

OPEN ONDEMAND 101

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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

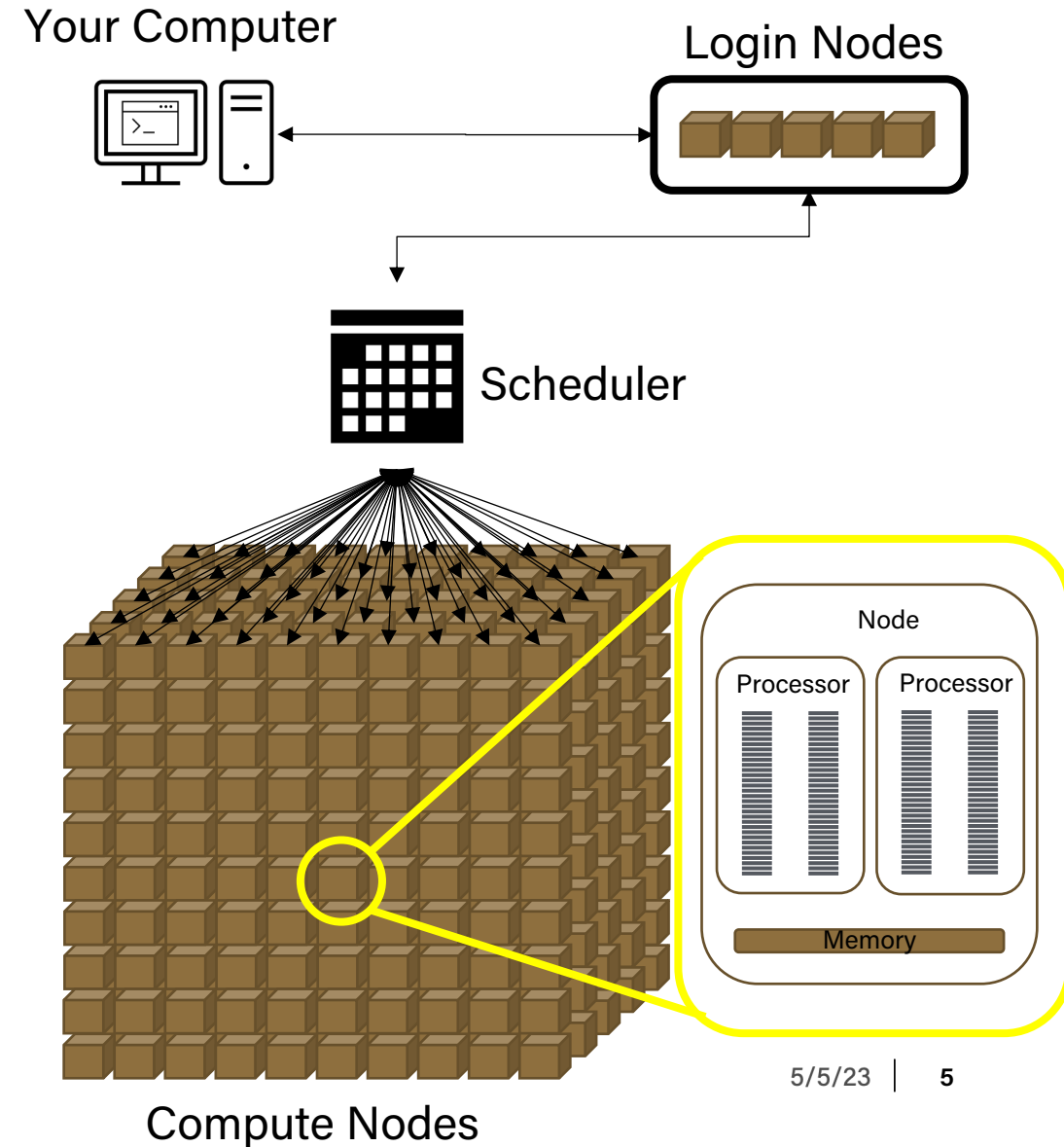
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Lowering the Barrier to HPC

Lowering the Barrier to HPC

Layout of a Cluster

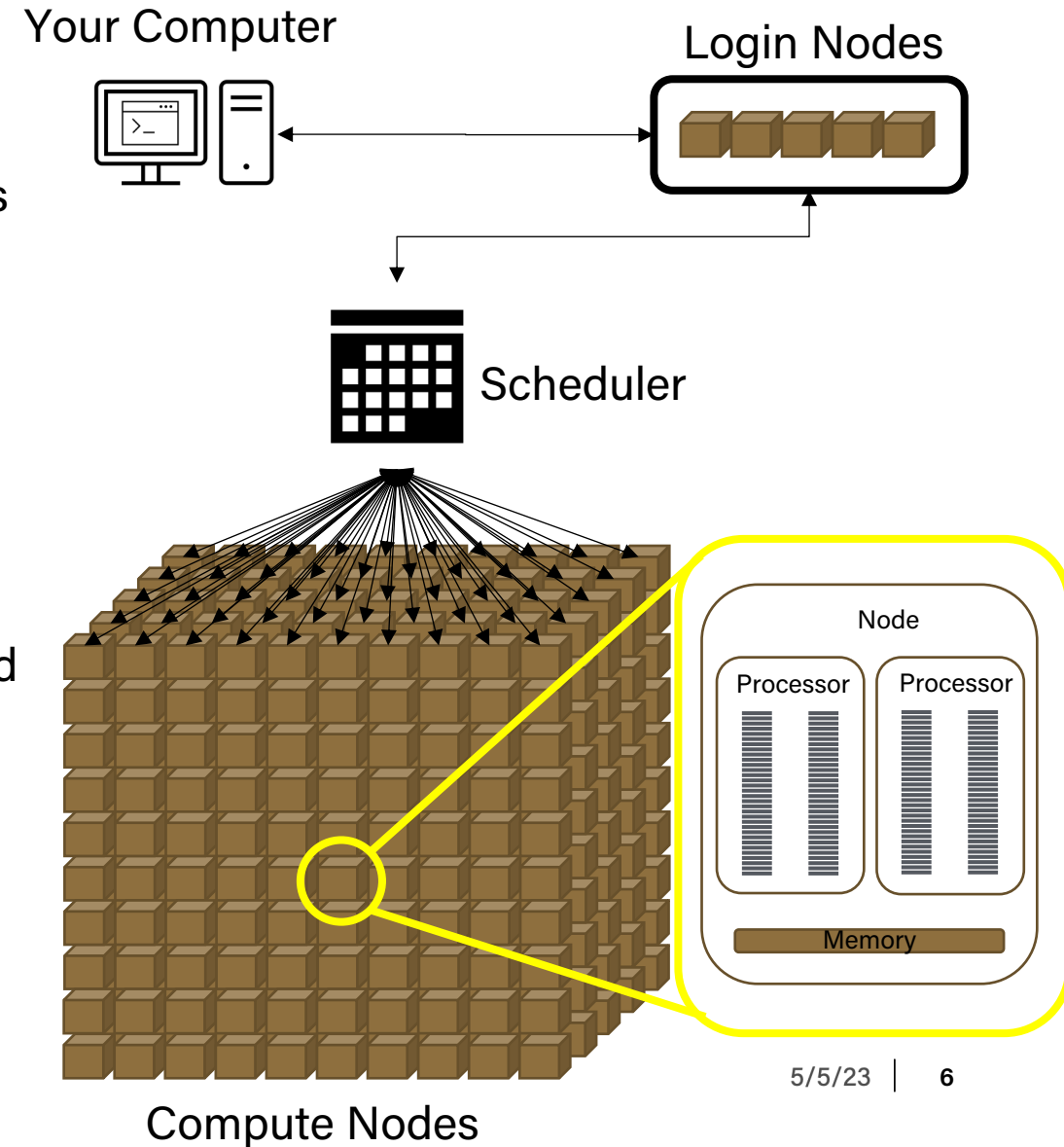
- HPC systems are often organized into clusters
 - We call them clusters because they are a multitude of independent nodes that can communicate with one another
 - Because each node is independent, we can have different types of nodes with specialized hardware
- When you login to a cluster, typically 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

