OPEN ONDEMAND 101

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PURDUE UNIVERSITY | Rosen Center for Advanced Computing

OOD 101

Outline

What to Expect from Open OnDemand 101?

Objectives

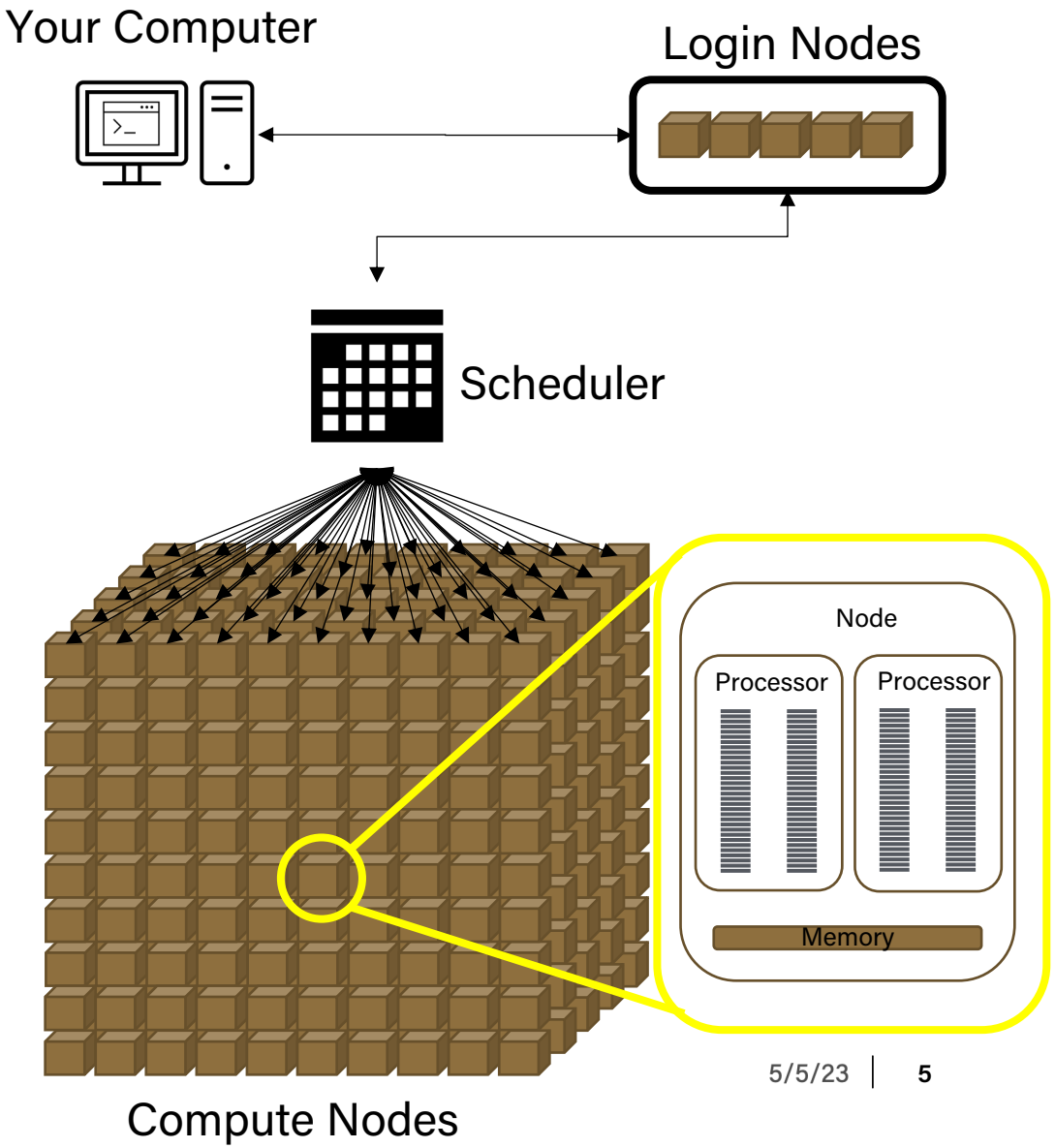
- Understand how science gateways like Open OnDemand address the challenges faced in typical high-performance computing (HPC) work
- Ensure you know how to login to Open OnDemand with your ACCESS account associated with your allocation here on Anvil
- Become comfortable with the purpose and location of different features in Open OnDemand
- Feel confident running your own workflows in Open OnDemand

OOD 101

Lowering the Barrier to HPC

Layout of a Cluster

- HPC systems are often organized into clusters
  - We call them clusters because they are a multitude of independent nodes that can communicate with one another
  - Because each node is independent, we can have different types of nodes with specialized hardware
- When you login to a cluster, typically you will land on login node along with all the other users on the cluster
  - In order to carve out dedicated resources for your work, you need to ask the scheduler to allocate you resources on the compute nodes

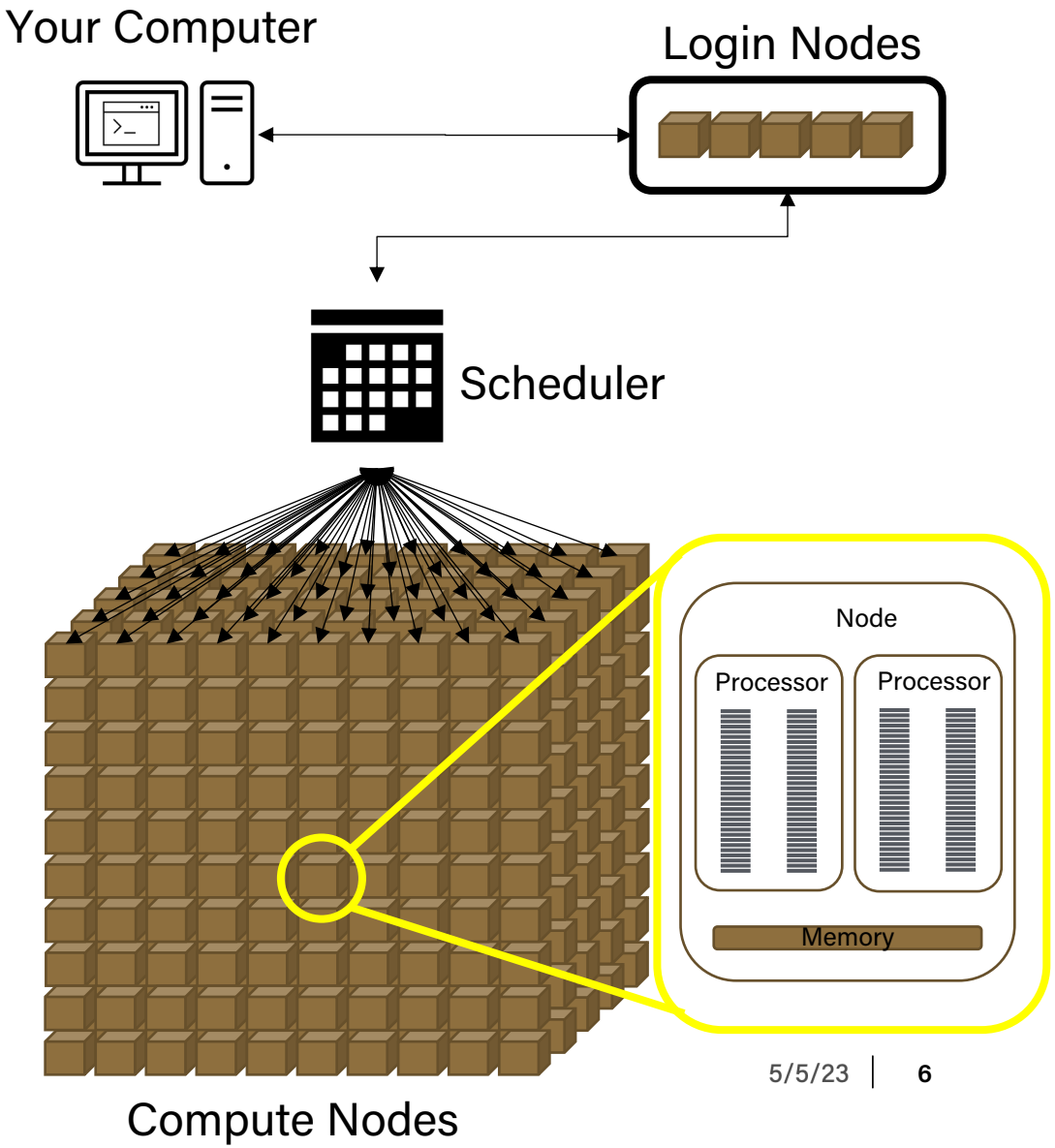


Lowering the Barrier to HPC

HPC Presents a Steep Learning Curve

- Working within HPC in this traditional manner presents many challenges to new users
  - Typically use an SSH client/Linux terminal
  - Learning new commands for interacting with the scheduler
  - Software runs without a graphical user interface (GUI)

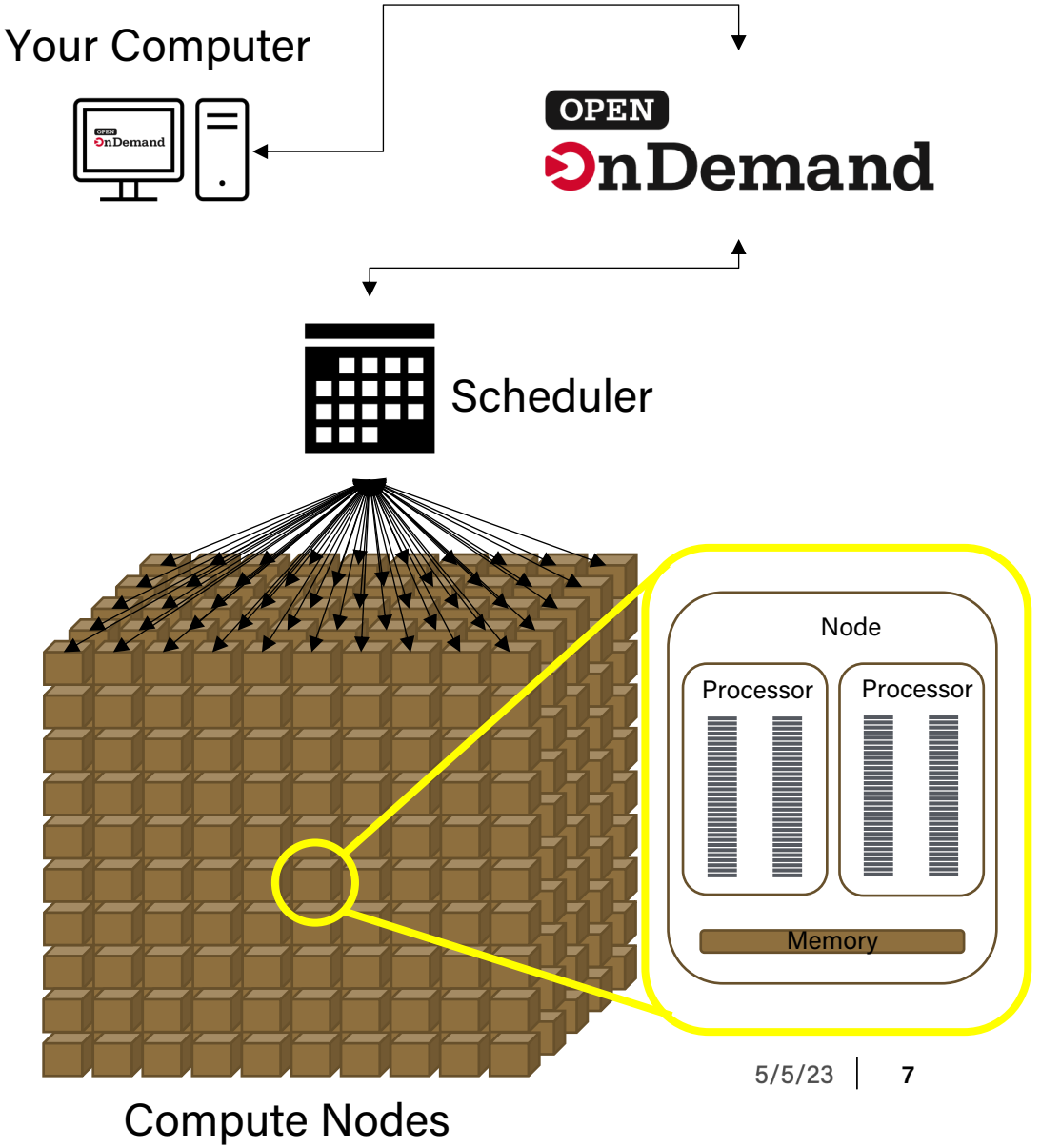
- This can lead to new domain scientists spending most of their time learning how to use the system as opposed to doing science



Lowering the Barrier to HPC

Science Gateways

- To make these resources easier to use, there has been a push for the creation of “science gateways”
- Science Gateways are typically web based interfaces that allow users to run science/engineering applications on HPC resources from their web browser
- Open OnDemand is an example of such a science gateway



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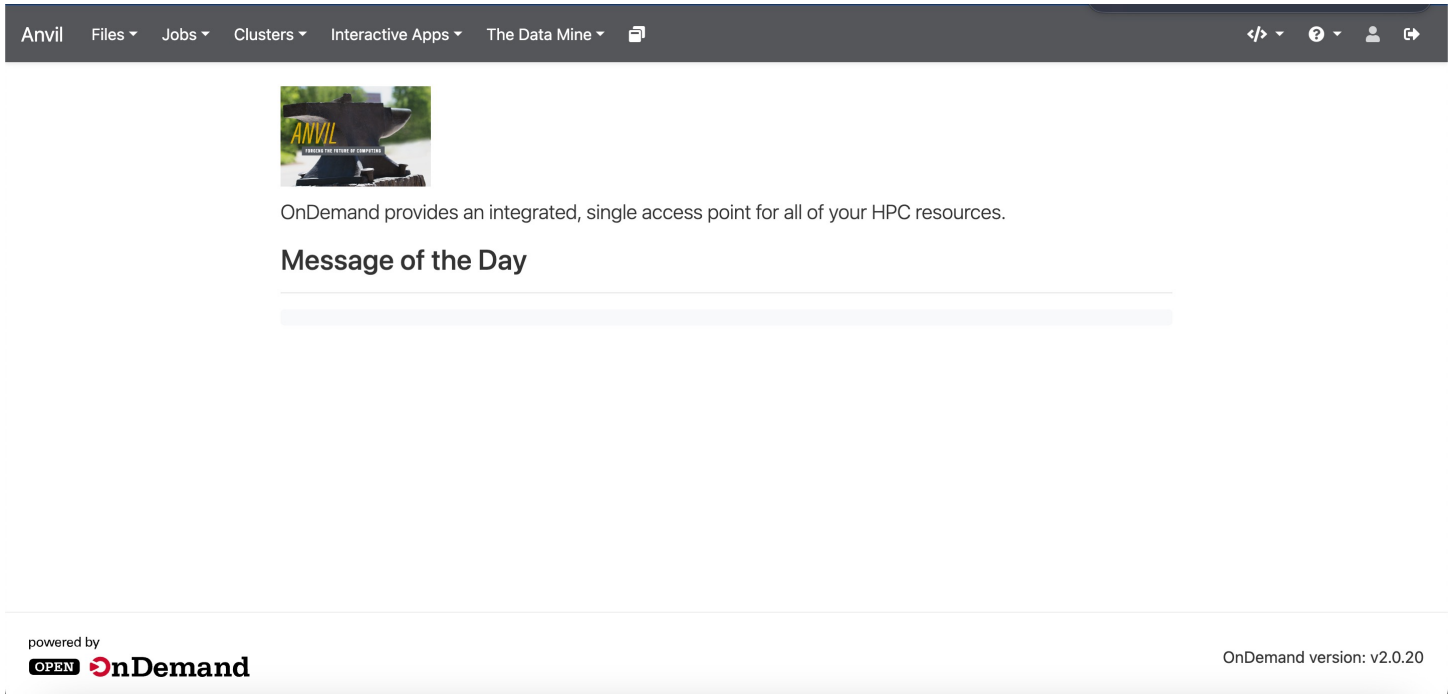
Using Open OnDemand: Dashboard

