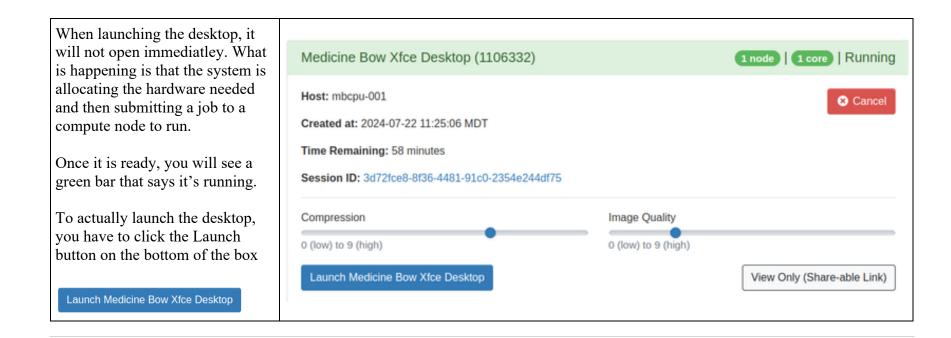
Open OnDemand's interactive desktop application enables users to use the MedicineBow HPC system as if it were a regular desktop computer that many are used to rather than a command line interface (CLI). However, since MedicineBow is a Linux based system, so

is the interactive desktop and may not be as familiar as a Windows or Mac desktop. On MedicineBow, the Xfce desktop environment is used to facilitate this functionality.
Before you use the interactive desktop be prepared that it will prompt you for:
 □ Project/Account □ Number of hours □ Desktop Configuration for your CPU and RAM requirements □ GPU requirements

Configuring the Desktop



Launching the Desktop



Exploring the Desktop



MATLAB

Launching MATLAB is as similar process, the options are a little different where version of the software is one of them and the CPU and RAM options can be manually selected instead of a drop down.

MATLAB

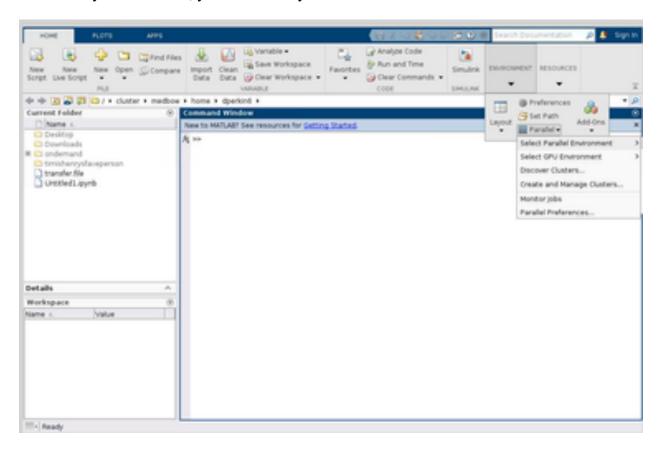
This app will launch a MATLAB GUI on the Medicine Bow cluster. You will be able to interact with the MATLAB GUI through a VNC session.

Matlab Version 2024a Select which version of Madab you would like to load. Project/Account: MOD Pick the slurm account you want to use. Number of hours The maximum number of hours your session will run. (1-168) Number of CPUs. 4 Number of CPUs to allocate to this session. (2-96) Total Memory (GB) * Yotal amount of memory in GB to allocate to this session. (8-512)

GPU Type

Parallel Computing in MATLAB

If you've used Matlab before, you'll be familiar with the window you see after launching. However, In order to use the parallel functionality of MATLAB, you have to set your environment.



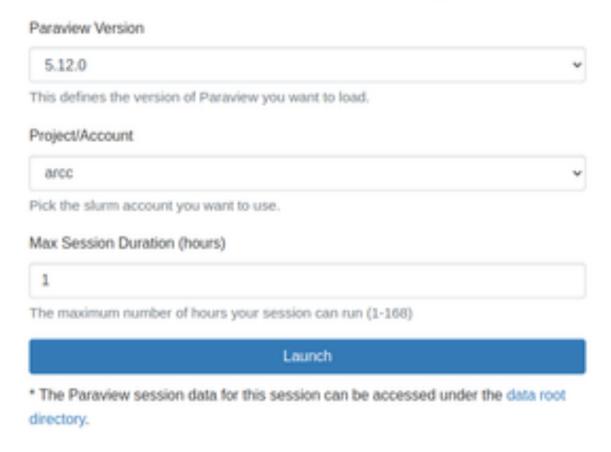
Also, be aware if you are running parallel, that by default, Matlab restricts you to 12 worker threads, so you'd need to override this if you needed by setting the poolobj = parapool ('local', 24);

ParaView

Once again the process of launching the Paraview GUI is similar, but with different options:

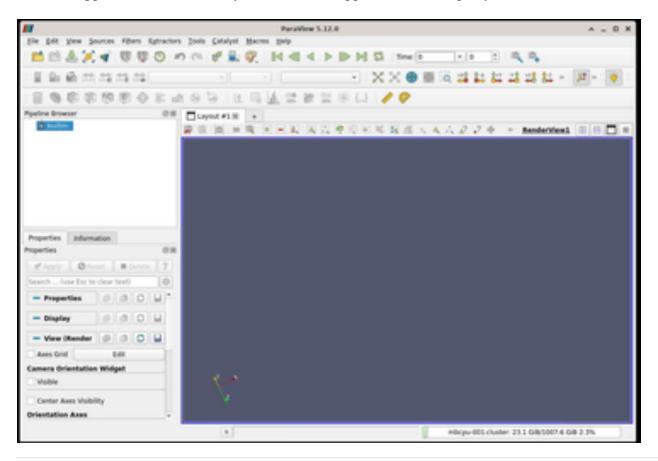
Paraview

This app will launch a ParaView GUI on the Medicine Bow cluster using a shared node. You will be able to interact with the ParaView GUI through a VNC session.

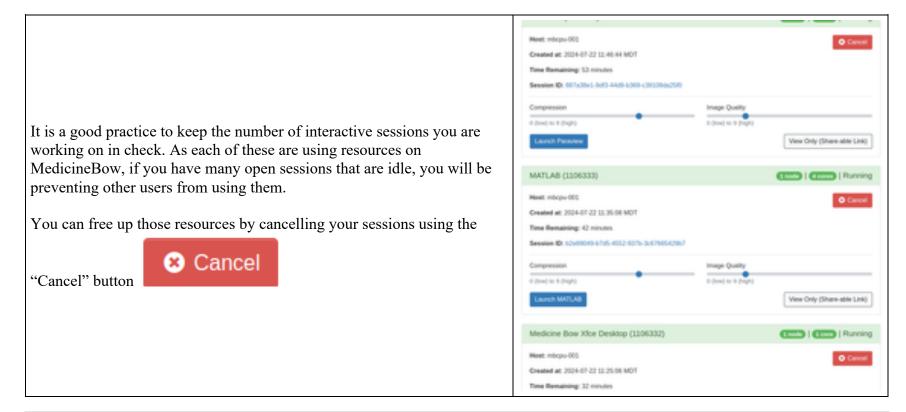


Using Paraview

Once the application is launched, you will see the application running in your browser window.



Managing Interactive Sessions



Next Steps

Previous	Workshop Home
Open OnDemand Job Composer	Intro to Open OnDemand