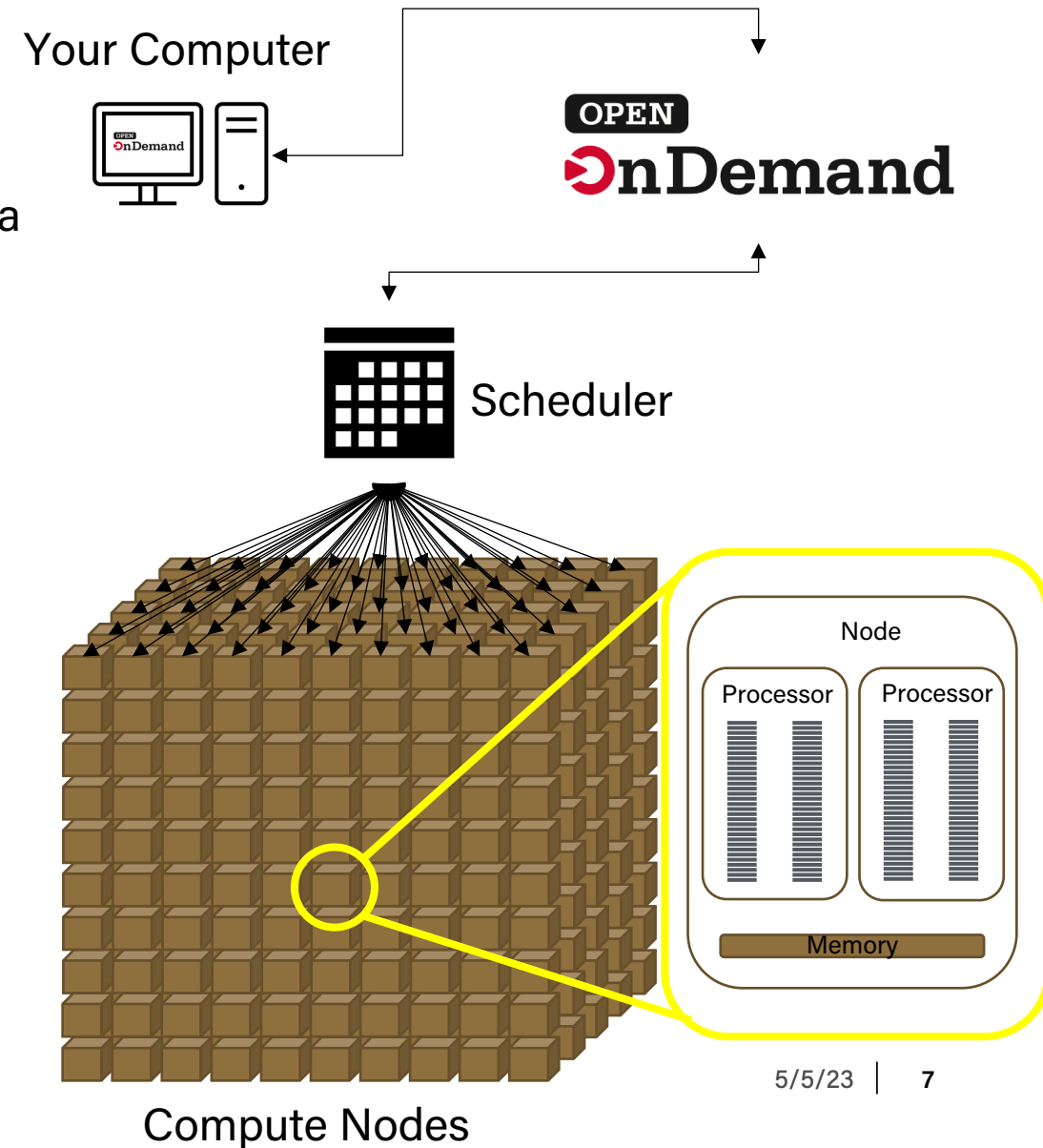
- Working within HPC in this traditional manner presents many challenges to new users
 - Typically use an SSH client/Linux terminal
 - Learning new commands for interacting with the scheduler
 - Software runs without a graphical user interface (GUI)
- This can lead to new domain scientists spending most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



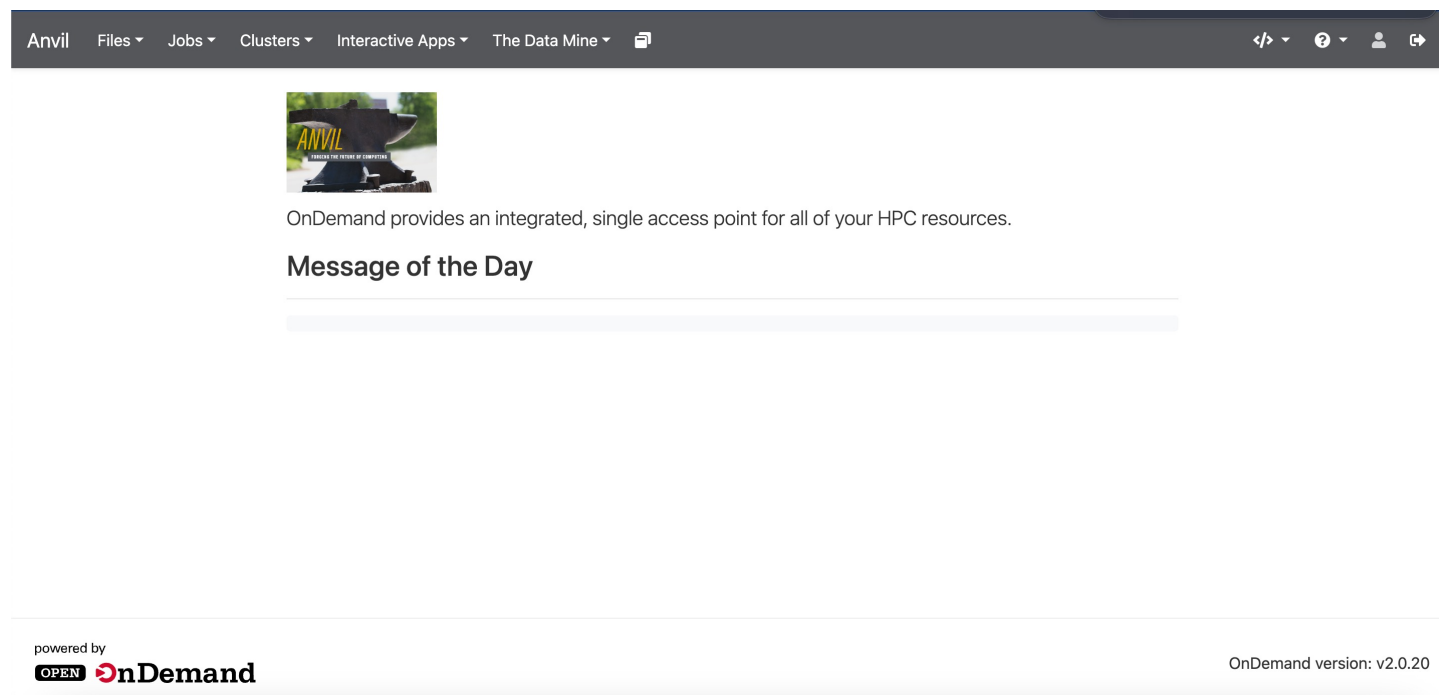
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Using Open OnDemand: Dashboard