Using Open OnDemand: Dashboard

Logging into Open OnDemand

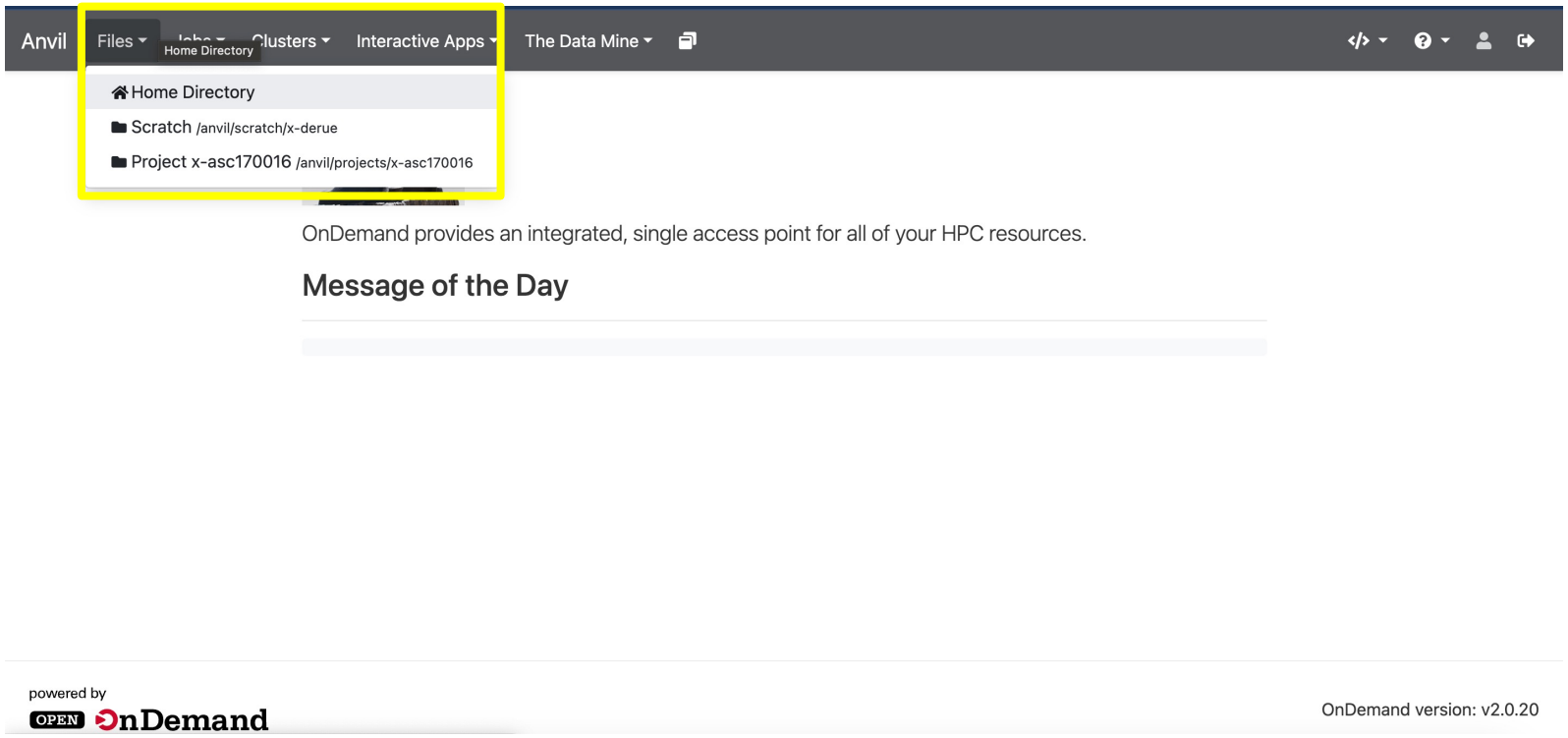
- We offer Open OnDemand on Anvil here at Purdue which can be found by navigating to:
  - ondemand.anvil.rcac.purdue.edu
- Upon navigating to this URL, you will need to login with your ACCESS username and password as well as use 2FA
- Once you are logged in, you will land on your dashboard page
  - My dashboard for can be seen on the right



Using Open OnDemand: Dashboard

Getting Familiar with The Dashboard

1. Directory Shortcuts
   - Allows you to quickly navigate between your important directories
   - Clicking these will open a file navigator allowing you to view your files or upload/download files to/from the cluster

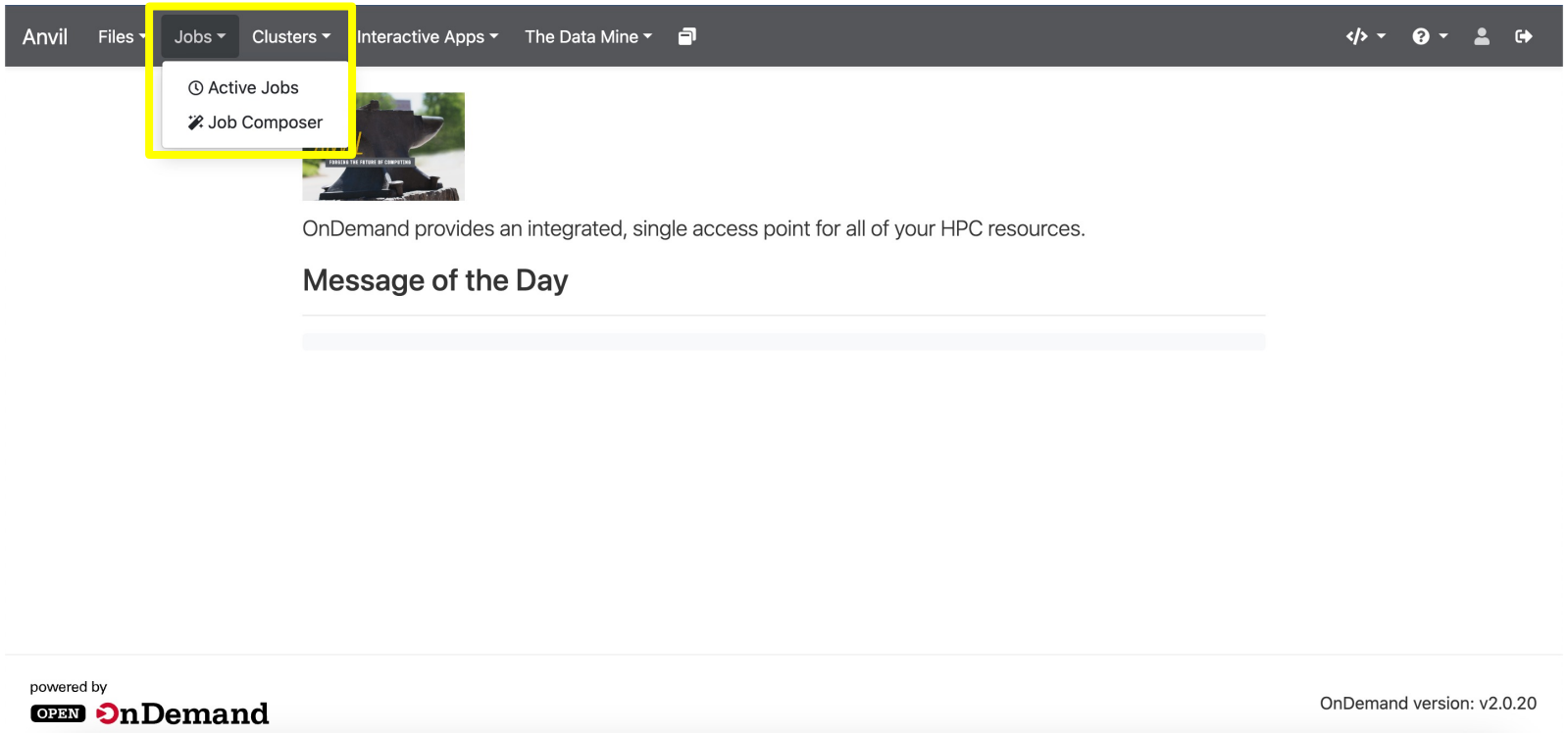


Using Open OnDemand: Dashboard

Getting Familiar with The Dashboard

2. Jobs Menu

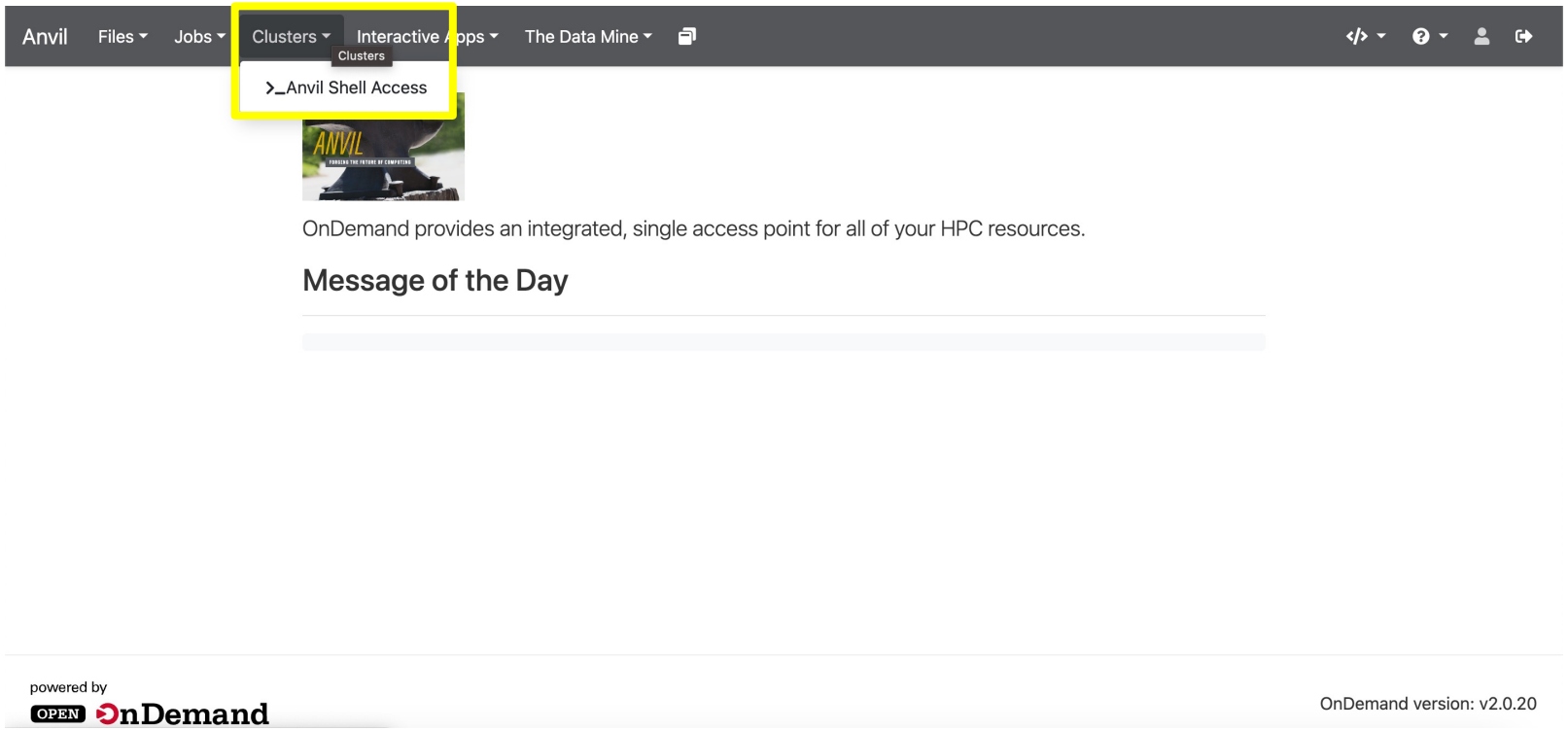
- Provides shortcuts to widgets for creating new Slurm jobs as well as viewing the status of your current ones



Using Open OnDemand: Dashboard

Getting Familiar with The Dashboard

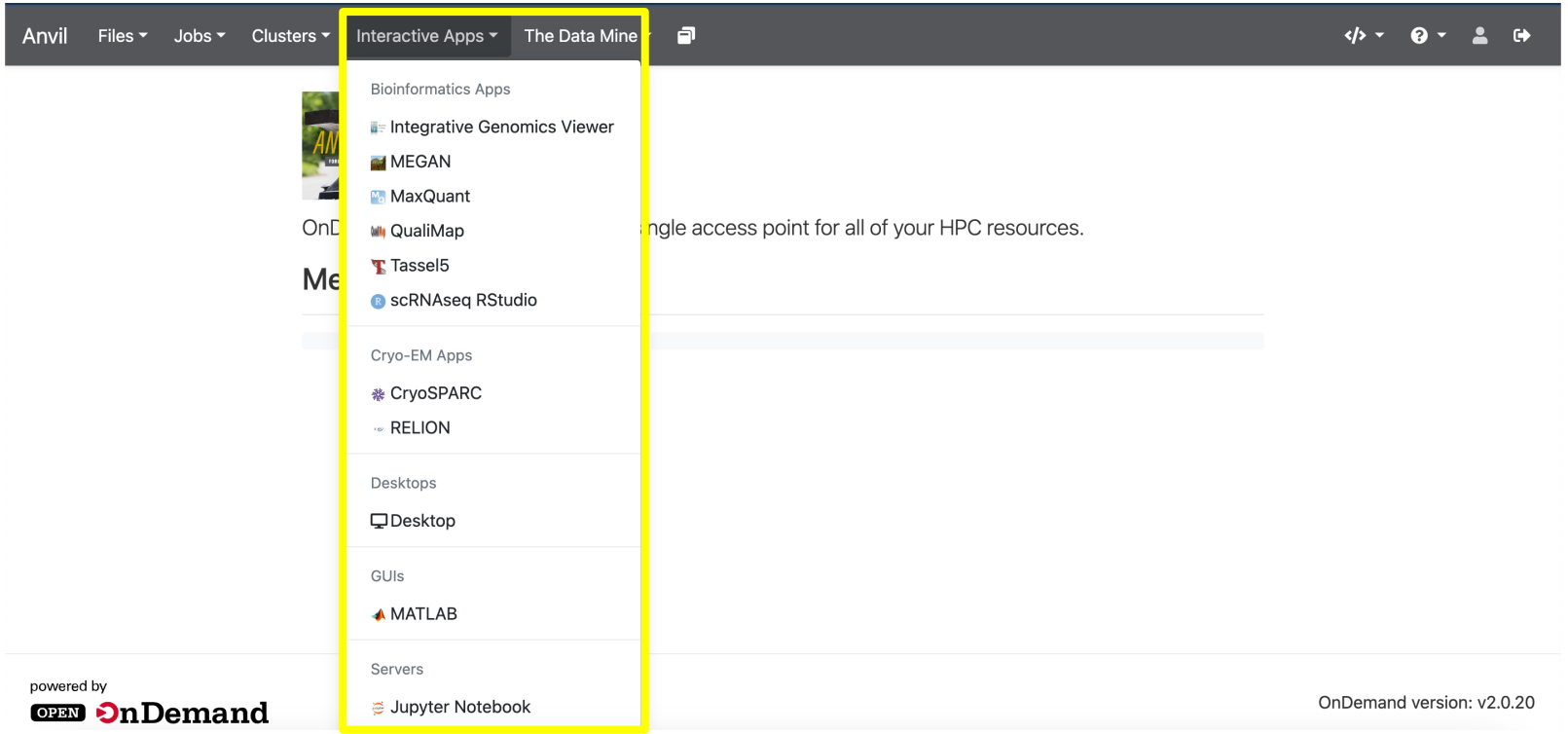
3. Cluster
   - Provides options for interacting with the cluster directly
   - Anvil Shell Access will provide you with a Unix shell on one of the login nodes



Using Open OnDemand: Dashboard

Getting Familiar with The Dashboard

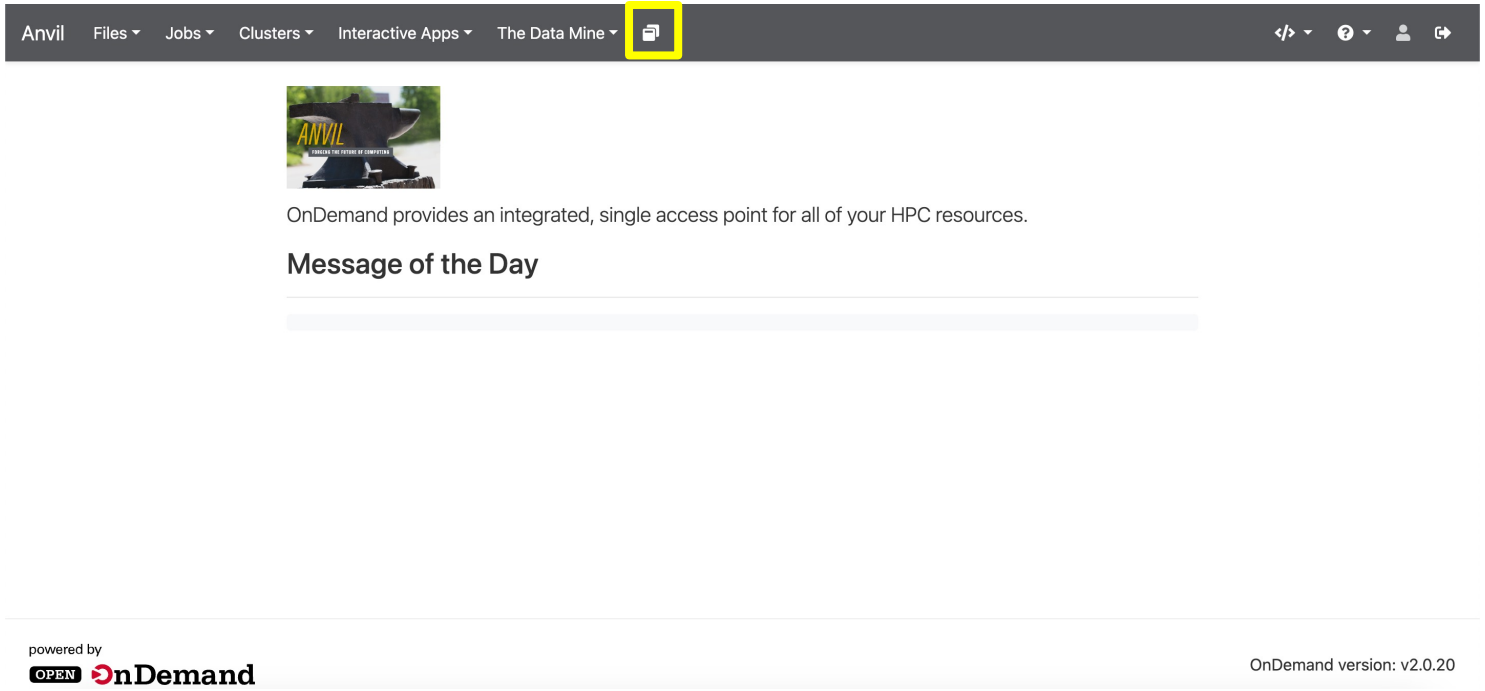
4. Interactive Application Menu
   - This dropdown lists all the applications we support on Open OnDemand
   - Clicking one of the applications will take you to a form through which you can request the resources you want to use