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



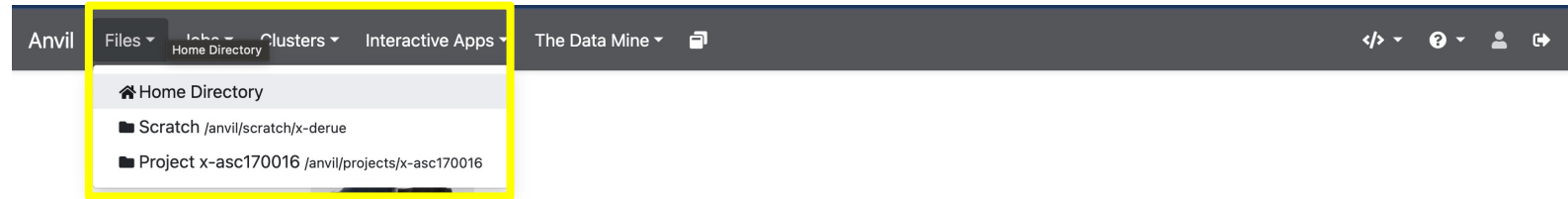
The screenshot shows the Open OnDemand dashboard interface. At the top, there is a navigation bar with the following items: Anvil, Files, Jobs, Clusters, Interactive Apps, and The Data Mine. Below the navigation bar, there is a central area with a logo for ANVIL (Advanced National Virtual Infrastructure Laboratory) and the text "OnDemand provides an integrated, single access point for all of your HPC resources." Below this, there is a section titled "Message of the Day" with a horizontal line underneath. At the bottom of the page, there is a footer that says "powered by OPEN OnDemand" and "OnDemand version: v2.0.20".