Using Open OnDemand: Dashboard

Getting Familiar with The Dashboard

5. My Interactive Sessions
   - This will take you to a page wherein you can access all your currently running application sessions



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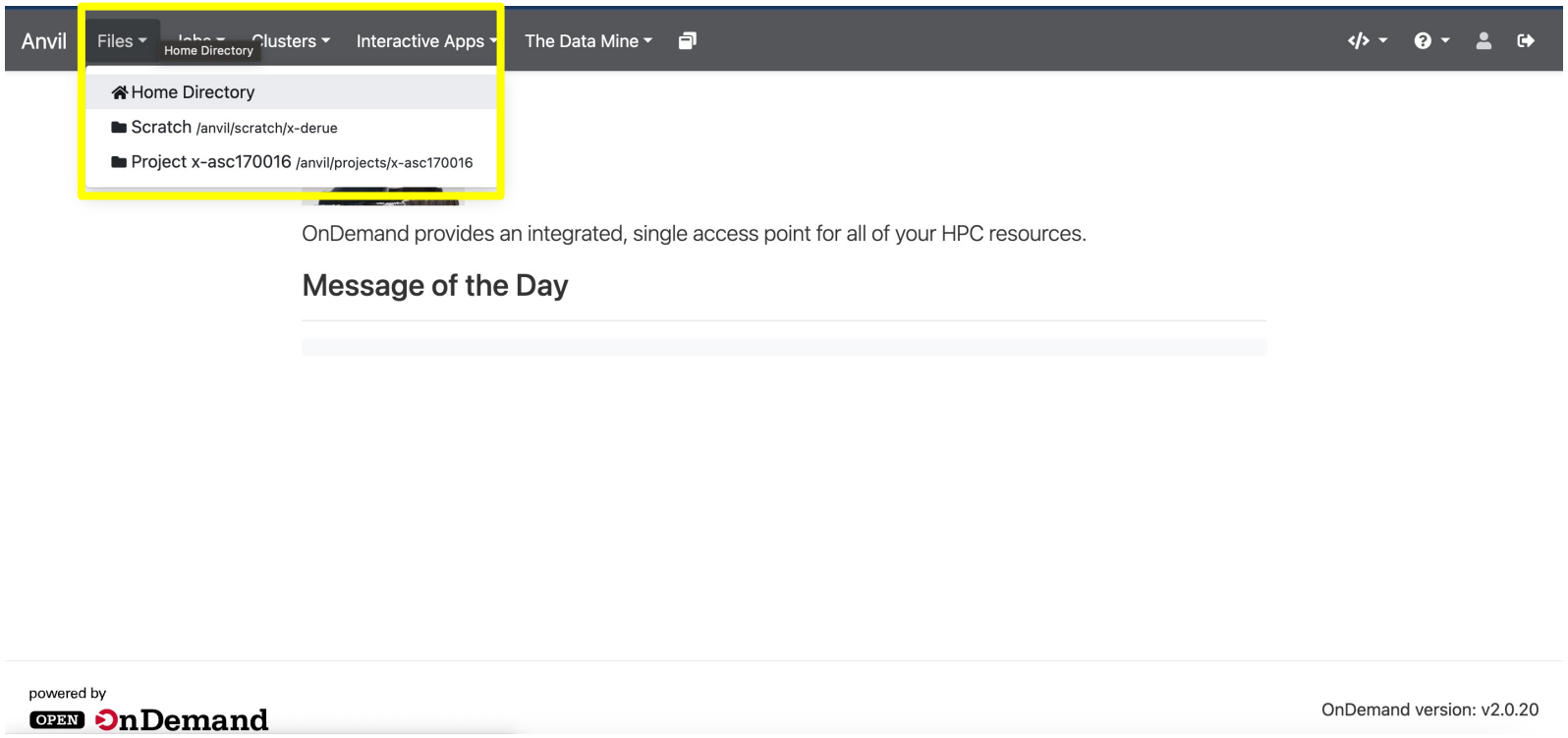
Using Open OnDemand: Files

Using Open OnDemand: Files

A Web-Based File Explorer

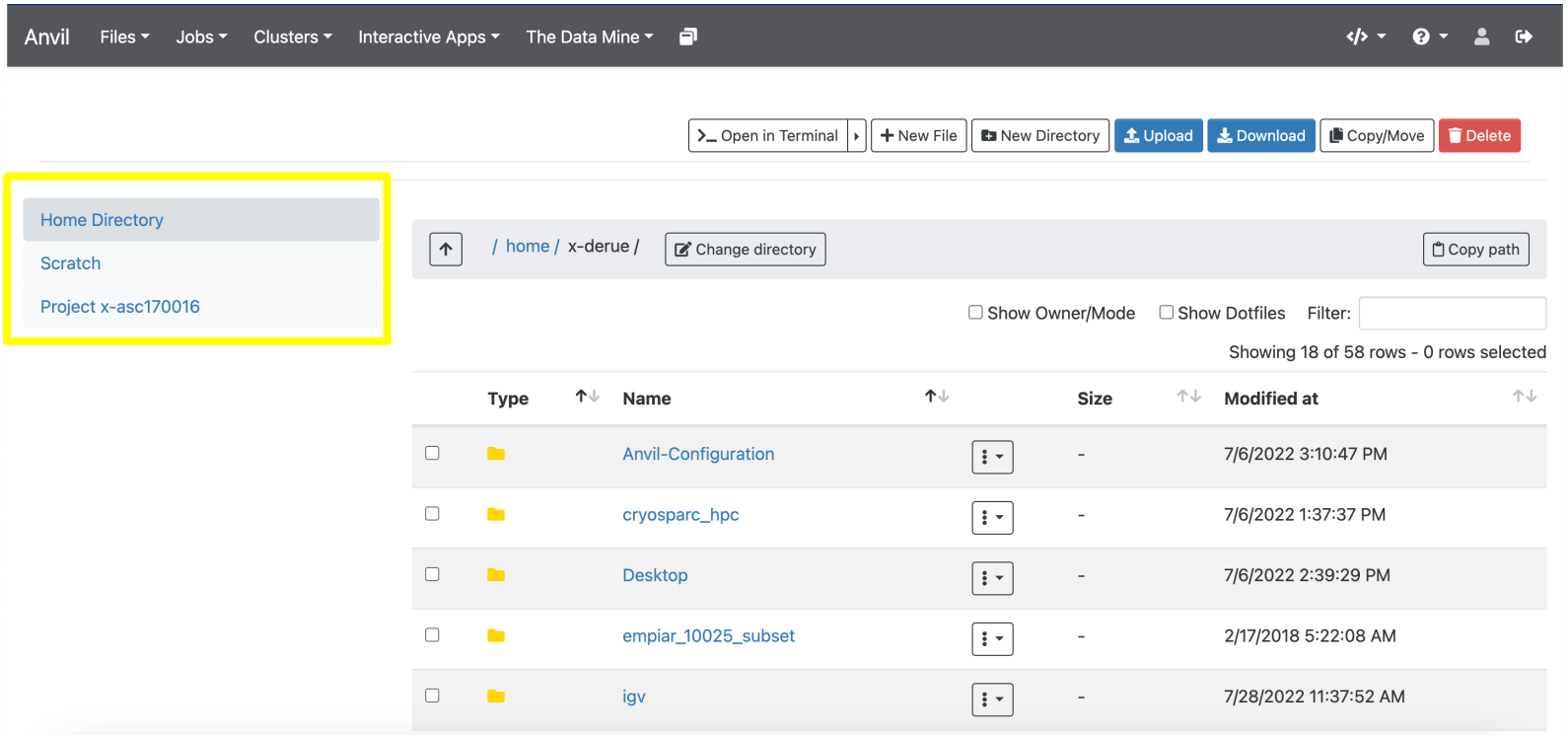
1. To access the File Explorer, click on one of the mounted locations listed in the Files dropdown
   - This will open a new tab containing the File Explorer



Using Open OnDemand: Files

A Web-Based File Explorer

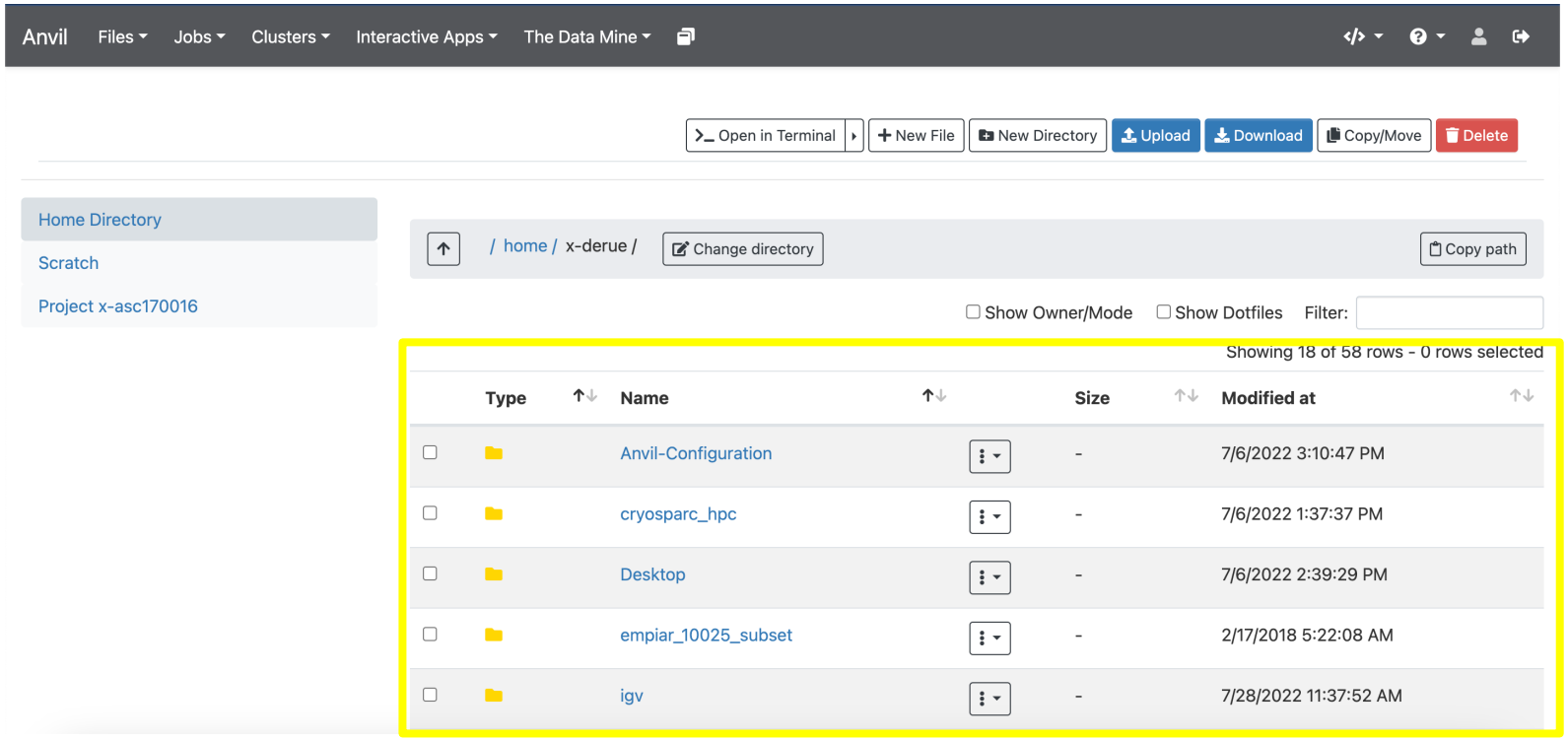
2. The menu along the left-hand side of the screen is for navigating to the top-level directories for your home, project, and scratch spaces
   - Even if you change the directory you are currently examining, this menu will continue to display the same shortcuts



Using Open OnDemand: Files

A Web-Based File Explorer

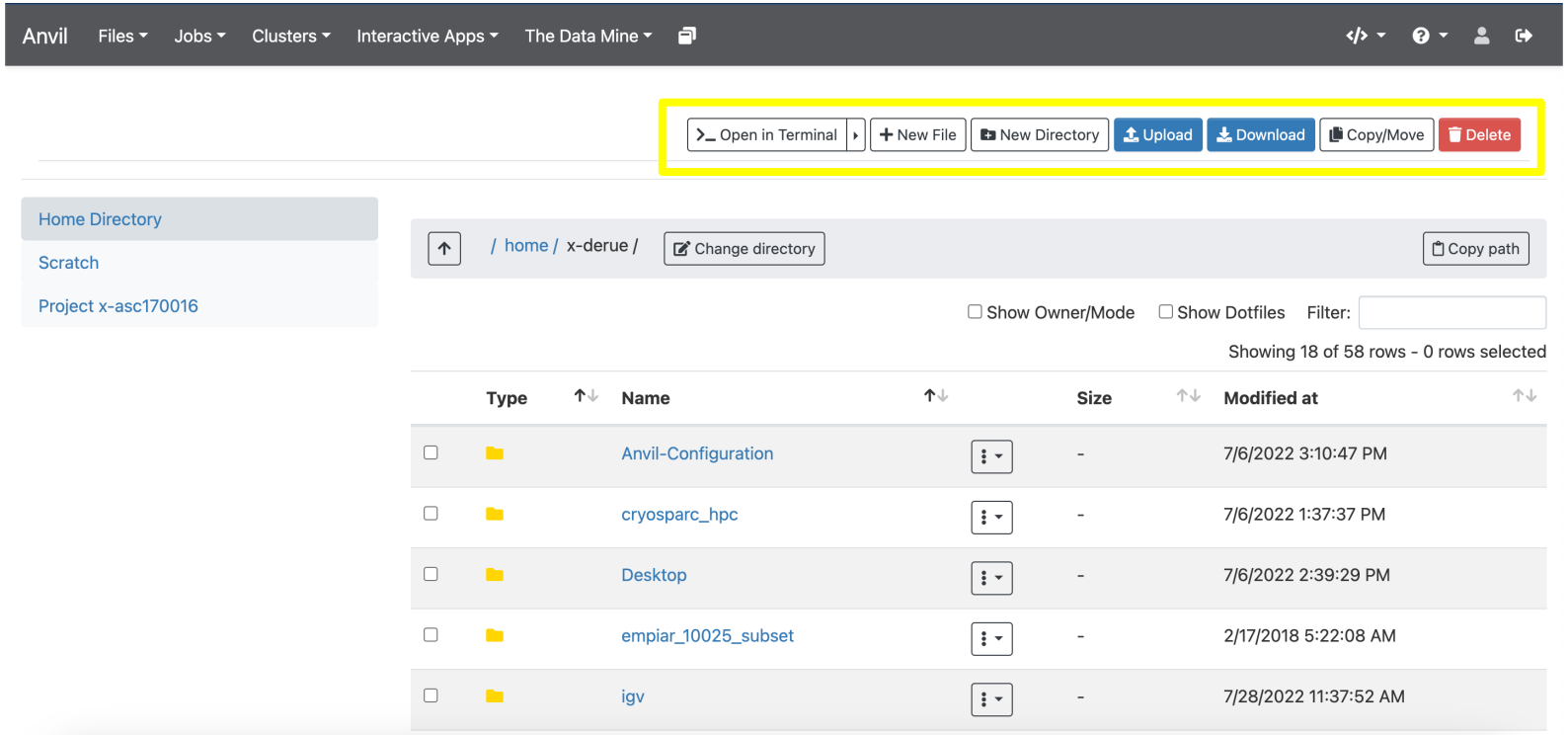
3. The central part of this webpage displays the contents of your present working directory as well along with some metadata like the last modified timestamps
   - The result of selecting a file depends on the type of file you select:
     - Selecting a text file will open that file in a viewer whereas selecting a binary file like an executable will download it



Using Open OnDemand: Files

A Web-Based File Explorer

4. The toolbar in the upper right corner provides tools for changing your current directory, opening your current directory in a terminal to apply shell commands to the files, and creating new files/directories that are either empty or uploaded from your local workstation.