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



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

Message of the Day

powered by
OPEN OnDemand

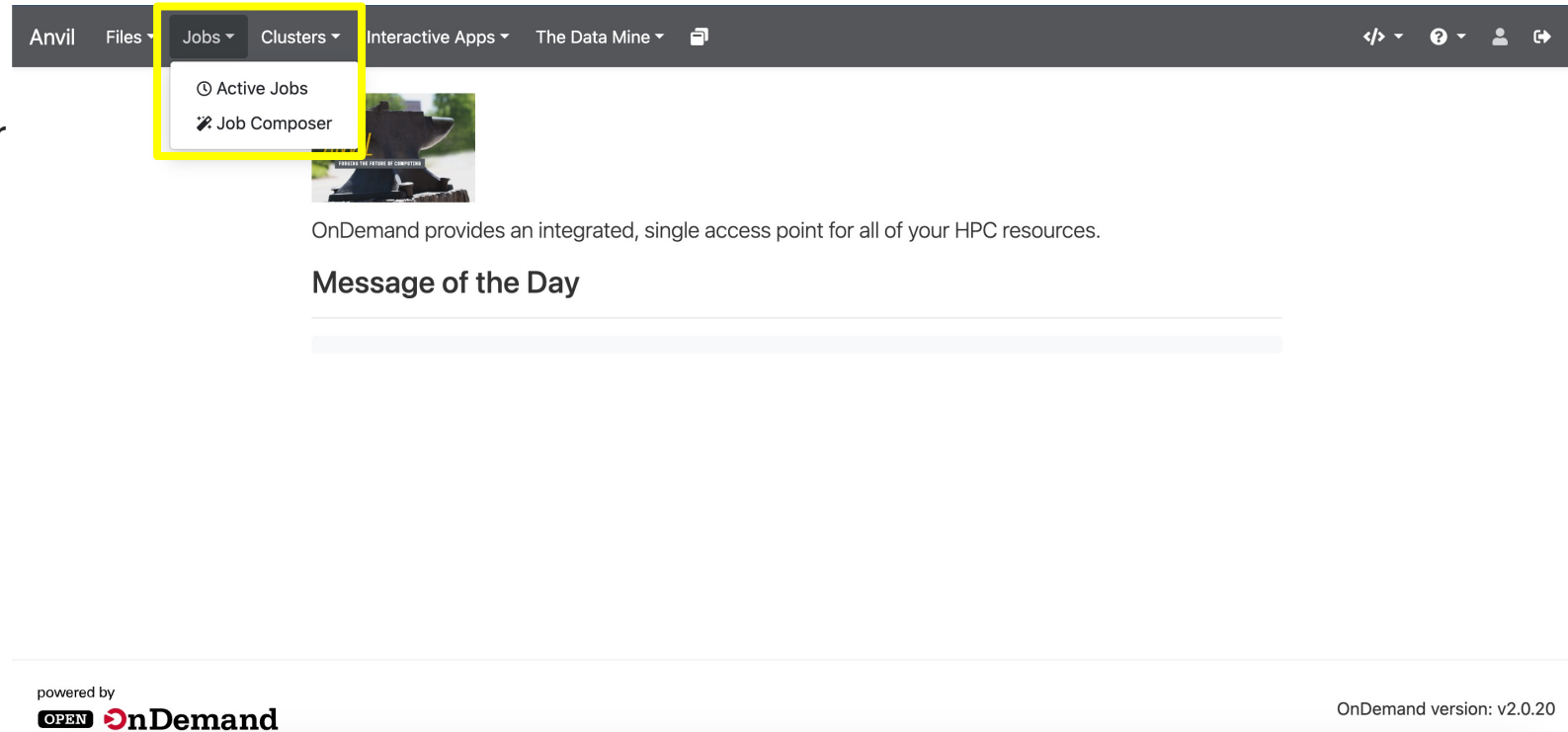
OnDemand version: v2.0.20

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



powered by **OPEN OnDemand**

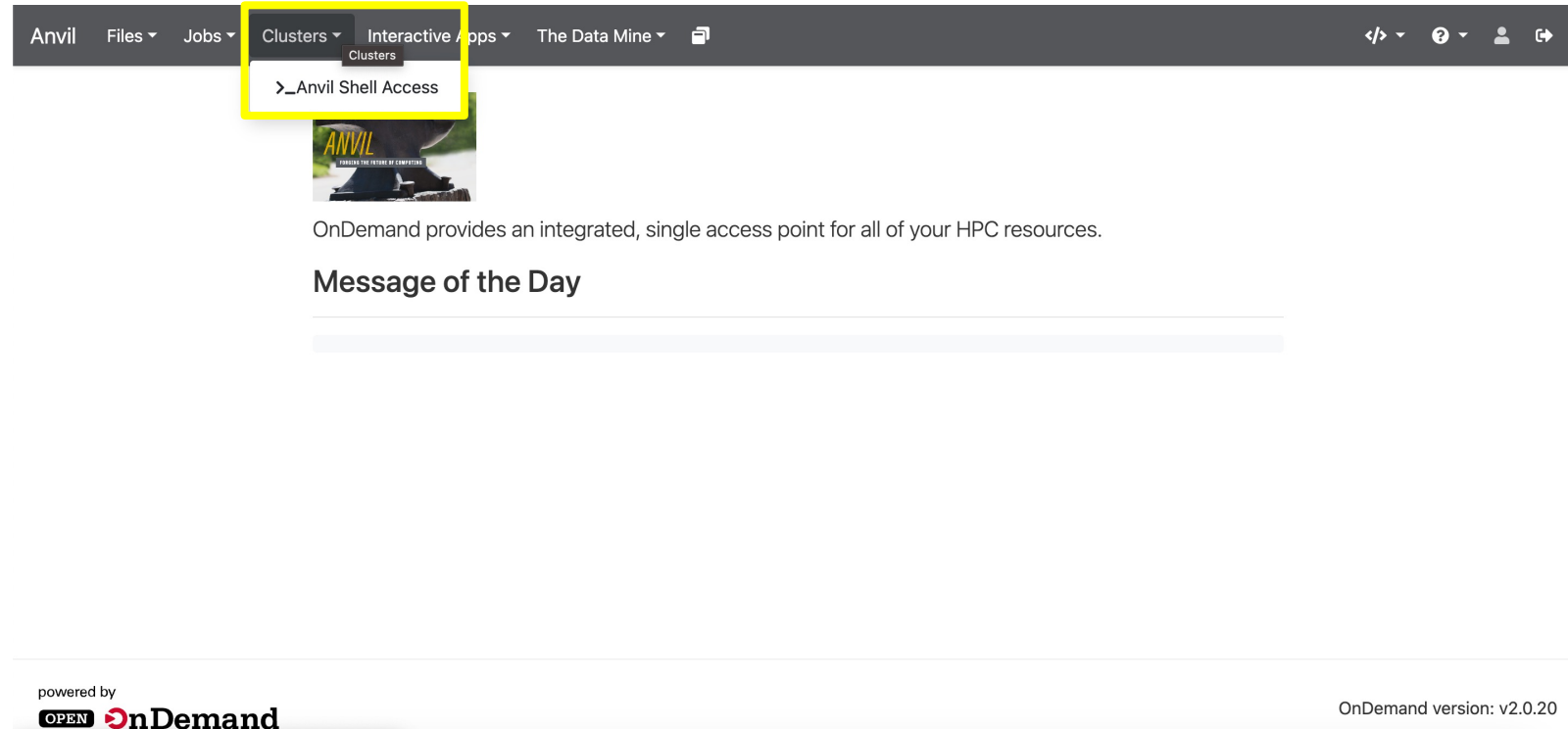
OnDemand version: v2.0.20

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



powered by
OPEN OnDemand

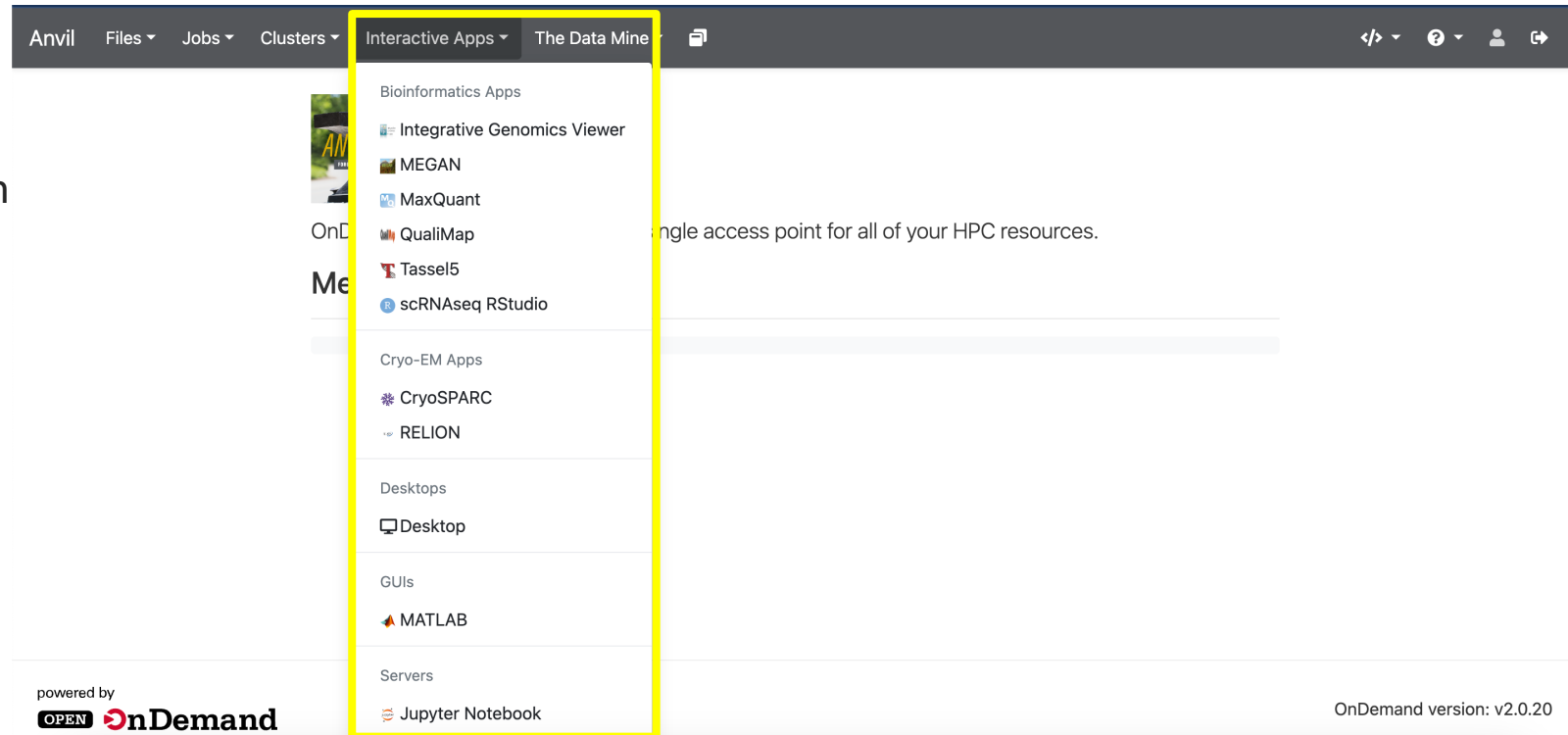
OnDemand version: v2.0.20

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

powered by
OPEN OnDemand

OnDemand version: v2.0.20

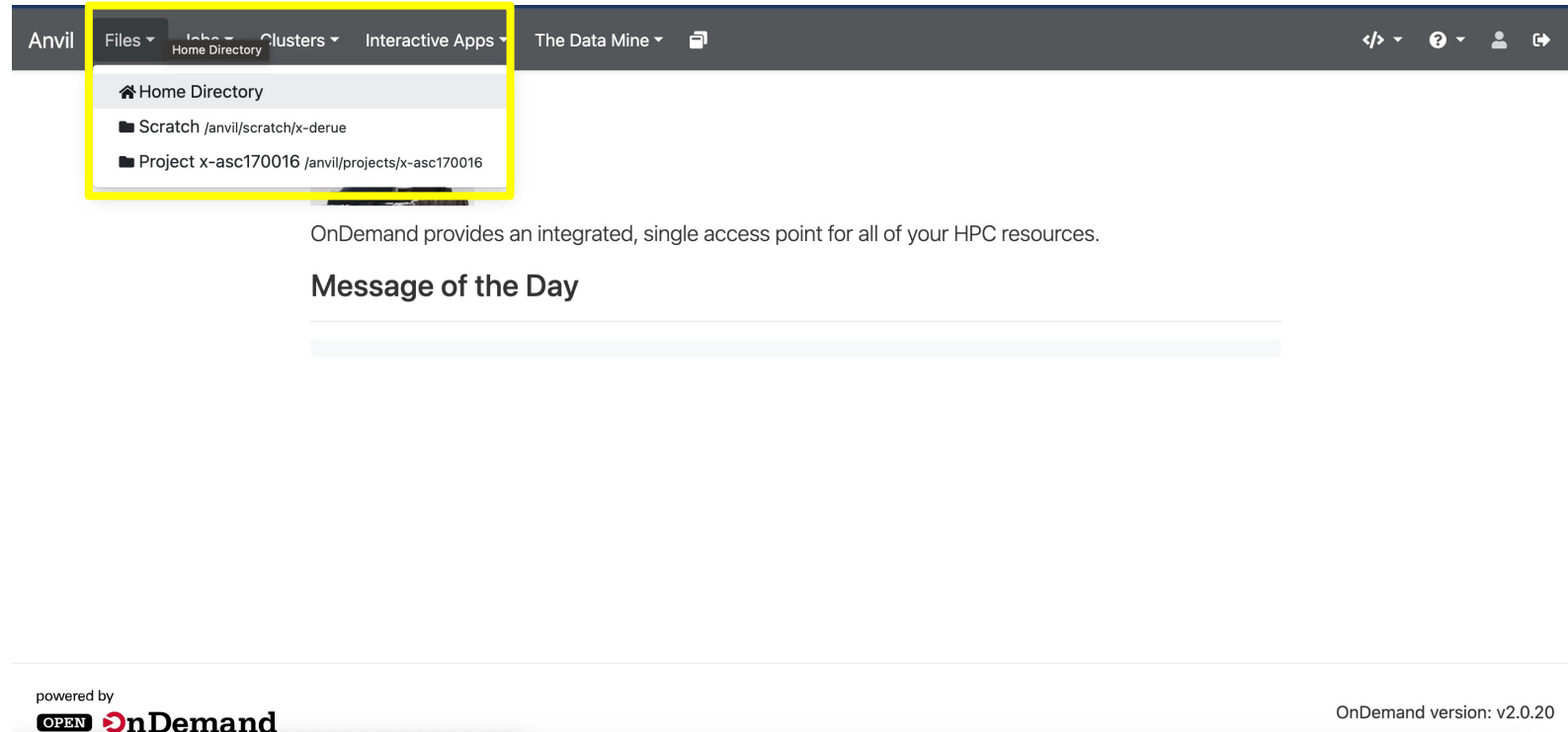
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Using Open OnDemand: Files