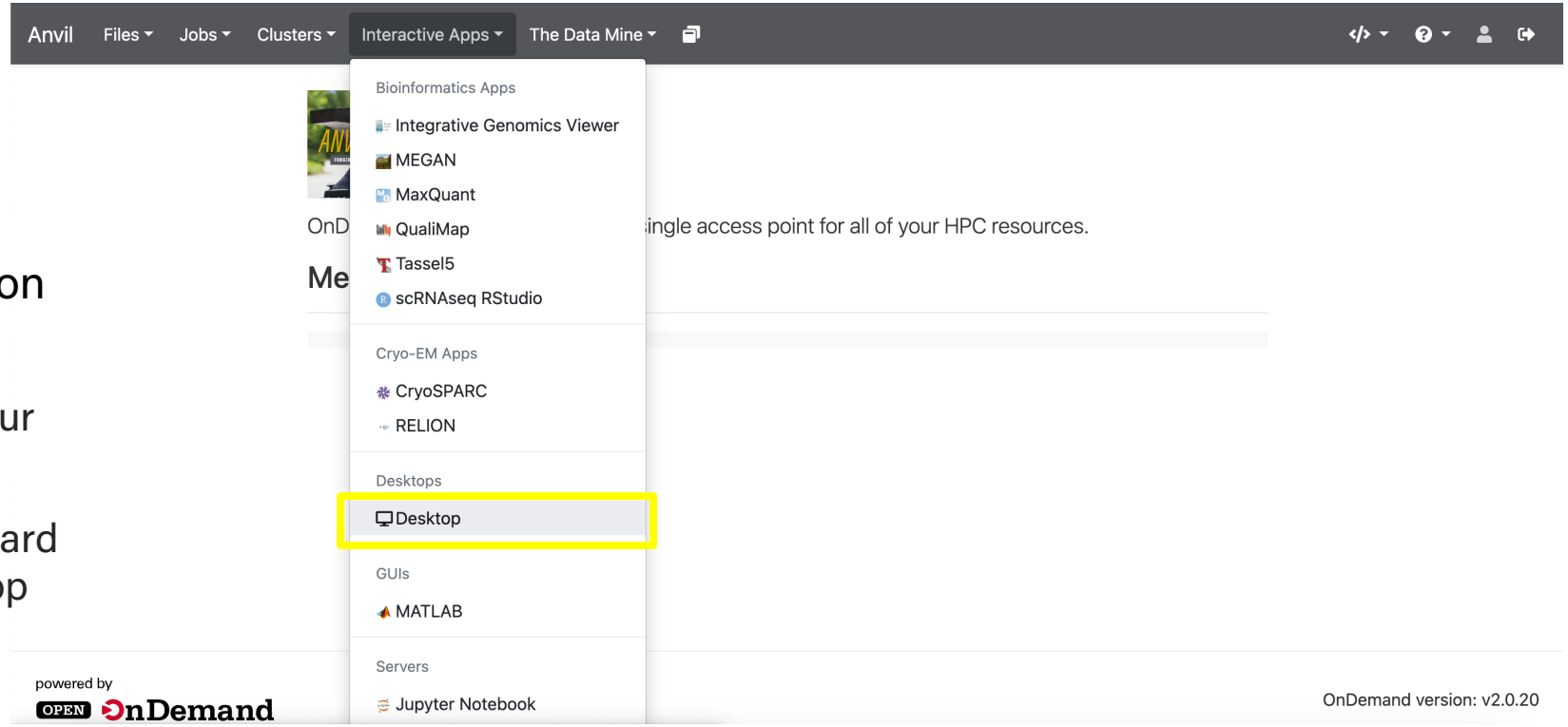
OOD 101

Using Open OnDemand: Applications

Using Open OnDemand: Applications

Application Forms

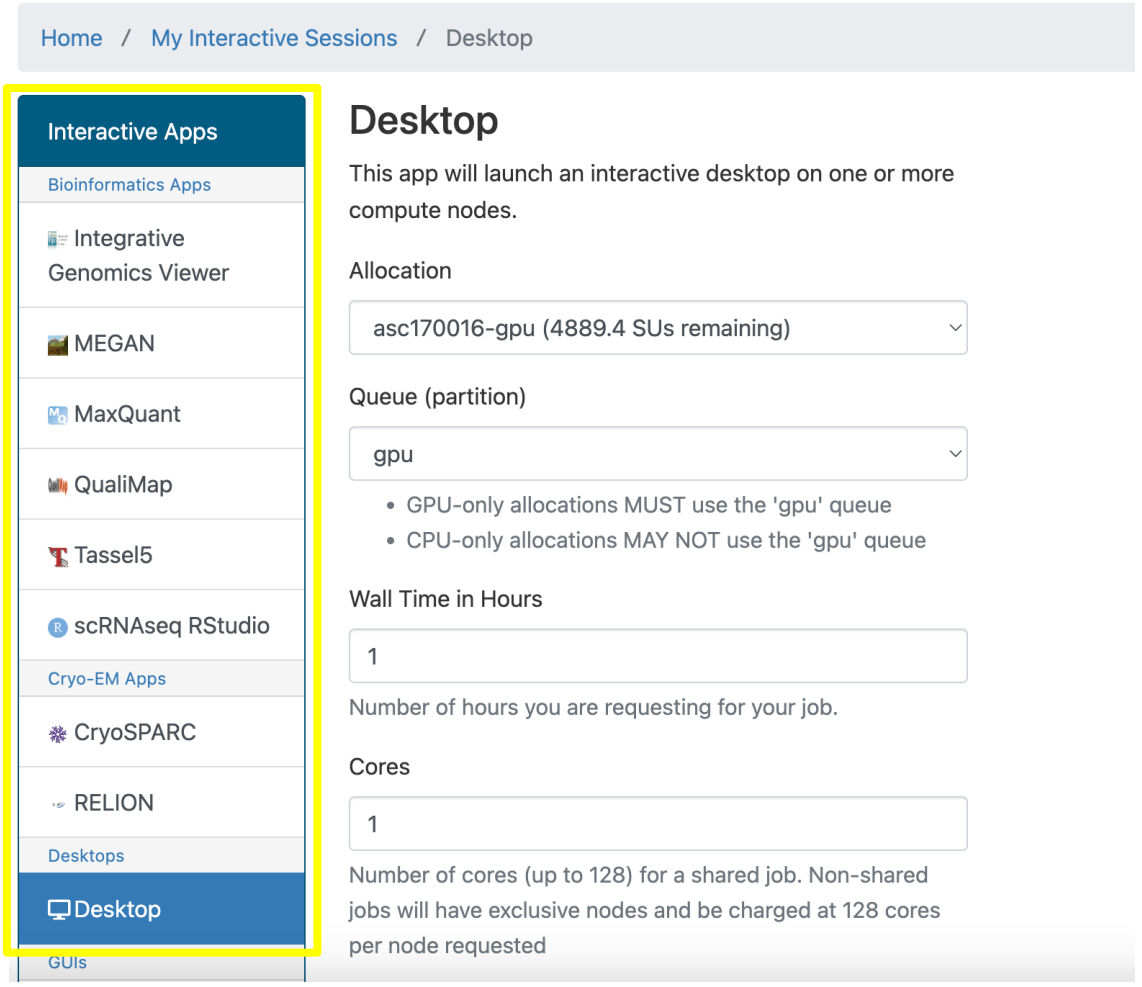
1. To access the App Form for “Desktop”, select it from the Interactive Apps dropdown on the Dashboard
   - The form will be opened in your current tab
   - You can return to the Dashboard by clicking on “Anvil” in the top left corner



Using Open OnDemand: Applications

Application Forms

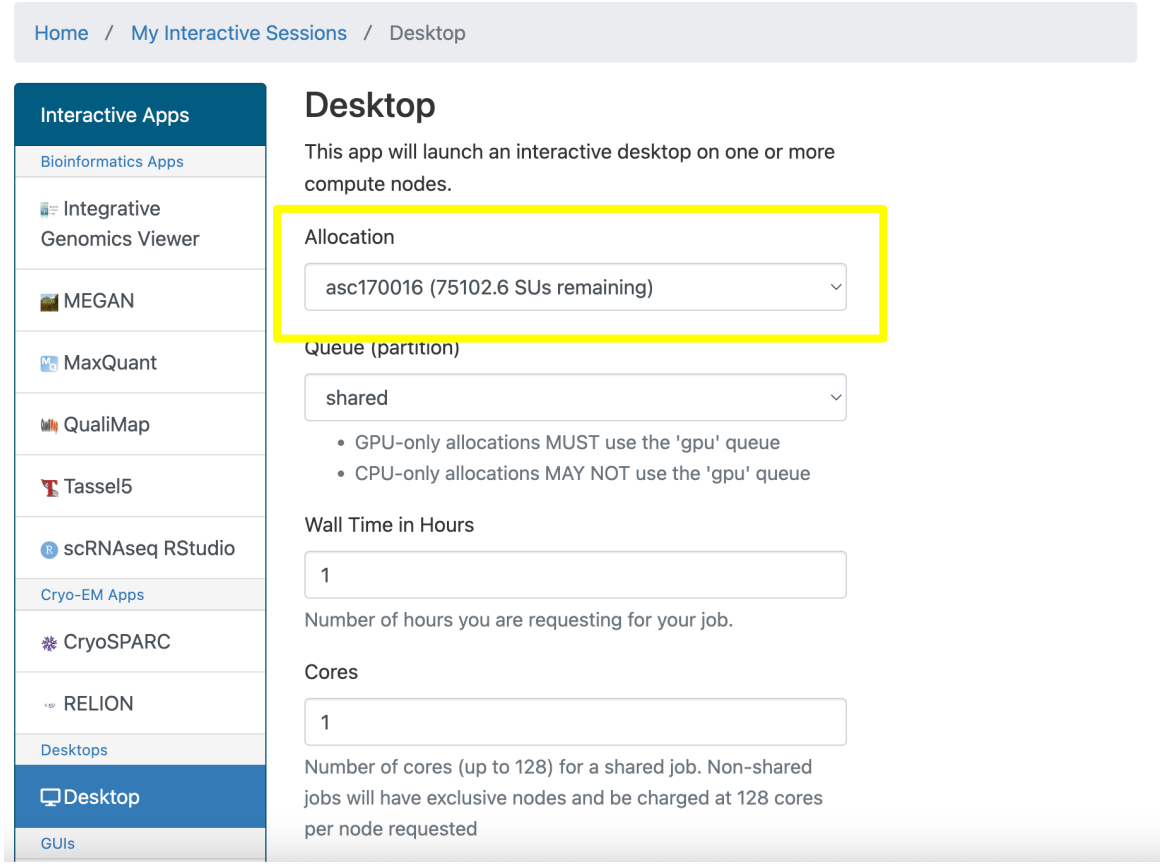
2. You can navigate to other Interactive Apps by selecting them from the left-hand menu



Using Open OnDemand: Applications

Application Forms

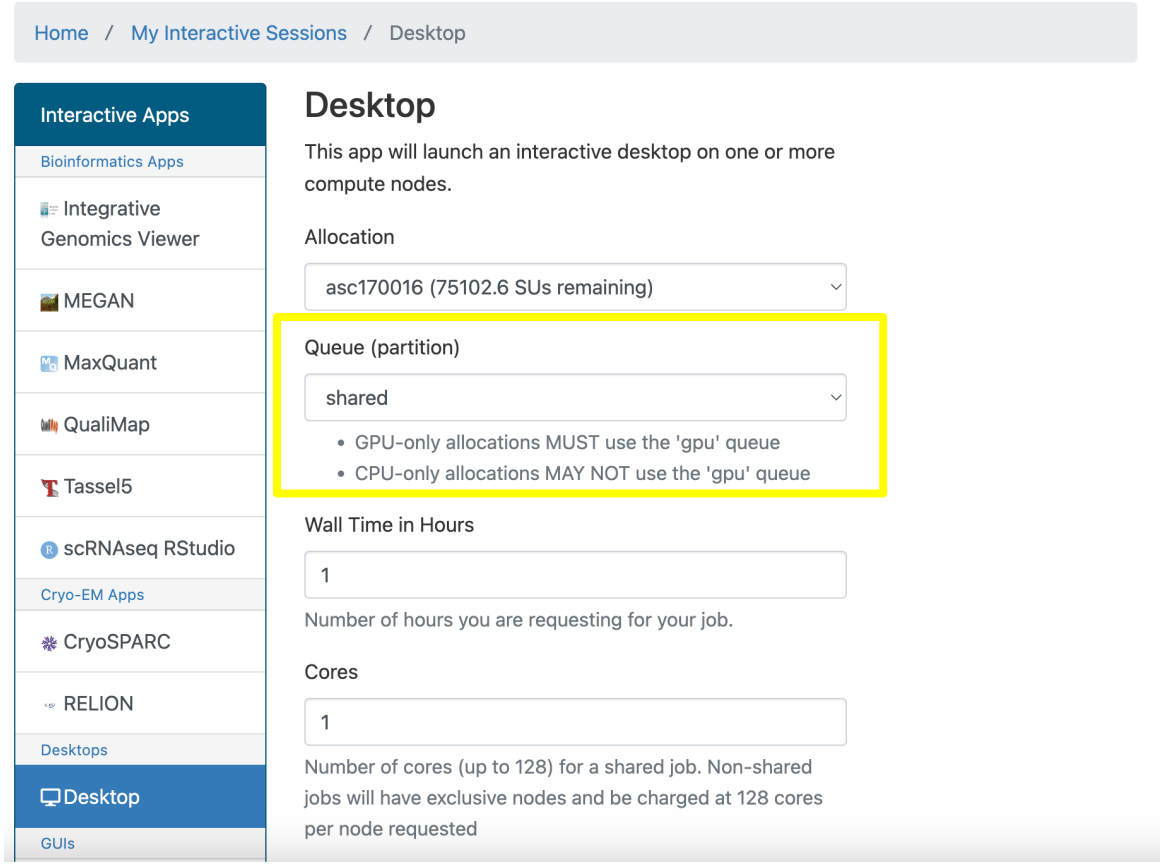
3. In order to request access to dedicated resources, you must select the allocation to charge your resource usage to. You may have more than one type of allocation (CPU vs. GPU). Ensure that you're selecting the correct one



Using Open OnDemand: Applications

Application Forms

4. In addition to your allocation, you must specify the partition to which you want to submit your job. Each of the partitions has a specialized use case, and submitting to the wrong partition can cause you to use more SUs than you intend. Refer to our knowledge guide for more information.