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



The screenshot shows the Anvil web interface. The top navigation bar includes 'Anvil', 'Files', 'Jobs', 'Clusters', 'Interactive Apps', and 'The Data Mine'. The 'Files' dropdown menu is open, showing three options: 'Home Directory', 'Scratch /anvil/scratch/x-derue', and 'Project x-asc170016 /anvil/projects/x-asc170016'. A yellow box highlights the dropdown menu. Below the navigation bar, there is a section titled 'Message of the Day' and a footer that reads 'powered by OPEN OnDemand' and 'OnDemand version: v2.0.20'.

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

The screenshot shows the Open OnDemand Files interface. At the top, there is a navigation bar with tabs for Anvil, Files, Jobs, Clusters, Interactive Apps, and The Data Mine. Below this is a toolbar with buttons for Open in Terminal, New File, New Directory, Upload, Download, Copy/Move, and Delete. The main area shows the current directory path as /home/x-derue/. On the left, a navigation menu is highlighted with a yellow box, containing links for Home Directory, Scratch, and Project x-asc170016. The main area displays a table of files and directories.

Type	↑↓	Name	↑↓	Size	↑↓	Modified at	↑↓
<input type="checkbox"/>	📁	Anvil-Configuration	⋮	-		7/6/2022 3:10:47 PM	
<input type="checkbox"/>	📁	cryosparc_hpc	⋮	-		7/6/2022 1:37:37 PM	
<input type="checkbox"/>	📁	Desktop	⋮	-		7/6/2022 2:39:29 PM	
<input type="checkbox"/>	📁	empiar_10025_subset	⋮	-		2/17/2018 5:22:08 AM	
<input type="checkbox"/>	📁	igv	⋮	-		7/28/2022 11:37:52 AM	

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

Type	↑↓	Name	↑↓	Size	↑↓	Modified at	↑↓
<input type="checkbox"/>	Folder	Anvil-Configuration	⋮	-		7/6/2022 3:10:47 PM	
<input type="checkbox"/>	Folder	cryosparc_hpc	⋮	-		7/6/2022 1:37:37 PM	
<input type="checkbox"/>	Folder	Desktop	⋮	-		7/6/2022 2:39:29 PM	
<input type="checkbox"/>	Folder	empiar_10025_subset	⋮	-		2/17/2018 5:22:08 AM	
<input type="checkbox"/>	Folder	igv	⋮	-		7/28/2022 11:37:52 AM	

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.

Type	Name	Size	Modified at
Folder	Anvil-Configuration	-	7/6/2022 3:10:47 PM
Folder	cryosparc_hpc	-	7/6/2022 1:37:37 PM
Folder	Desktop	-	7/6/2022 2:39:29 PM
Folder	empiar_10025_subset	-	2/17/2018 5:22:08 AM
Folder	igv	-	7/28/2022 11:37:52 AM

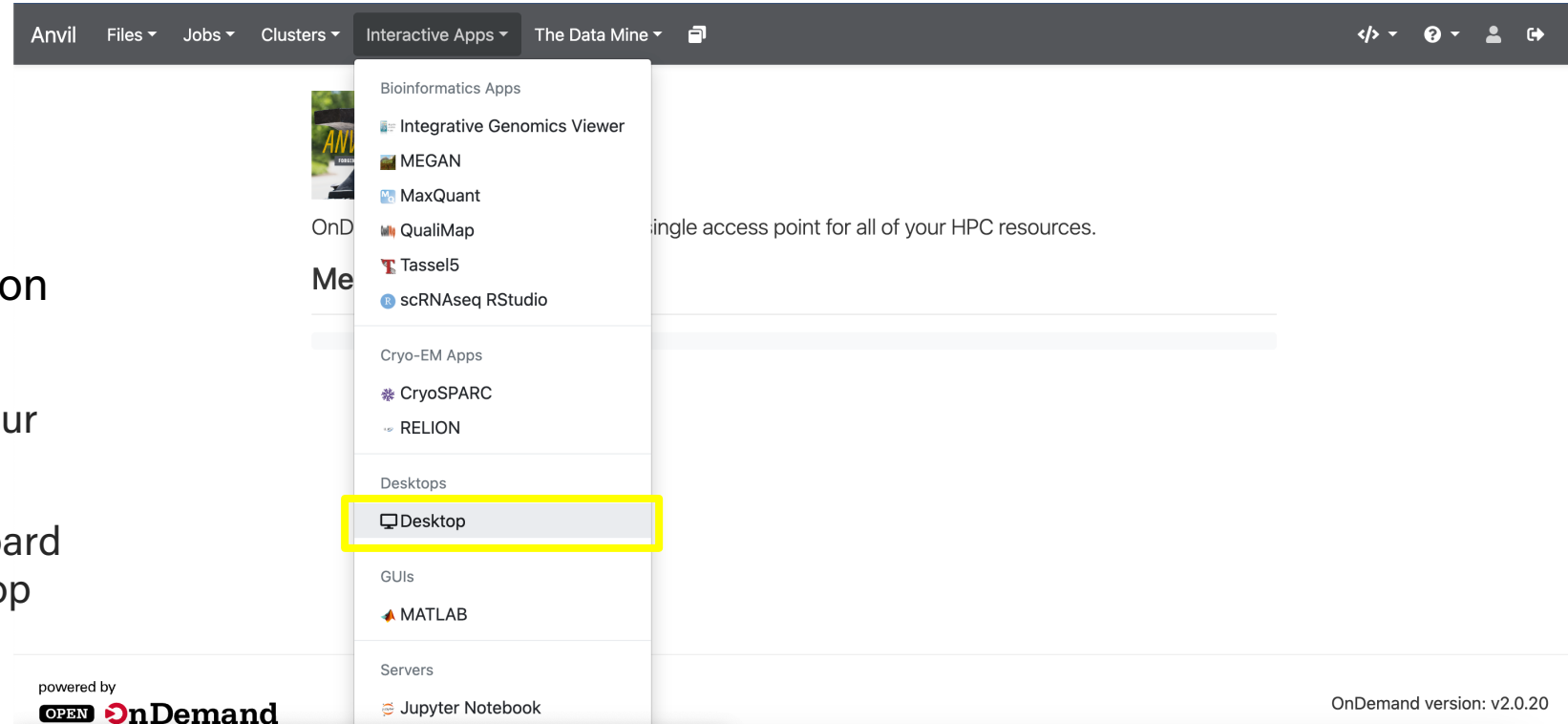
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Using Open OnDemand: Applications

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

Home / My Interactive Sessions / Desktop

Interactive Apps

- Bioinformatics Apps
 - Integrative Genomics Viewer
 - MEGAN
 - MaxQuant
 - QualiMap
 - Tassel5
 - scRNAseq RStudio
- Cryo-EM Apps
 - CryoSPARC
 - RELION
- Desktops
 - Desktop**
- GUIs

Desktop

This app will launch an interactive desktop on one or more compute nodes.