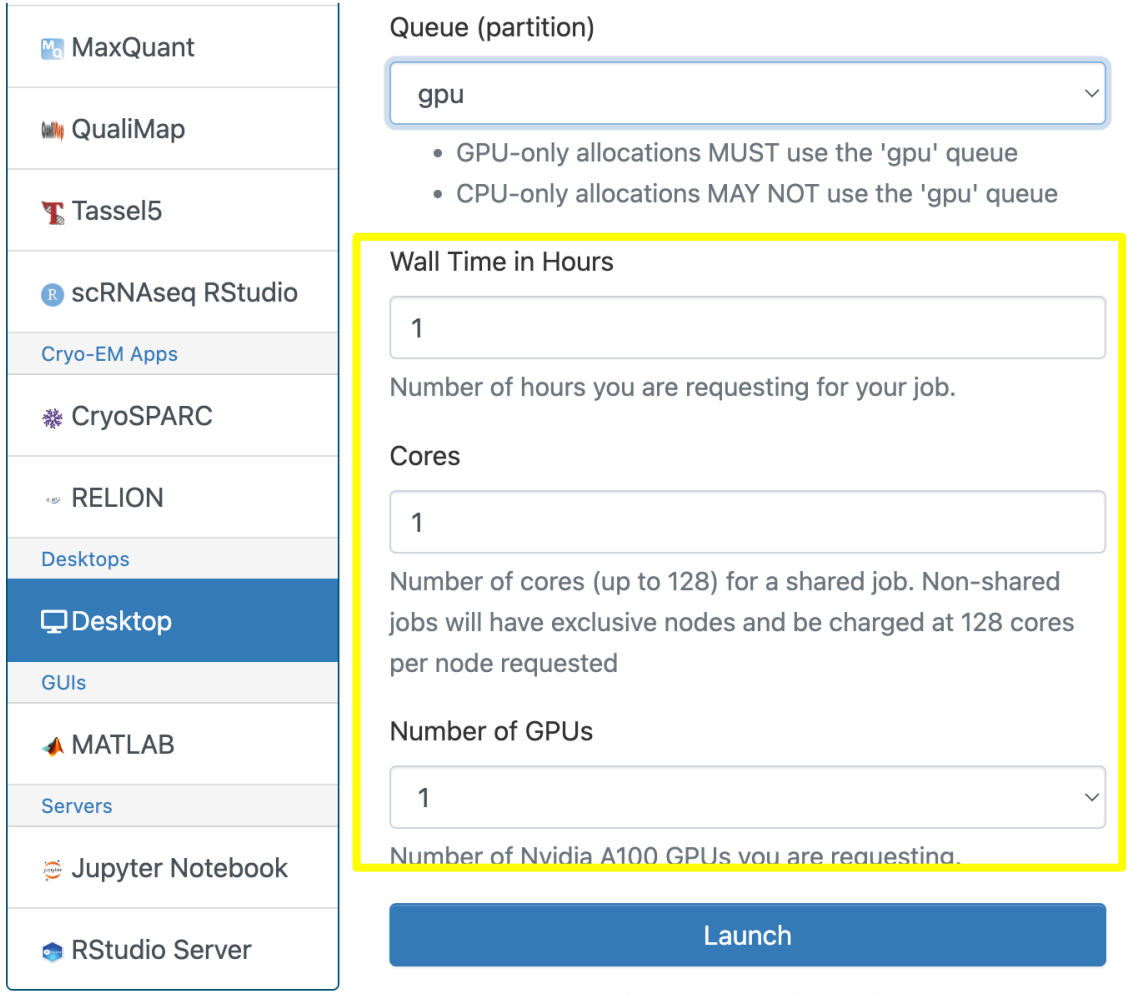


https://www.rcac.purdue.edu/knowledge/anvil/run/partitions

Using Open OnDemand: Applications

Application Forms

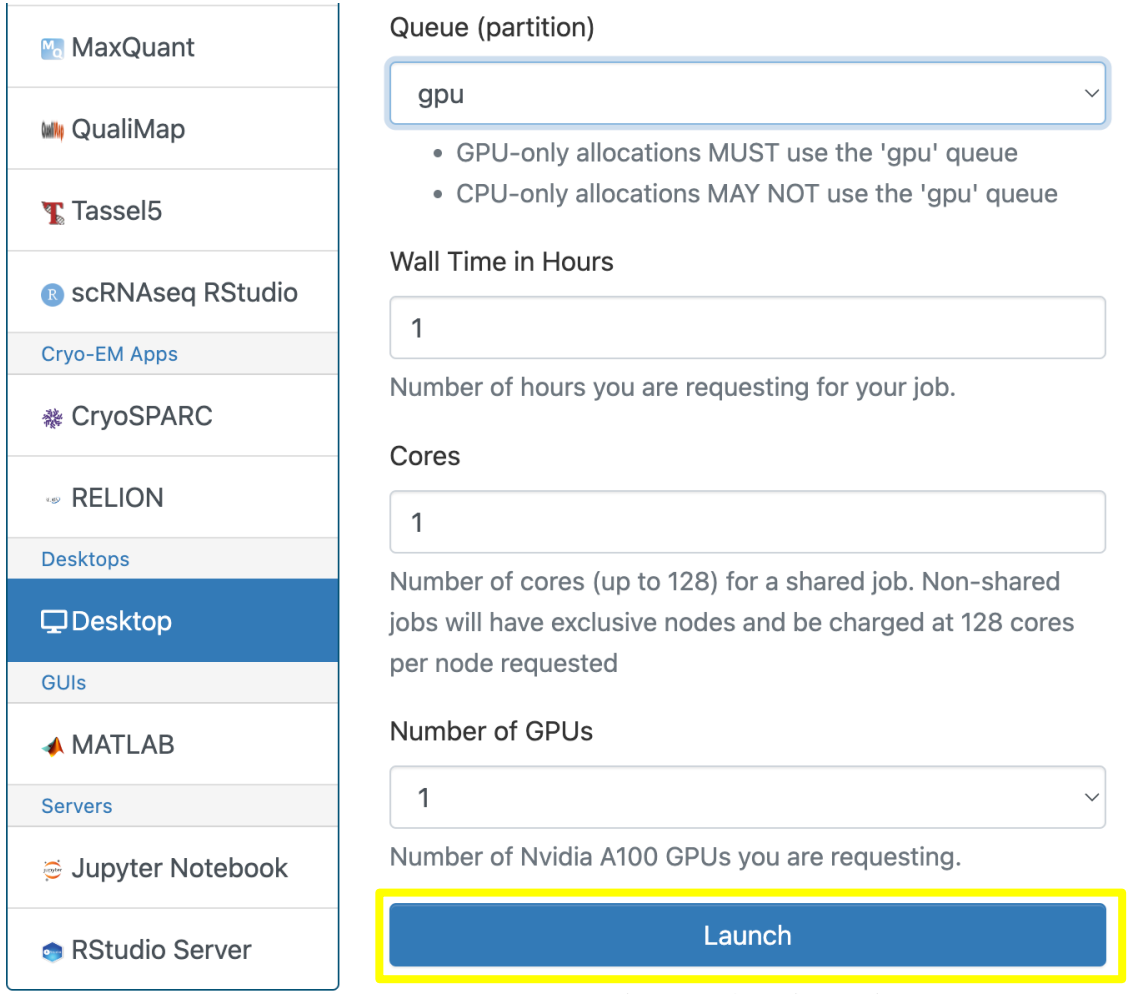
5. You must also specify the number/type of resources you wish to have allocated and for how long you intend to use them
   - You will be given memory proportional to the number of CPUs requested on the node type in the partition you select
     - Shared/Wholenode: ~2 GB/CPU
     - GPU: ~3.5GB/CPU
     - Highmem: 8GB/CPU



Using Open OnDemand: Applications

Application Forms

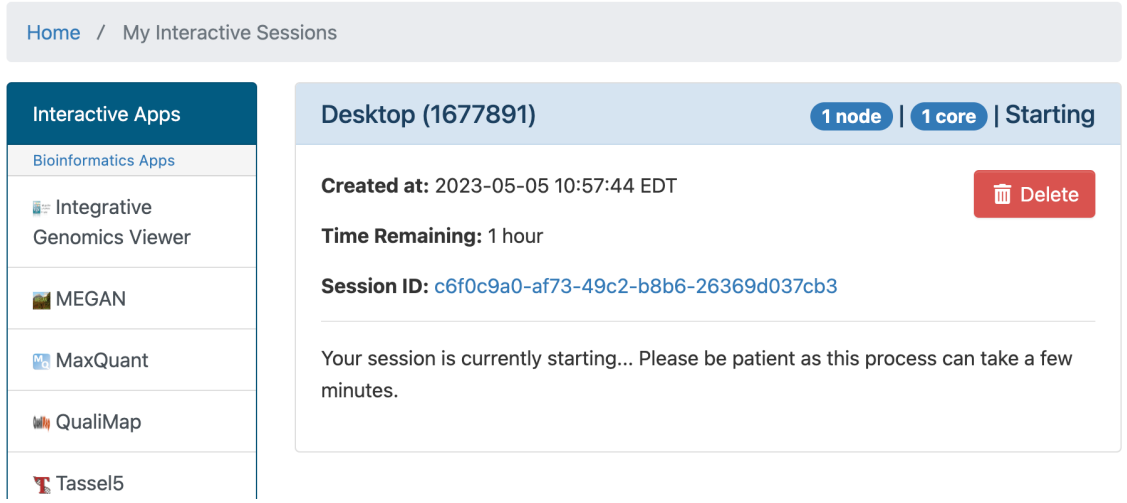
6. After selecting the options you would like for your session, click launch to send your request to the scheduler

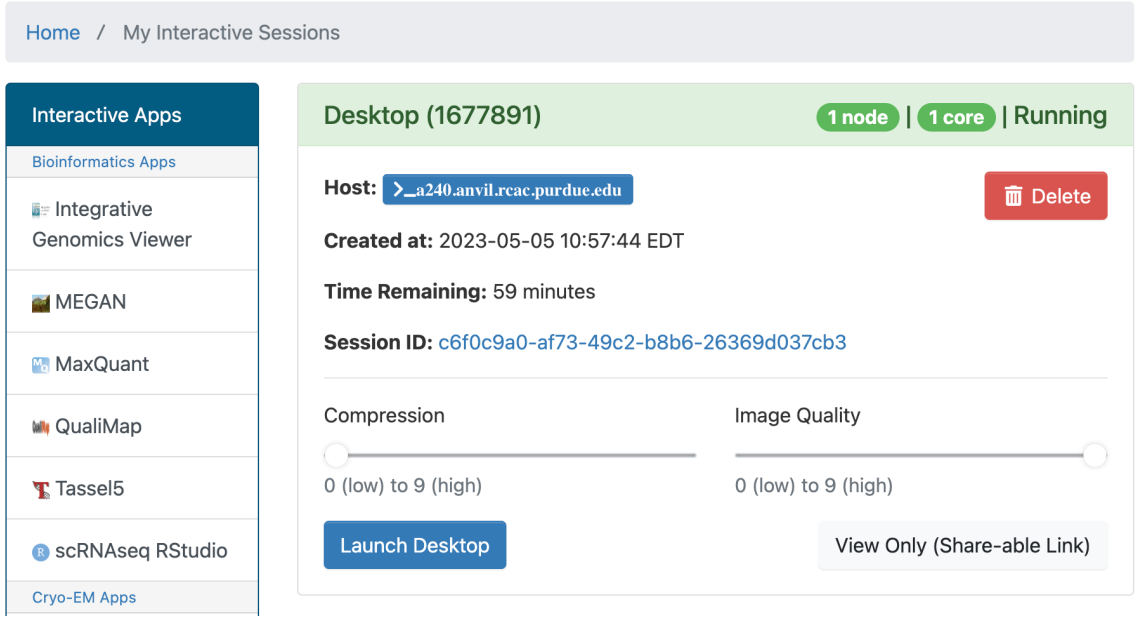


Using Open OnDemand: Applications

Application Forms

7. This will create a "card" for this session which will assign it two IDs
   - The first ID is the Slurm scheduler's job ID and is parenthesized next to the application name
   - The second ID is the Session ID and is the name of the directory where Open OnDemand will track information about the session
     - Clicking this session ID will open this directory in the File Explorer
   - When the scheduler finds resources for your job, the card will transform into the second image, and you can access the application by clicking the blue button labelled "Launch..."





Specific Applications: Compute Desktop

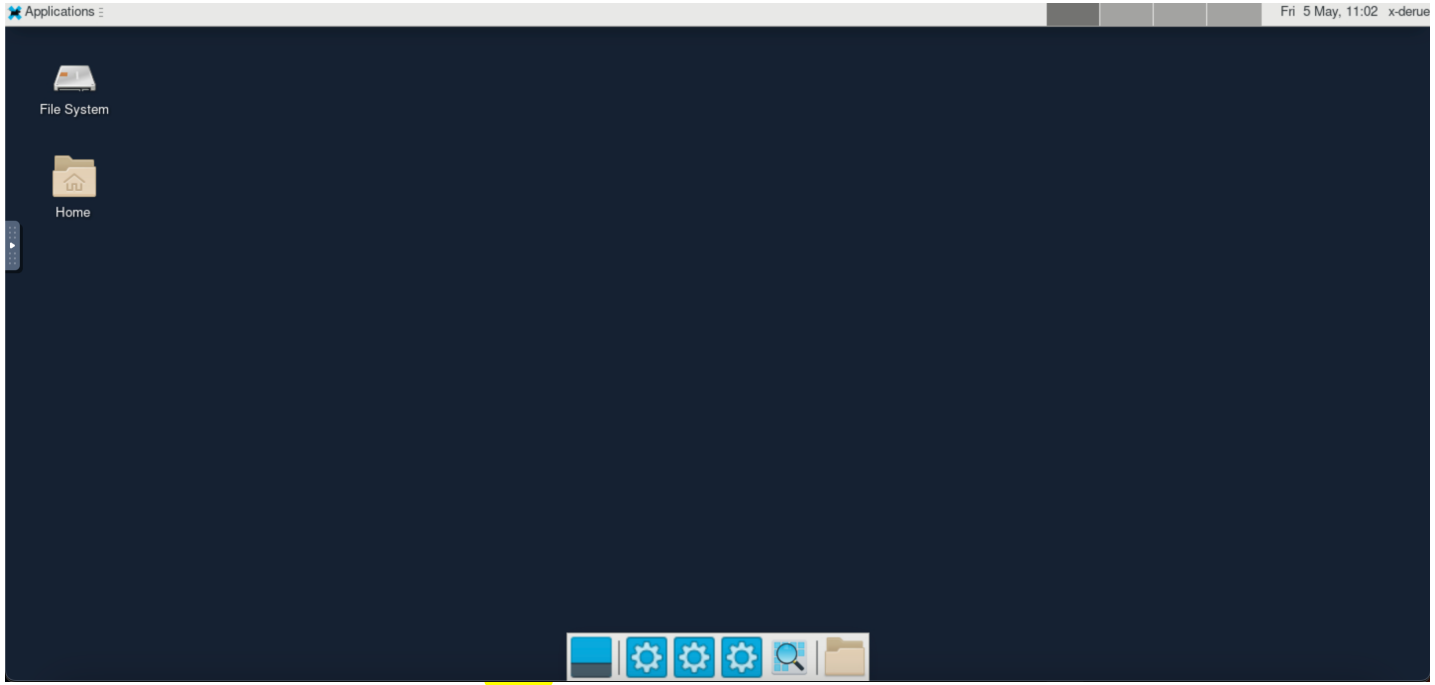
The Desktop application is an extremely useful application for interfacing with Anvil

- This application will launch a lightweight graphical desktop that you can use to interact with the HPC cluster as you would your own local workstation
- It includes a native file explorer, Firefox as an internet browser, a terminal, and a typical Desktop that you can save files to
- This application can be used to launch software that requires a GUI
  - This can be used on system-wide installations by RCAC as well as with software you personally install

Using Open OnDemand: Applications

Specific Applications: Compute Desktop

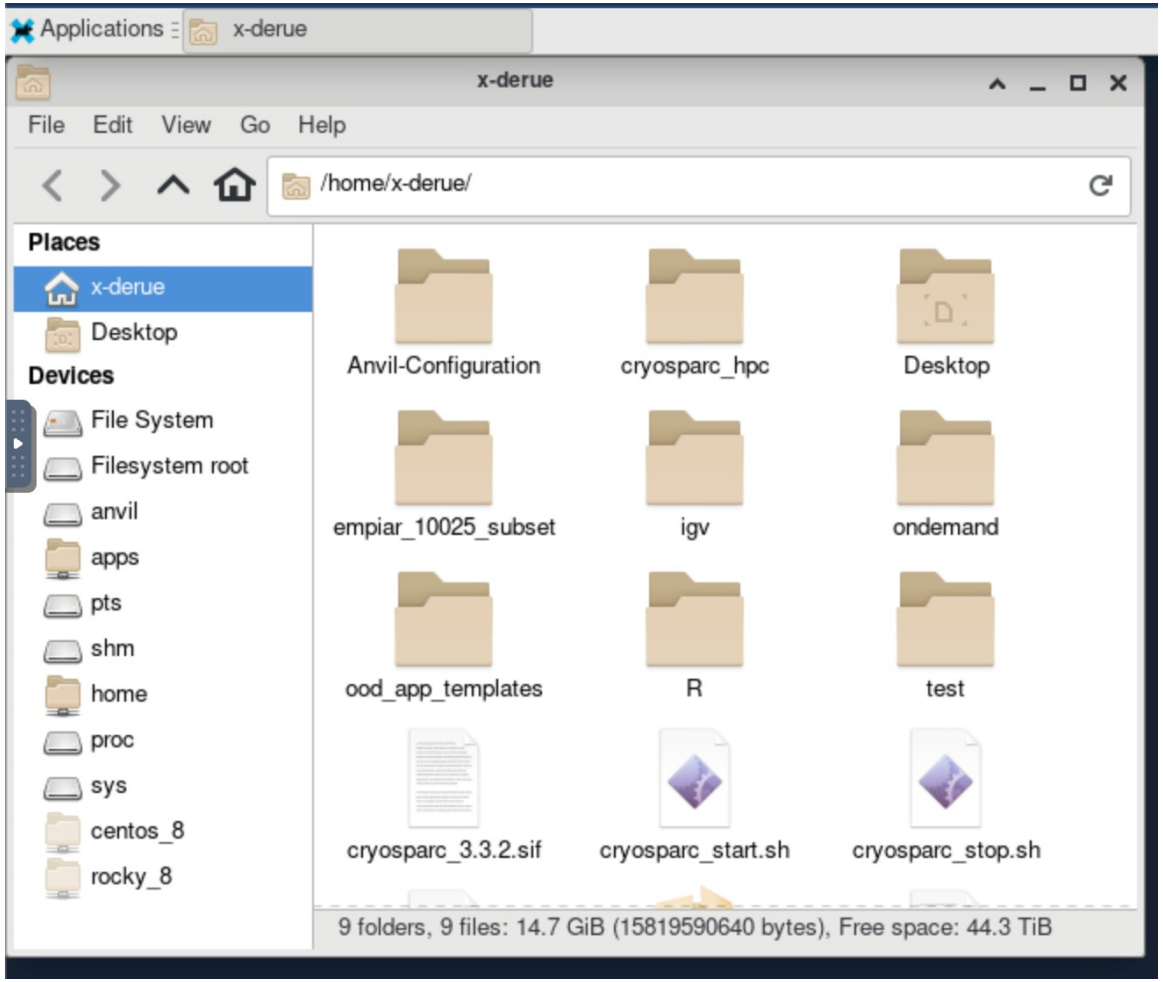
1. When you first launch the Compute Desktop, you will be presented with a desktop that appears as the one on the right
    - You can access your files by selecting the folder icon in the taskbar along the bottom, or by selecting the directory icon labelled “Home”.