Allocation

asc170016-gpu (4889.4 SUs remaining) ▾

Queue (partition)

gpu ▾

- GPU-only allocations MUST use the 'gpu' queue
- CPU-only allocations MAY NOT use the 'gpu' queue

Wall Time in Hours

1

Number of hours you are requesting for your job.

Cores

1

Number of cores (up to 128) for a shared job. Non-shared jobs will have exclusive nodes and be charged at 128 cores per node requested

Using Open OnDemand: Applications

Application Forms

- 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

Home / My Interactive Sessions / Desktop

Interactive Apps

- Bioinformatics Apps
- Integrative Genomics Viewer
- MEGAN
- MaxQuant
- QualiMap
- Tassel5
- scRNAseq RStudio
- Cryo-EM Apps
- CryoSPARC
- RELION
- Desktops**
- GUIs

Desktop

This app will launch an interactive desktop on one or more compute nodes.

Allocation

asc170016 (75102.6 SUs remaining) ▼

Queue (partition)

shared ▼

- GPU-only allocations MUST use the 'gpu' queue
- CPU-only allocations MAY NOT use the 'gpu' queue

Wall Time in Hours

1

Number of hours you are requesting for your job.

Cores

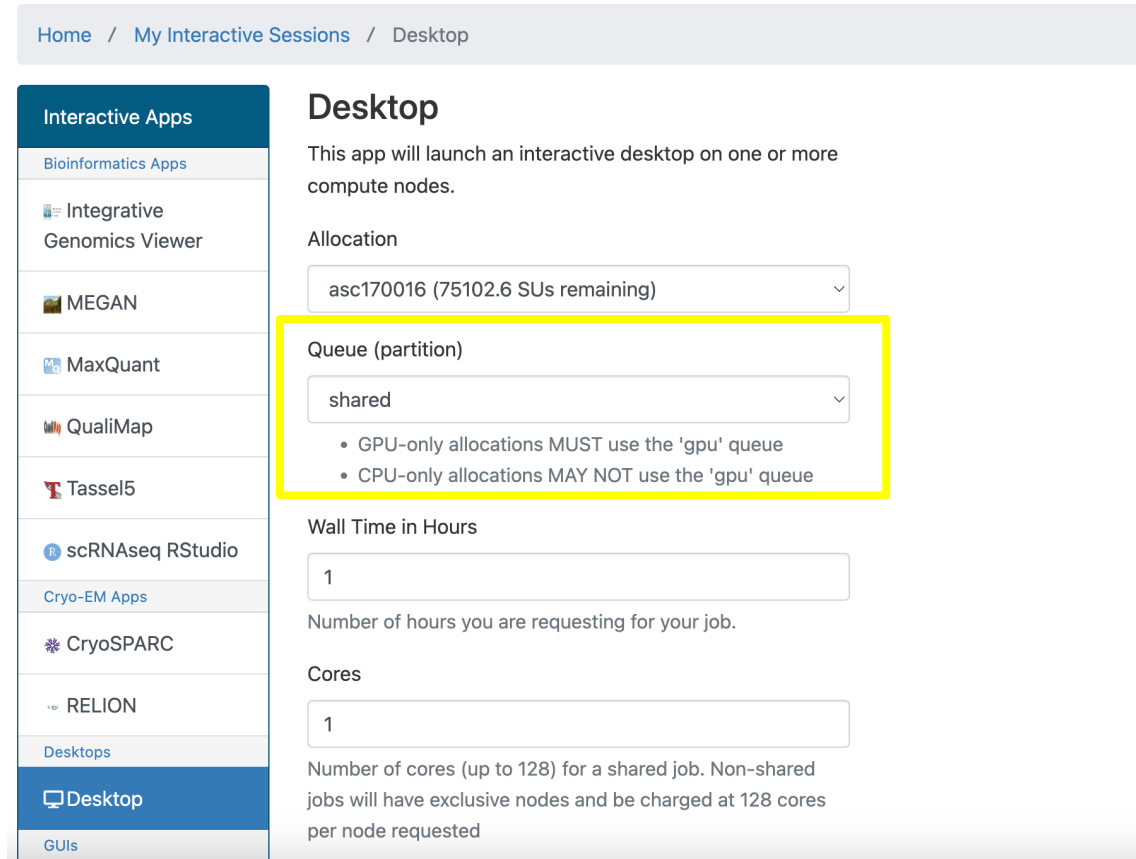
1

Number of cores (up to 128) for a shared job. Non-shared jobs will have exclusive nodes and be charged at 128 cores per node requested

Using Open OnDemand: Applications

Application Forms

- 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.



Home / My Interactive Sessions / Desktop

Interactive Apps

- Bioinformatics Apps
- Integrative Genomics Viewer
- MEGAN
- MaxQuant
- QualiMap
- Tassel5
- scRNAseq RStudio
- Cryo-EM Apps
- CryoSPARC
- RELION
- Desktops**
- Desktop
- GUIs

Desktop

This app will launch an interactive desktop on one or more compute nodes.

Allocation: asc170016 (75102.6 SUs remaining)

Queue (partition): shared

- GPU-only allocations MUST use the 'gpu' queue
- CPU-only allocations MAY NOT use the 'gpu' queue

Wall Time in Hours: 1

Number of hours you are requesting for your job.

Cores: 1

Number of cores (up to 128) for a shared job. Non-shared jobs will have exclusive nodes and be charged at 128 cores per node requested

<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

MaxQuant
QualiMap
Tassel5
scRNAseq RStudio
Cryo-EM Apps
CryoSPARC
RELION
Desktops
Desktop
GUIs
MATLAB
Servers
Jupyter Notebook
RStudio Server

Queue (partition)

gpu

- GPU-only allocations MUST use the 'gpu' queue
- CPU-only allocations MAY NOT use the 'gpu' queue

Wall Time in Hours

1

Number of hours you are requesting for your job.

Cores

1

Number of cores (up to 128) for a shared job. Non-shared jobs will have exclusive nodes and be charged at 128 cores per node requested

Number of GPUs

1











Number of Nvidia A100 GPUs you are requesting.

Launch

Using Open OnDemand: Applications

Application Forms

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

 MaxQuant
 QualiMap
 Tassel5
 scRNAseq RStudio
Cryo-EM Apps
 CryoSPARC
 RELION
Desktops
 Desktop
GUIs
 MATLAB
Servers
 Jupyter Notebook
 RStudio Server

Queue (partition)

- GPU-only allocations MUST use the 'gpu' queue
- CPU-only allocations MAY NOT use the 'gpu' queue

Wall Time in Hours

Number of hours you are requesting for your job.

Cores

Number of cores (up to 128) for a shared job. Non-shared jobs will have exclusive nodes and be charged at 128 cores per node requested

Number of GPUs

Number of Nvidia A100 GPUs you are requesting.

Using Open OnDemand: Applications

Application Forms

- 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..."



Rosen Center for
Advanced Computing

Home / My Interactive Sessions

Interactive Apps

Bioinformatics Apps

- Integrative Genomics Viewer
- MEGAN
- MaxQuant
- QualiMap
- Tassel5

Desktop (1677891) **1 node** | **1 core** | Starting

Created at: 2023-05-05 10:57:44 EDT Delete

Time Remaining: 1 hour

Session ID: c6f0c9a0-af73-49c2-b8b6-26369d037cb3

Your session is currently starting... Please be patient as this process can take a few minutes.