Using Open OnDemand: Applications

Specific Applications: Compute Desktop

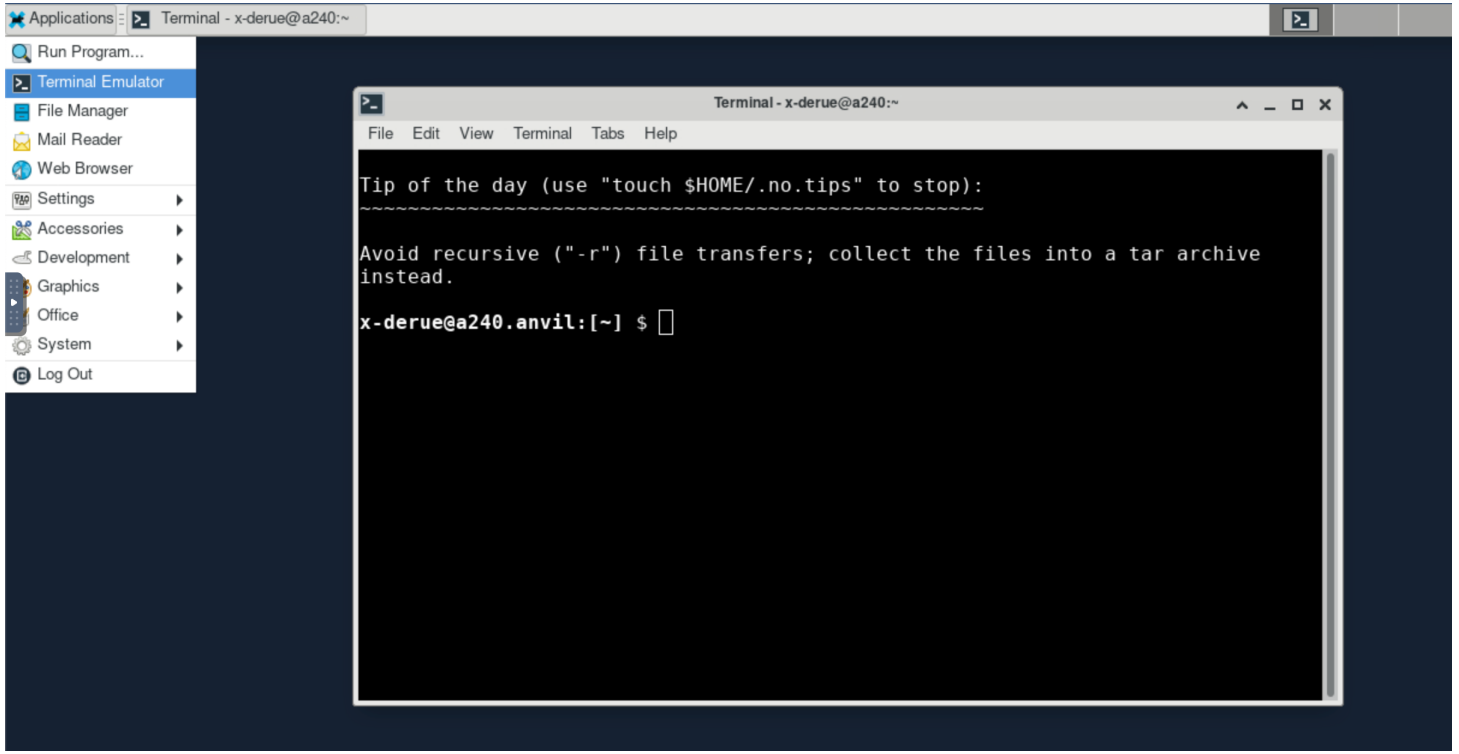
2. From this file menu, you can access any file on the cluster, but by default it will open to your home directory
   - You can change the directory you are viewing by clicking on other directories or by typing the absolute path into the search bar at the top



Using Open OnDemand: Applications

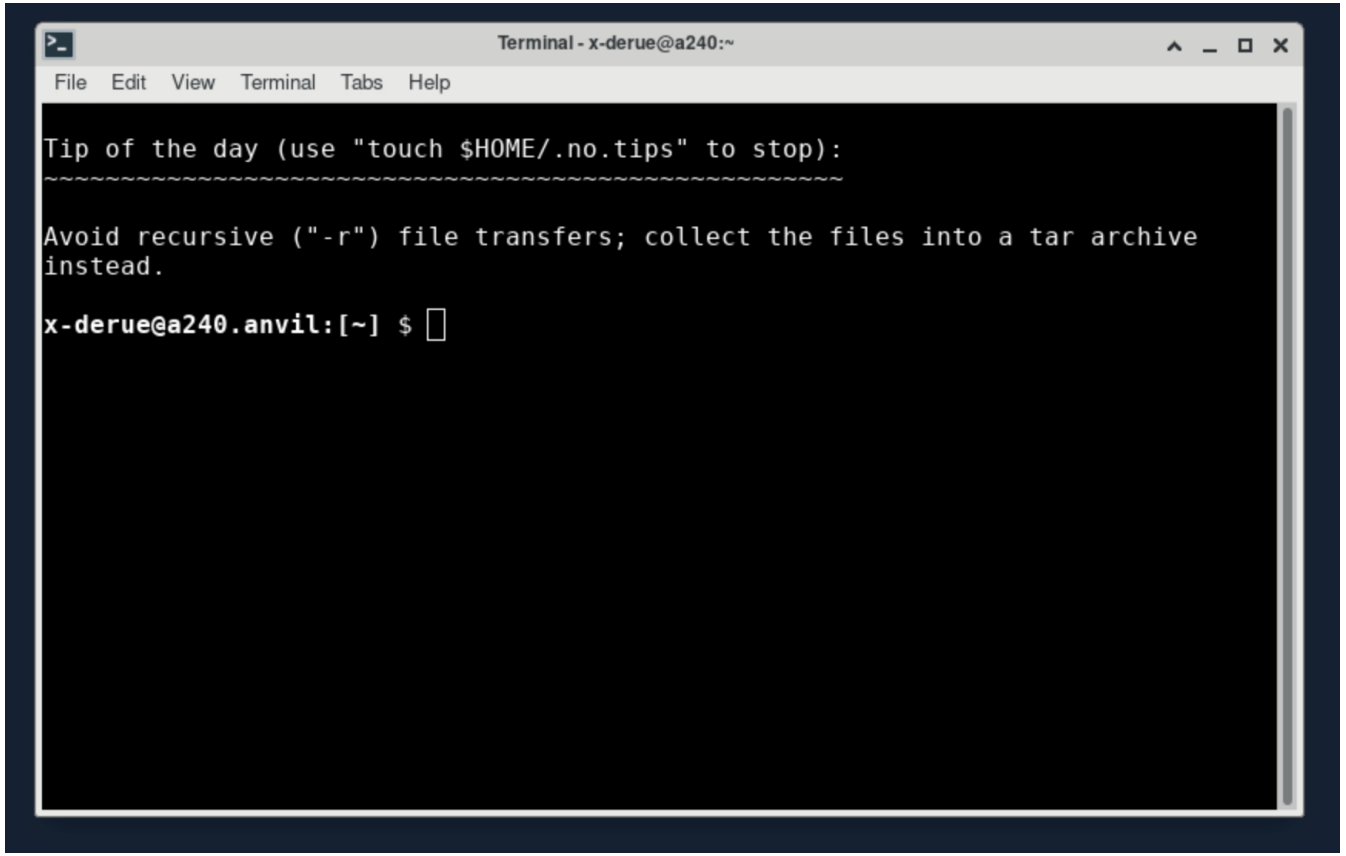
Specific Applications: Compute Desktop

3. You can launch a terminal on the desktop by selecting Applications menu in the top right, and then selecting "Terminal Emulator" from the sub-menu.
    - This is extremely useful for launching GUI applications from the command-line



Specific Applications: Compute Desktop

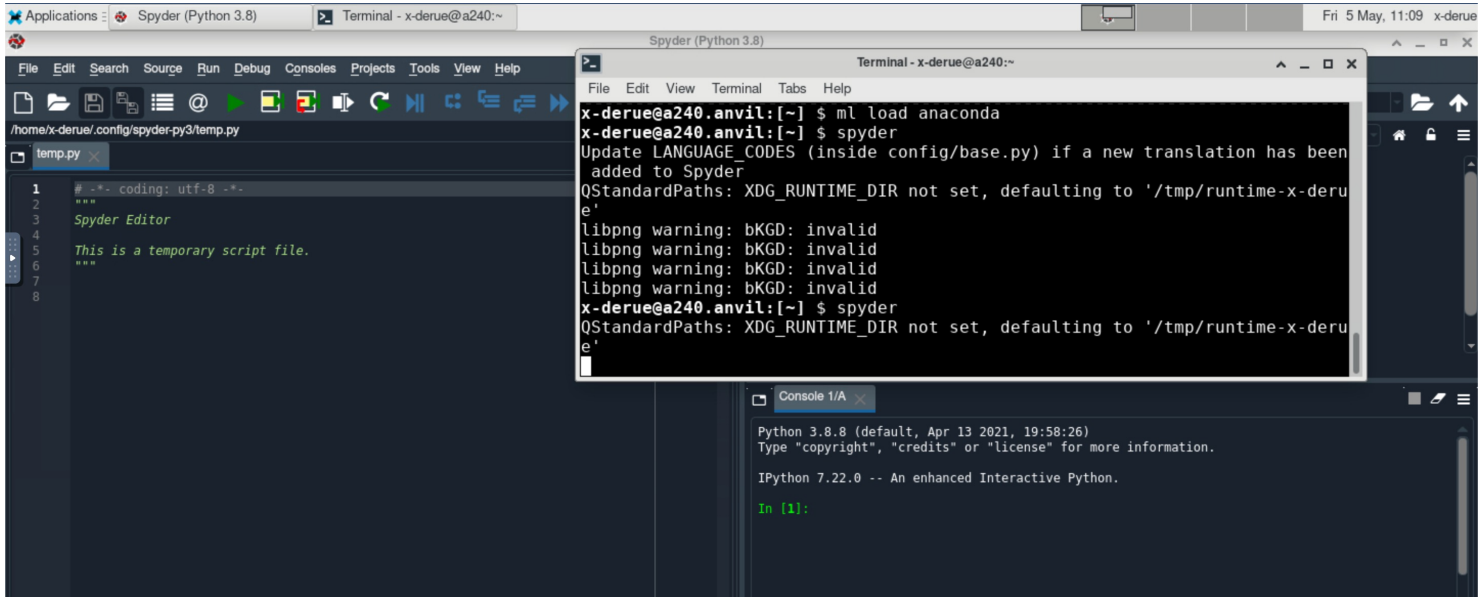
4. Notice that the prompt says that host is a240.anvil. This is the name of the compute node that we are on
   - If we were to try to do the same thing through ThinLinc (desktop.anvil.rcac.purdue.edu), which provides a similar interface, the terminal would indicate that we are on a login node (not a compute node) with a label of loginXX.anvil.



Using Open OnDemand: Applications

Specific Applications: Compute Desktop

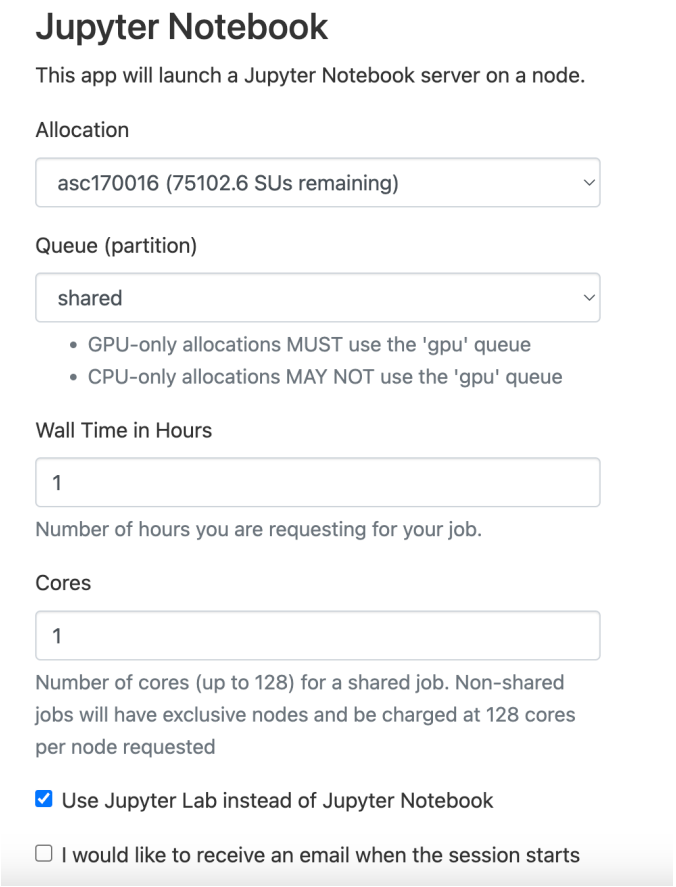
5. By loading a module (anaconda) for software that I know provides a GUI, I can launch that GUI by typing the name of the command to do so.
   - Usually, you can find such commands in the user manual for software you personally install
   - This allows me to run scientific software the same way many users do on ThinLinc, but I get all the resources dedicated to my application which improves performance!



Using Open OnDemand: Applications

Specific Applications: Jupyter

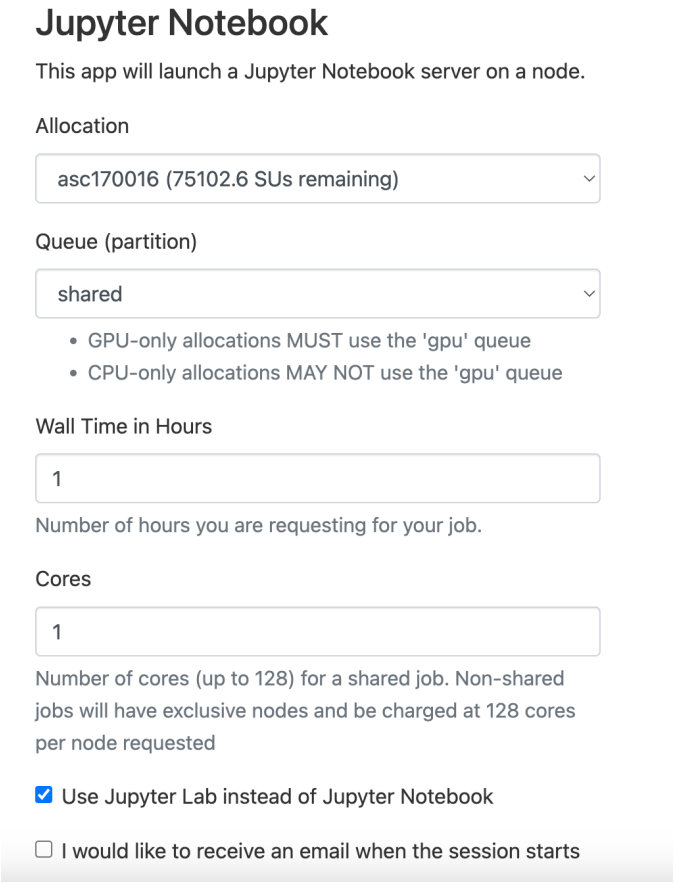
1. Jupyter is by far the most popular application for Open OnDemand on Anvil
   - Very useful application for interactive work with languages like Python, R, Julia, etc.
   - App form is very similar to the previous one, but it does have an option to select whether you want to run “Jupyter Lab” or “Jupyter Notebook”.
     - Notebook is the original Jupyter application and is a more bare-bones method of using Jupyter



Using Open OnDemand: Applications

Specific Applications: Jupyter

2. We have installed a few system wide Jupyter kernels for Python as well as R.
   - You cannot install additional packages into these kernels, but you can create your own anaconda environment containing the packages you want
   - For more information about how to expose your anaconda environments to Jupyter see our knowledge guide article on the topic.