Home / My Interactive Sessions

Interactive Apps

Bioinformatics Apps

- Integrative Genomics Viewer
- MEGAN
- MaxQuant
- QualiMap
- Tassel5
- scRNAseq RStudio
- Cryo-EM Apps

Desktop (1677891) **1 node** | **1 core** | Running

Host: >_a240.anvil.rcac.purdue.edu Delete

Created at: 2023-05-05 10:57:44 EDT

Time Remaining: 59 minutes

Session ID: c6f0c9a0-af73-49c2-b8b6-26369d037cb3

Compression Image Quality

0 (low) to 9 (high) 0 (low) to 9 (high)

Launch Desktop View Only (Share-able Link)

Using Open OnDemand: Applications

Specific Applications: Compute Desktop

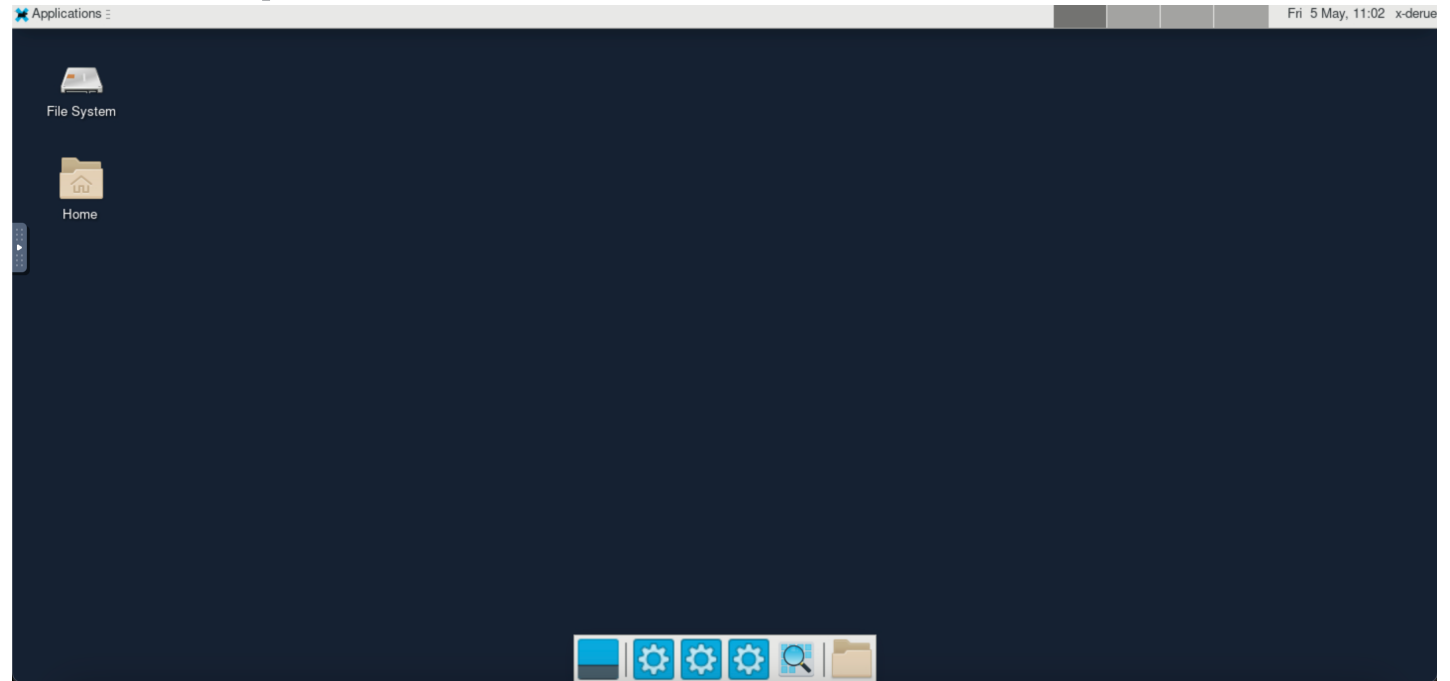
The Desktop application is an extremely useful application for interfacing with Anvil

- 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

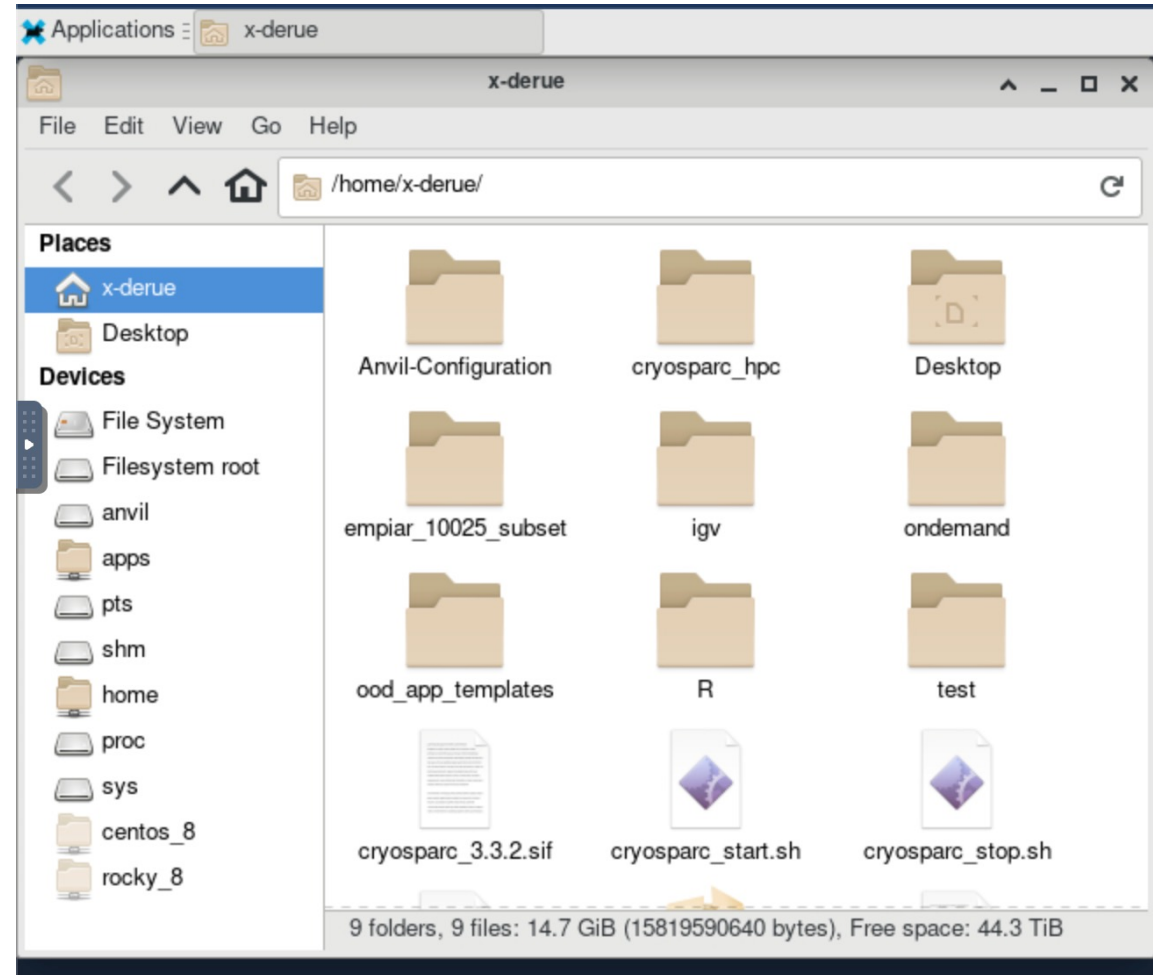
1. When you first launch the Compute Desktop, you will be presented with a desktop that appears as the one on the right
 - You can access your files by selecting the folder icon in the taskbar along the bottom, or by selecting the directory icon labelled "Home".