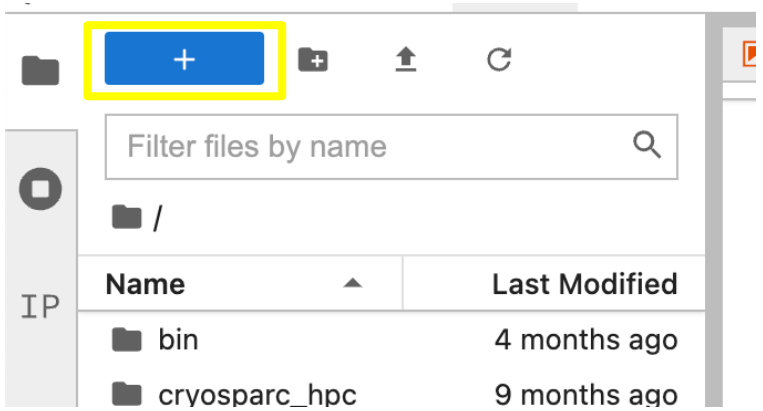


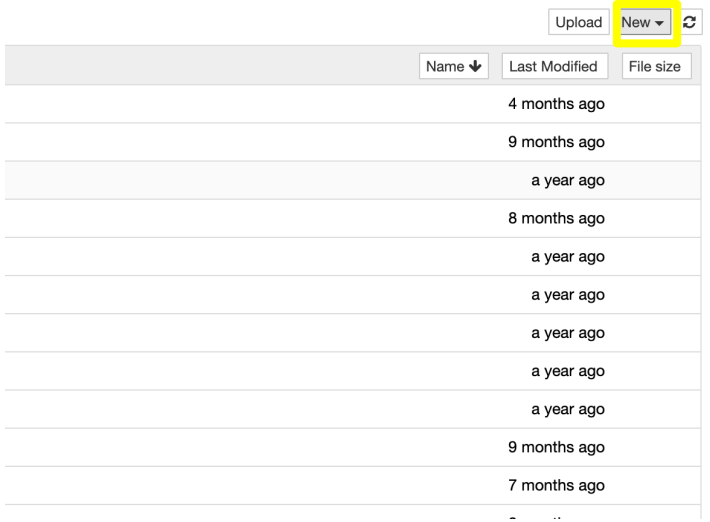
https://www.rcac.purdue.edu/knowledge/anvil/run/examples/apps/python/packages

Using Open OnDemand: Applications

Specific Applications: Jupyter

3. Regardless of whether you choose to use Jupyter Notebook or Jupyter Lab, it will open to your home directory.
   - To create a new notebook in Jupyter Lab click the blue “+” button in the top left corner (Shown in the top-most picture)
   - To create a new notebook in Jupyter Notebook, select the ”New” button in the top right corner. (Shown in the bottom-most picture)

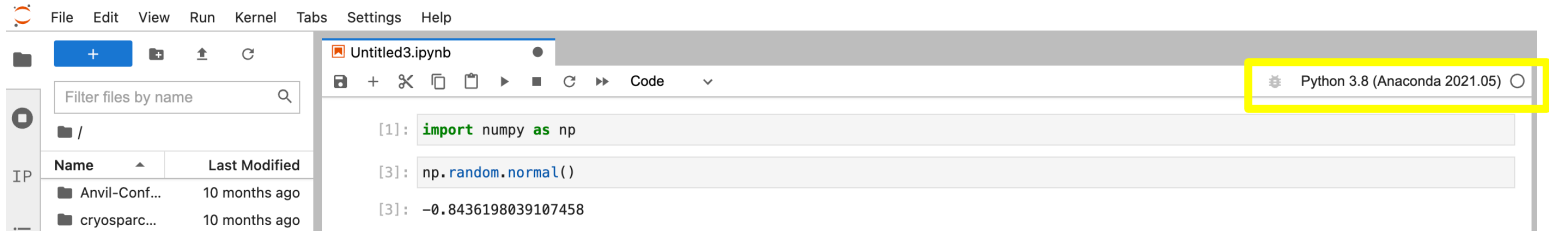


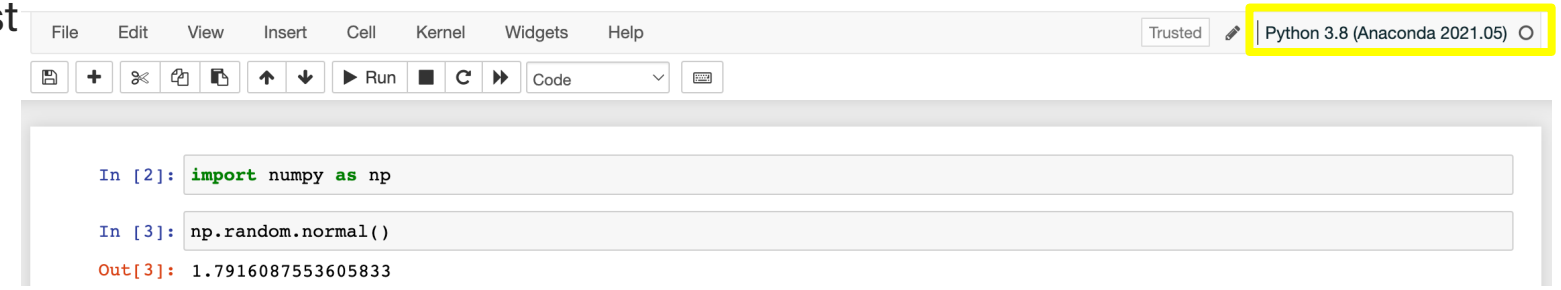


Using Open OnDemand: Applications

Specific Applications: Jupyter

4. After we have created a new notebook, we will be presented with our new notebook in an interface shown to the right
   - Jupyter Lab is shown in top-most picture and Jupyter Notebook shown below that
   - To select the kernel you wish to use, click on the name of the kernel shown to the right in a yellow box, and an option to select a new kernel will appear





OOD 101

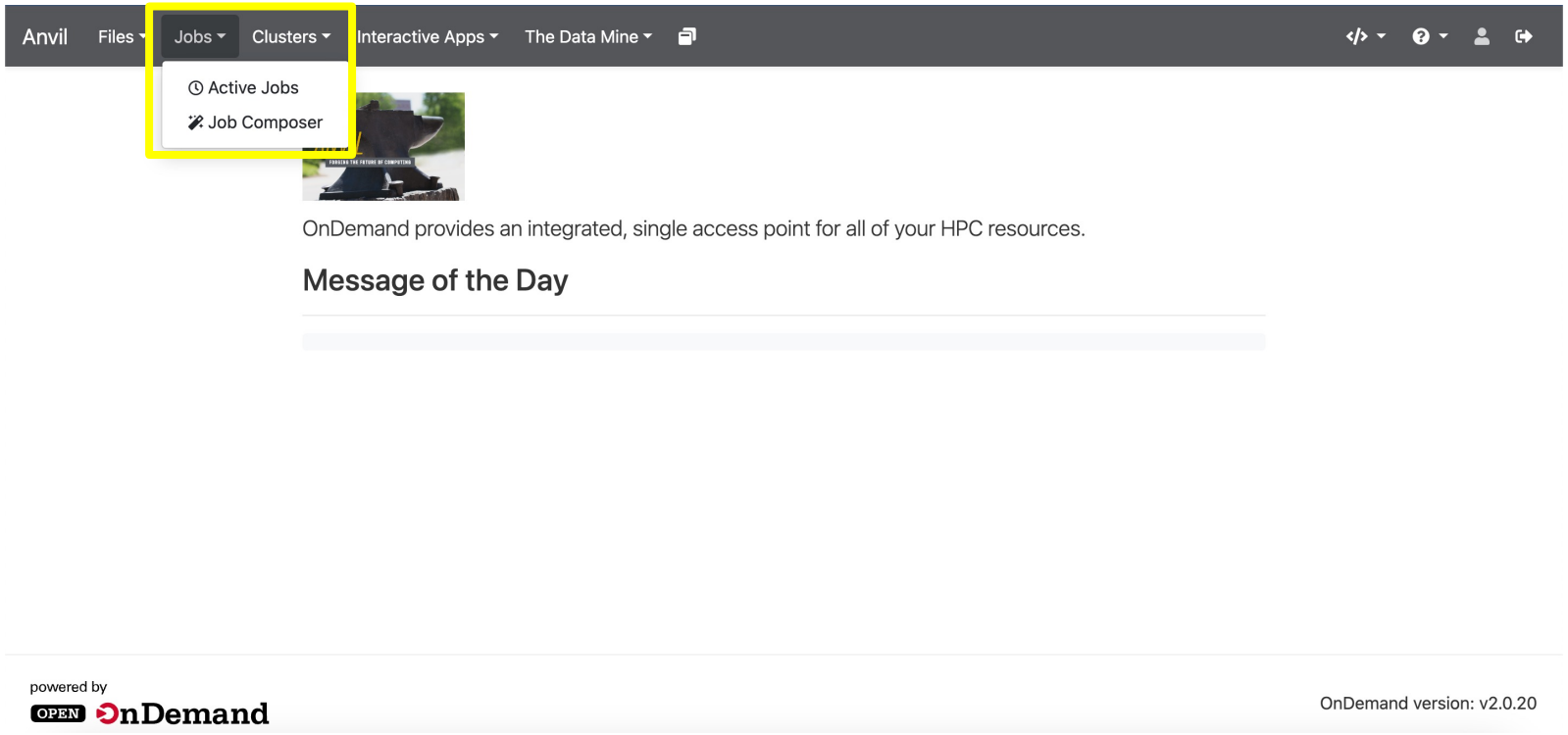
Using Open OnDemand: Job Composer

Using Open OnDemand: Job Composer

A Widget For Talking to the Scheduler

Often, we may also want to run non-interactive jobs. In such cases Open OnDemand provides an interface for creating such jobs as well as monitoring your interactive and non-interactive jobs.

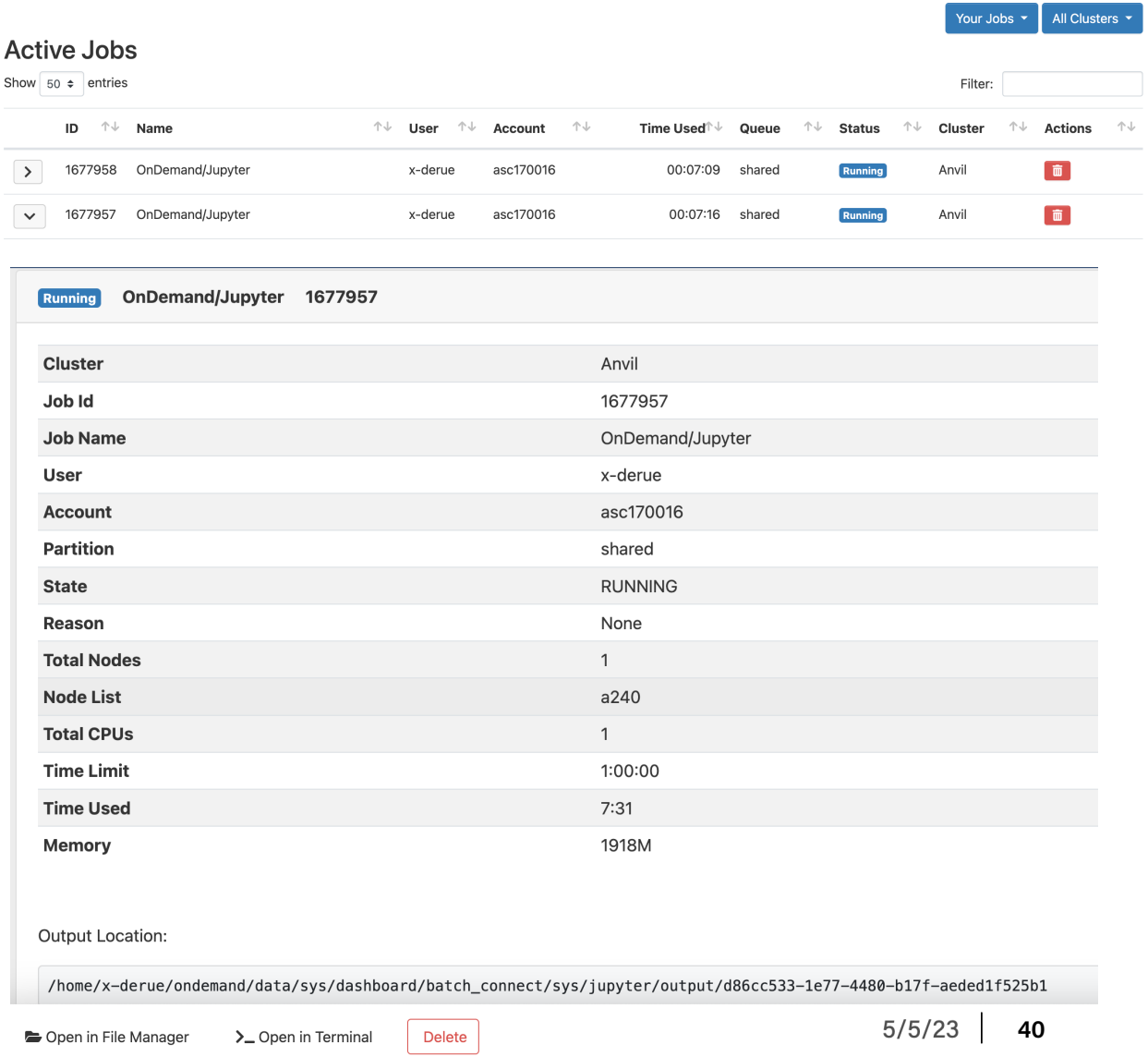
We can access these tools using the Jobs menu



Using Open OnDemand: Job Composer

A Widget For Talking to the Scheduler

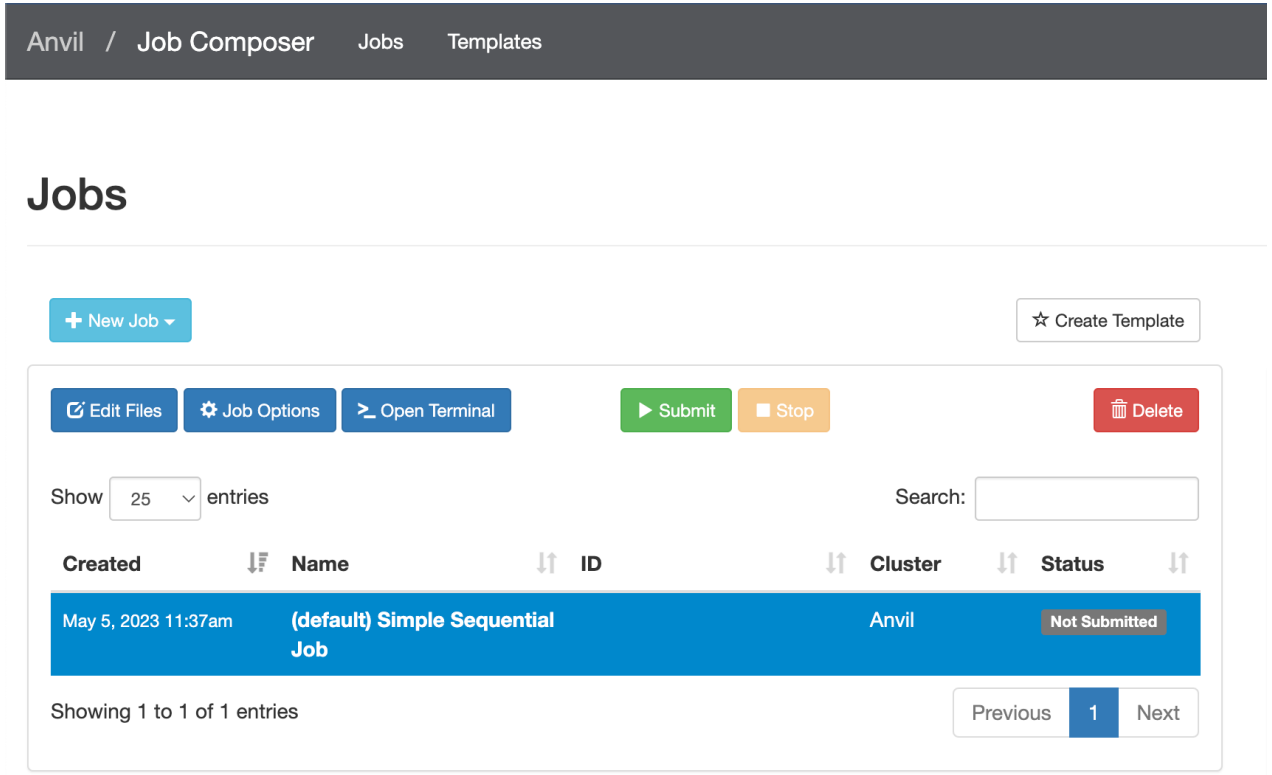
1. The Active Jobs widget will allow you to query certain usage statistics from the scheduler that you would otherwise need to do through the command line interface (CLI)
   - When a job fails due to an error, this is a useful tool to discover what may have happened
     - You can look at the amount of memory that was requested to see if perhaps there was an out of memory error
     - You can also use the “Open in File Manager” button to view the output.log file that may contain information about the error that occurred



Using Open OnDemand: Job Composer

A Widget For Talking to the Scheduler

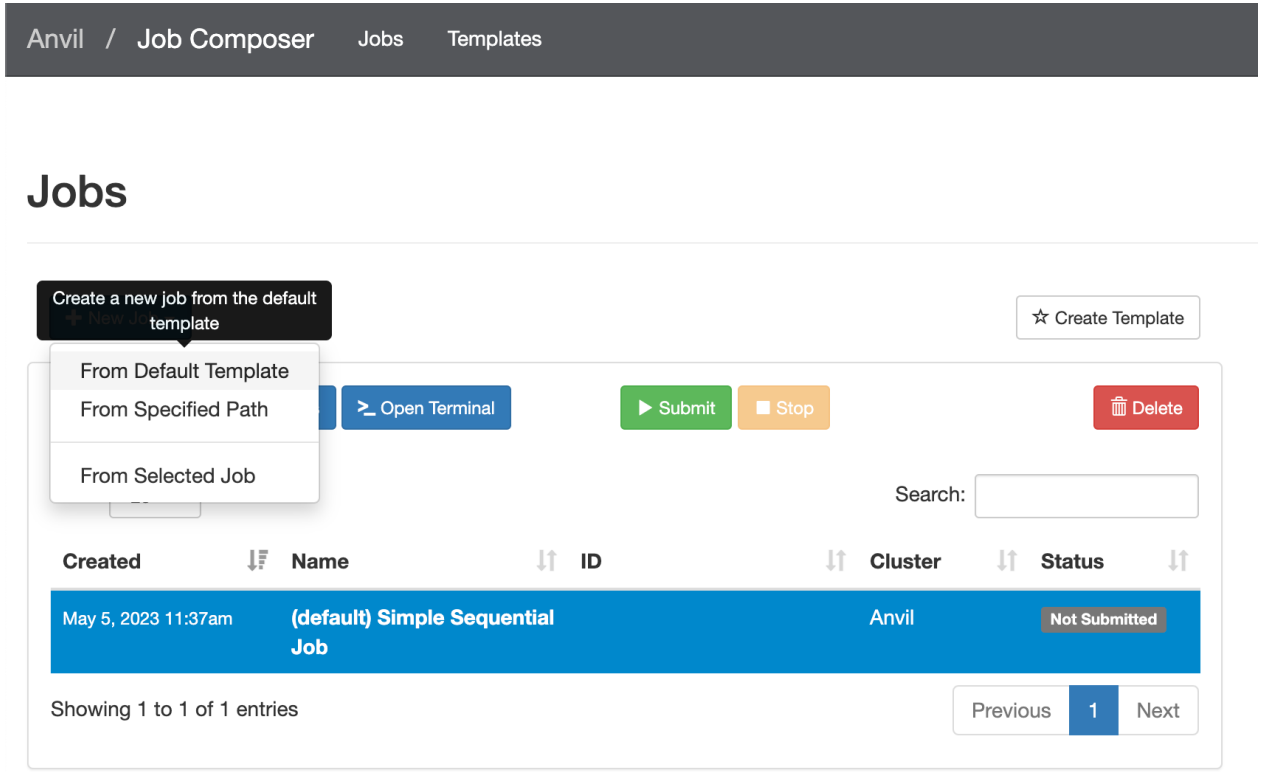
2. The Job Composer widget is used for submitting non-interactive jobs to the scheduler. This is very useful when you have some work to accomplish as part of your workflow that doesn't need to be done interactively.
   - An example of this might be post processing the output of some work that was generated interactively
   - This tool provides a simple default template for submitting a "Hello World" job script, but allows you to save template job scripts for workflows you may regularly repeat



Using Open OnDemand: Job Composer

A Widget For Talking to the Scheduler

3. Selecting the "+ New Job" button will allow you to begin working on creating a new job either from one of your existing templates, or from the default hello world template.
   - This will create a new entry in your table of jobs with a status of "Not Submitted"



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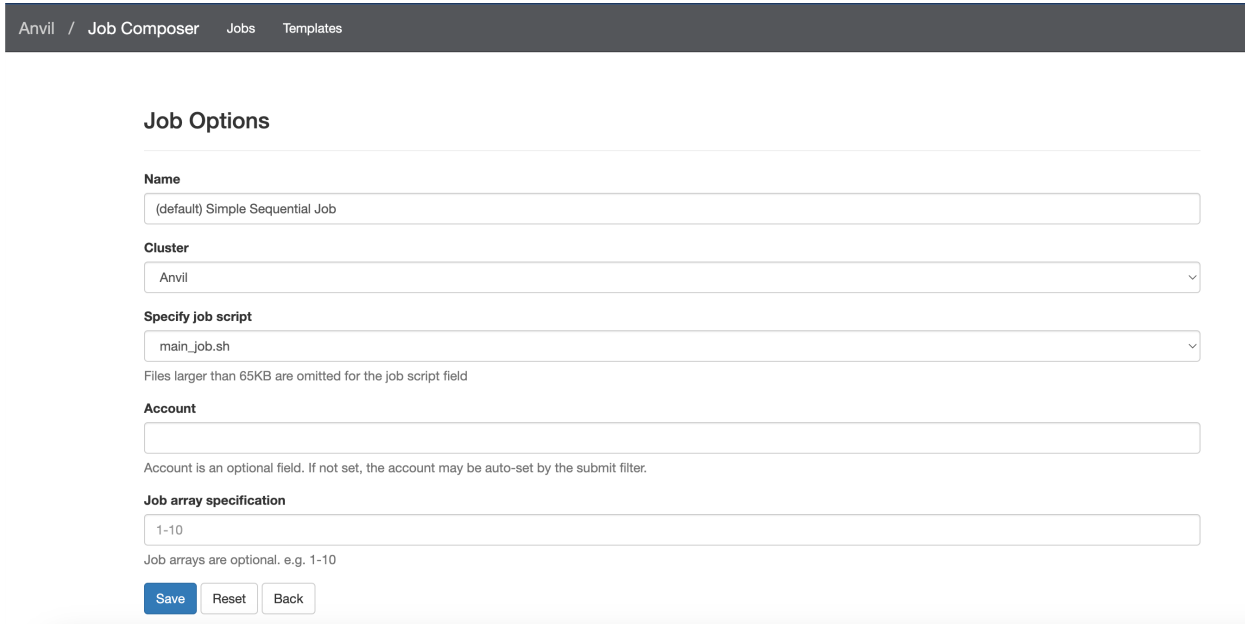
4. If we select the newly created job in the table, we can then click on the “Job Options” button to bring up configurable options for that job.
    - The most important fields here are the job name, which is for your own reference, and the “Account”
        - “Account” is the name of your allocation. You can enter the name of one of the queues which you are able to select from the Allocation dropdown on any of the app forms



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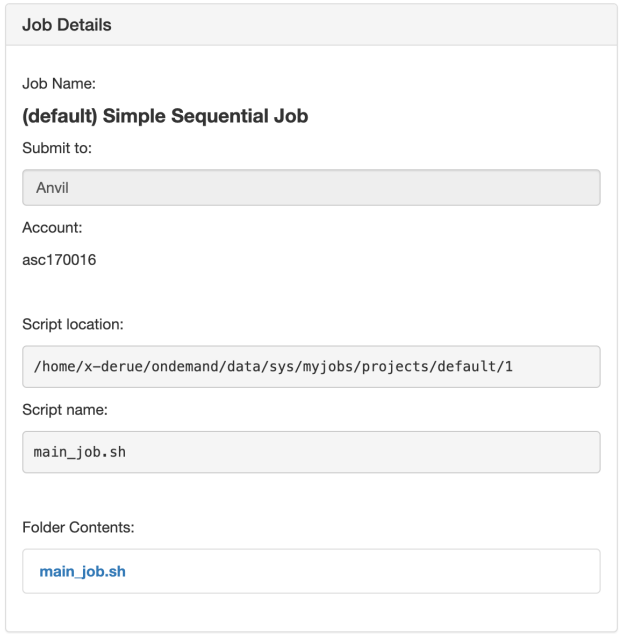
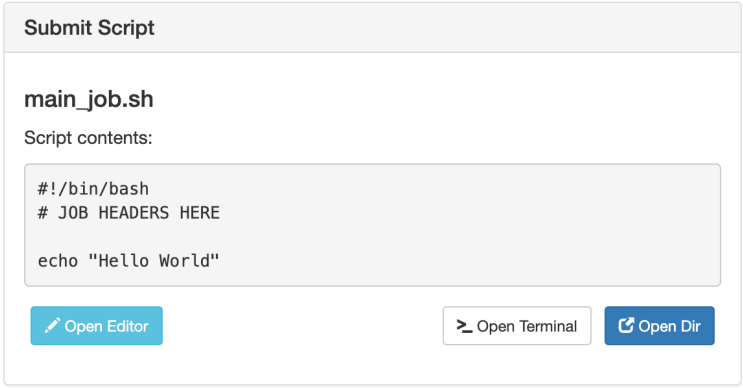
5. After saving the job options, we can scroll along the boxes on the right side of the table to do two things
   - We can see some details about the job
   - We can edit the job script that this job will run
     - This is the most important part of this workflow because this is defining what we want our non-interactive job to do
     - Select “Open Editor” to change the contents of this script





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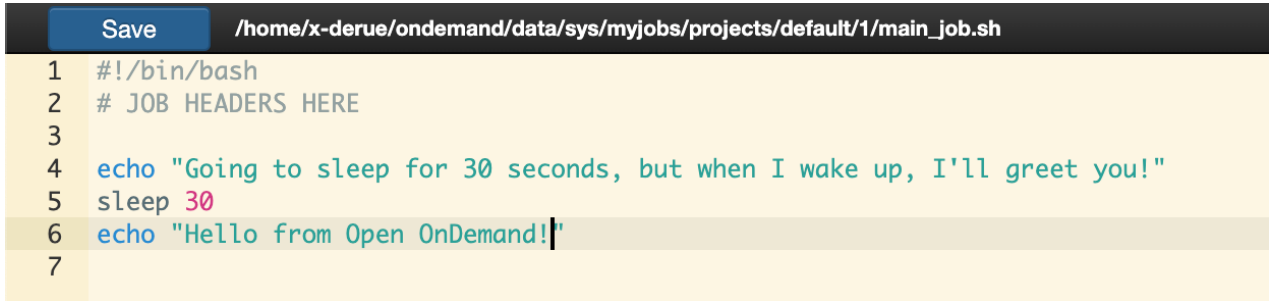
6. Within your job script, you will want to put all the commands which you want to be ran as part of the job, as well as any options to Slurm, and then hit “Save”
   - For more information about how to do this, see the user guide page for example Slurm job scripts



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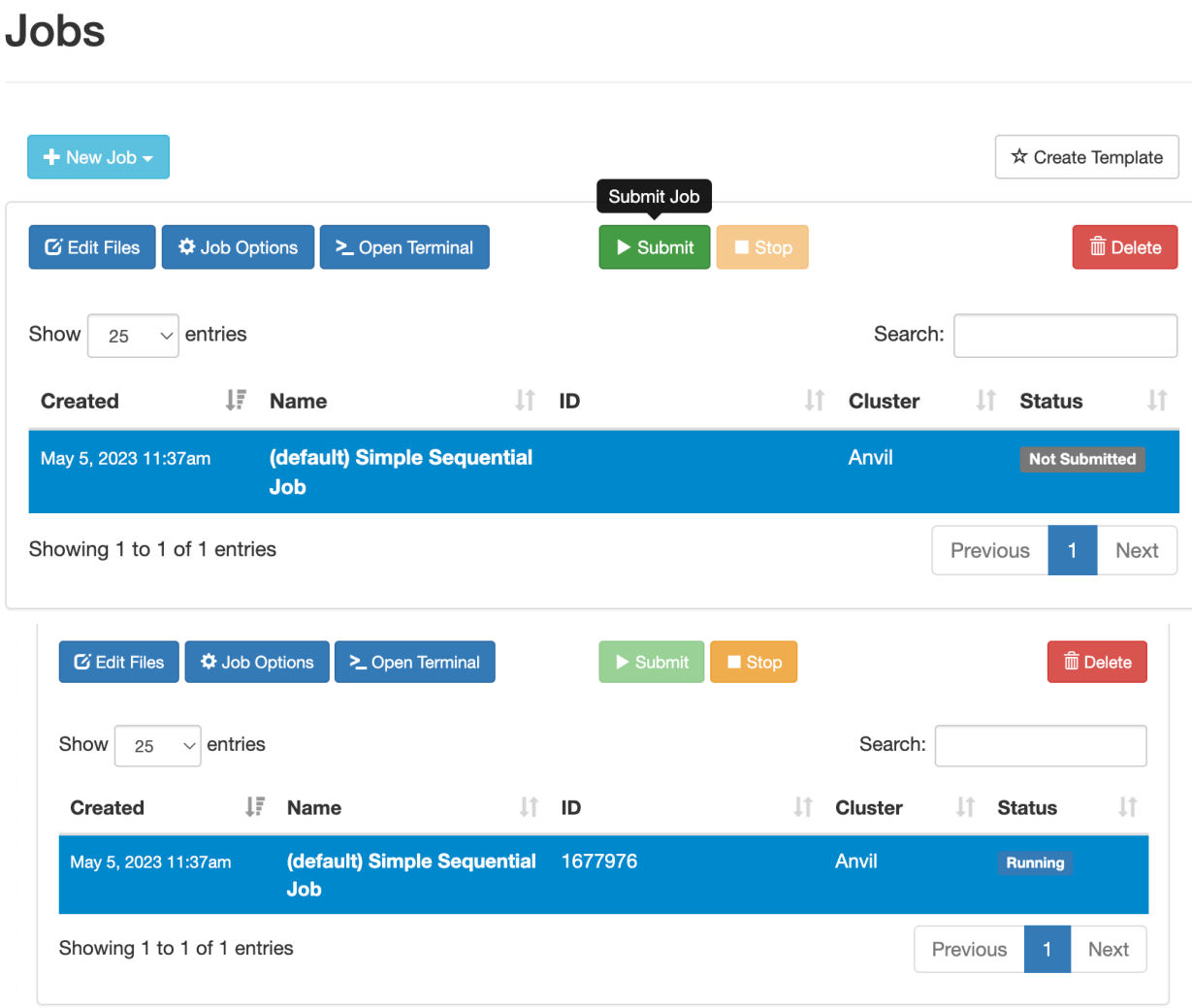
7. After we have made our edits to the job script, we can close this tab and return to the job composer page. Now all that remains is to select this job and hit submit!
   - After this point the status of the job updates from “Not Submitted” to “Running”, and when the job terminates, this will update finally to “Completed”



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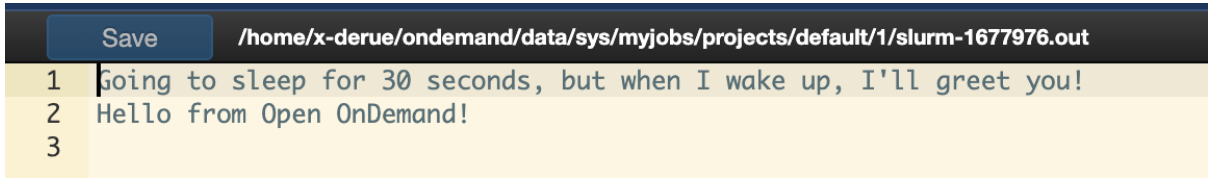
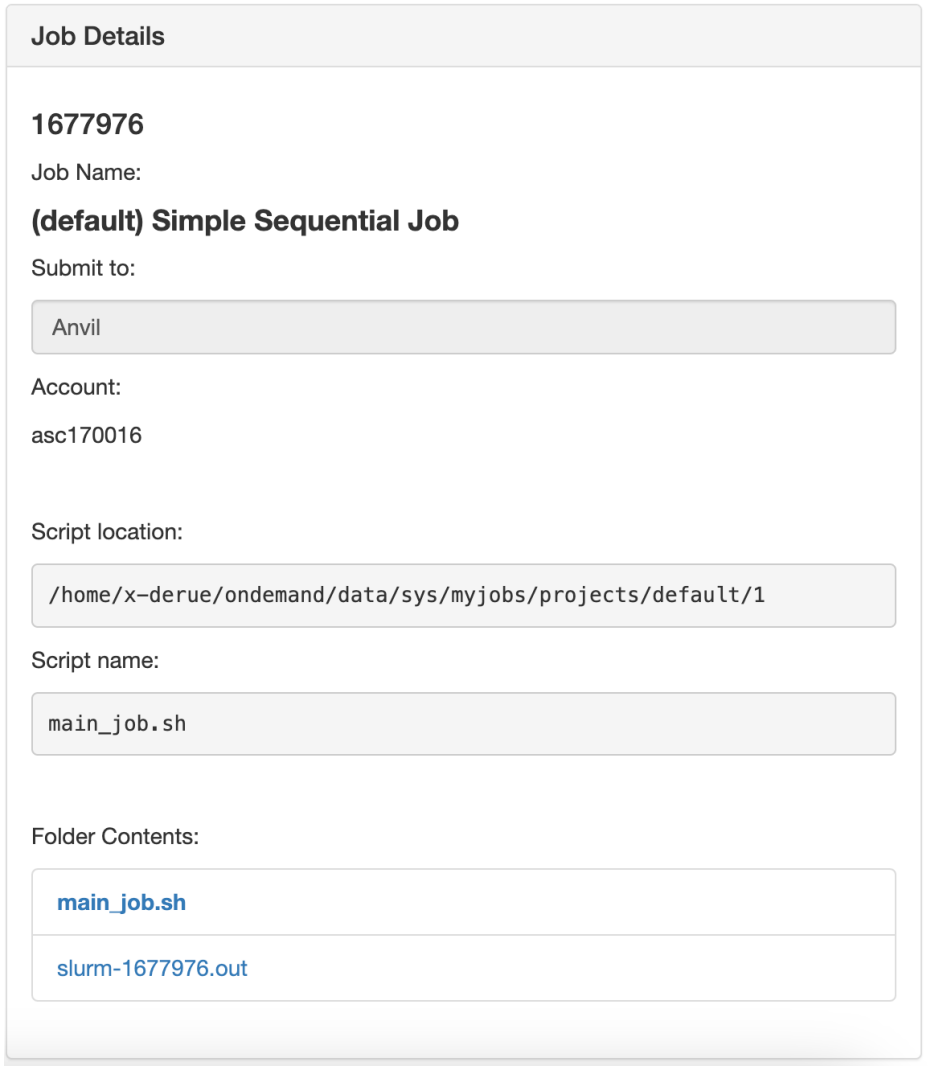
8. After the job completes, we can view the job details along the right-hand side of the page
    - We see that the “Folder Contents” has been updated with a new output file: “slurm-2677561.out”
        - If we click the link to this file, we will see that our job successfully generated the expected output:





OOD 101

Conclusions

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- Open OnDemand helps to lower the barrier of entry to HPC for domain scientists seeking to do computational work
- We can use Open OnDemand to manage our directories as well as transfer files to/from the cluster
- Open OnDemand is especially useful for running interactive style jobs that require a graphical user interface
- We can use Open OnDemand to manage our non-interactive jobs as well

OOD 101

Questions?

THANK YOU

Feel free to reach out to rderue@purdue.edu with questions.

Slides are posted at: https://www.rcac.purdue.edu/training/