Using Open OnDemand: Applications

Specific Applications: Compute Desktop

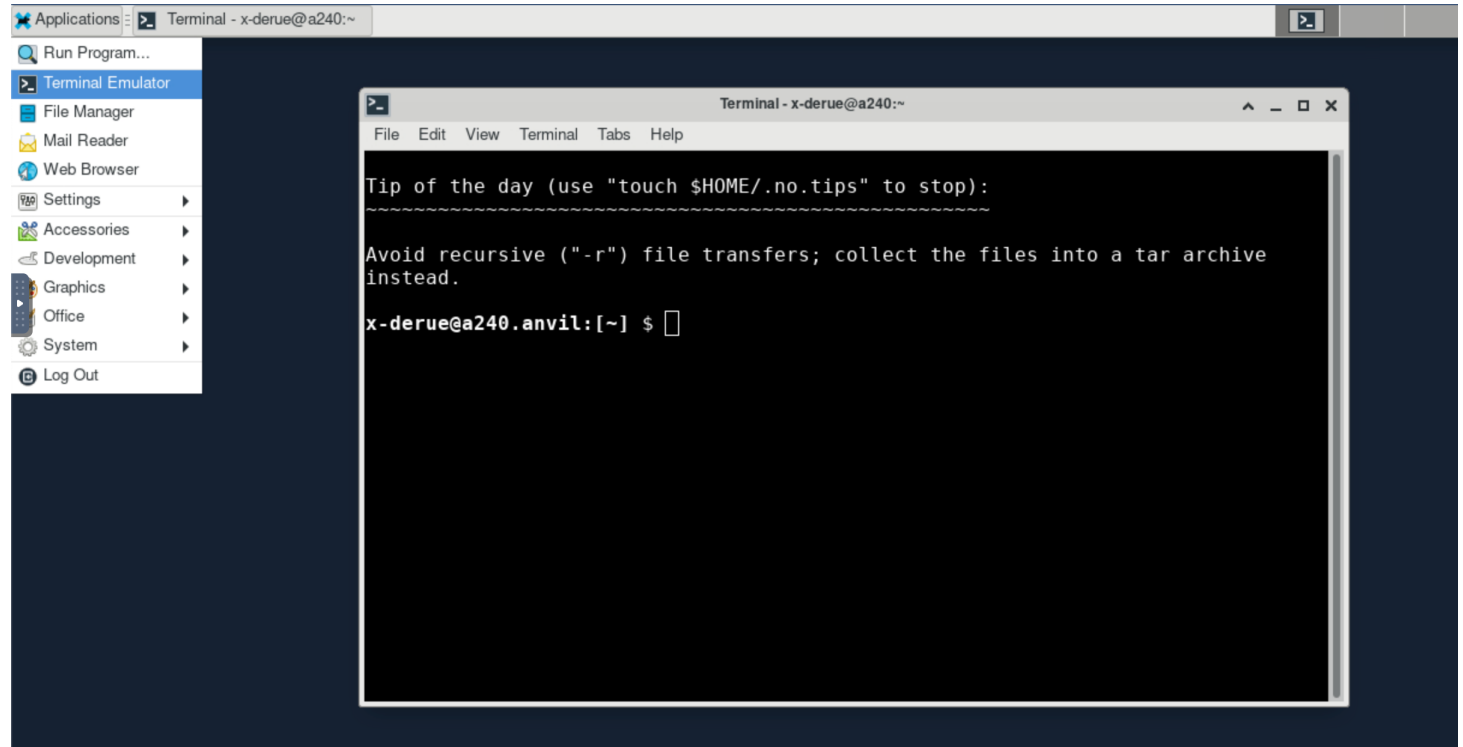
- From this file menu, you can access any file on the cluster, but by default it will open to your home directory
 - You can change the directory you are viewing by clicking on other directories or by typing the absolute path into the search bar at the top



Using Open OnDemand: Applications

Specific Applications: Compute Desktop

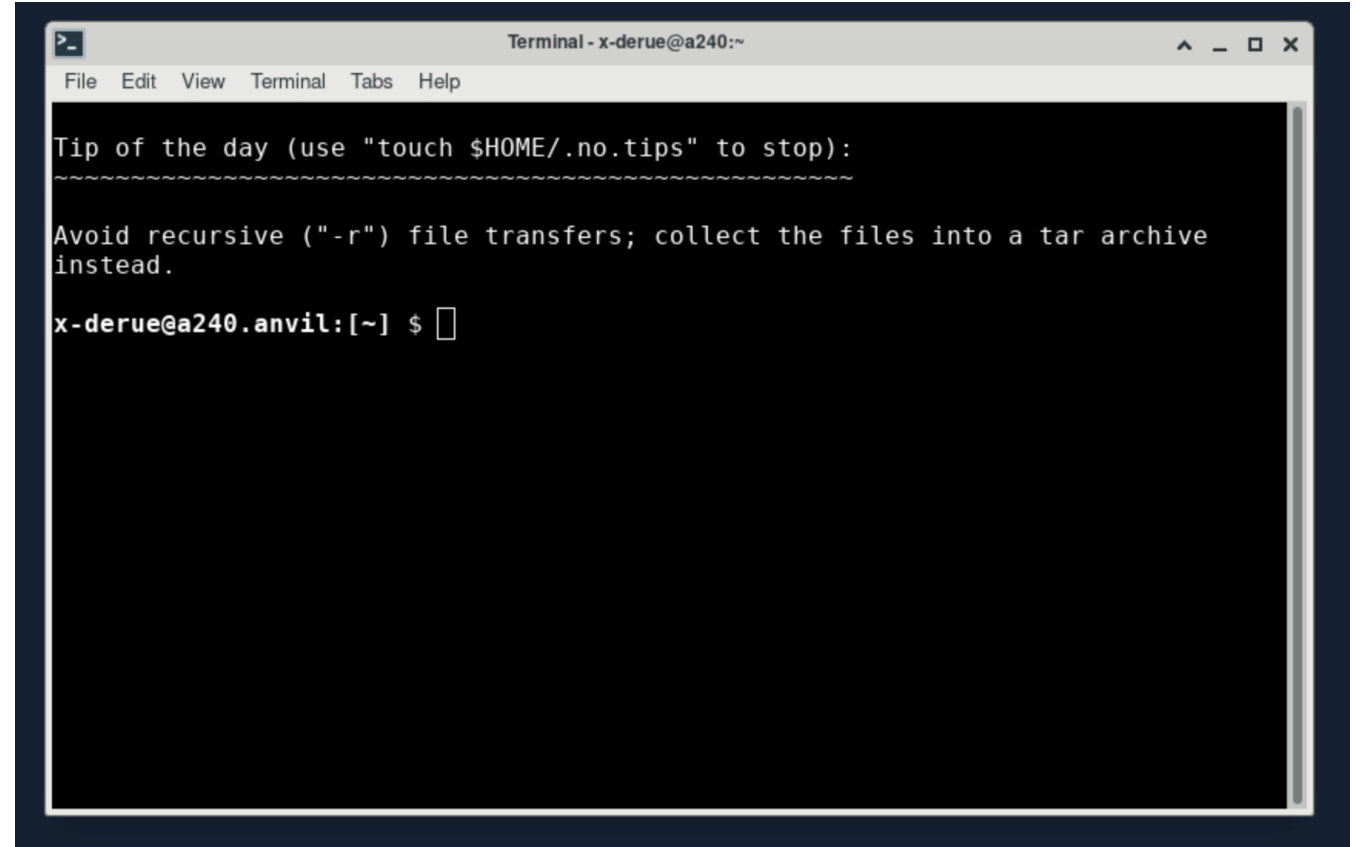
3. You can launch a terminal on the desktop by selecting Applications menu in the top right, and then selecting "Terminal Emulator" from the sub-menu.
 - This is extremely useful for launching GUI applications from the command-line



Using Open OnDemand: Applications

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.



```
Terminal - x-derue@a240:~
File Edit View Terminal Tabs Help

Tip of the day (use "touch $HOME/.no.tips" to stop):
-----
Avoid recursive ("-r") file transfers; collect the files into a tar archive
instead.

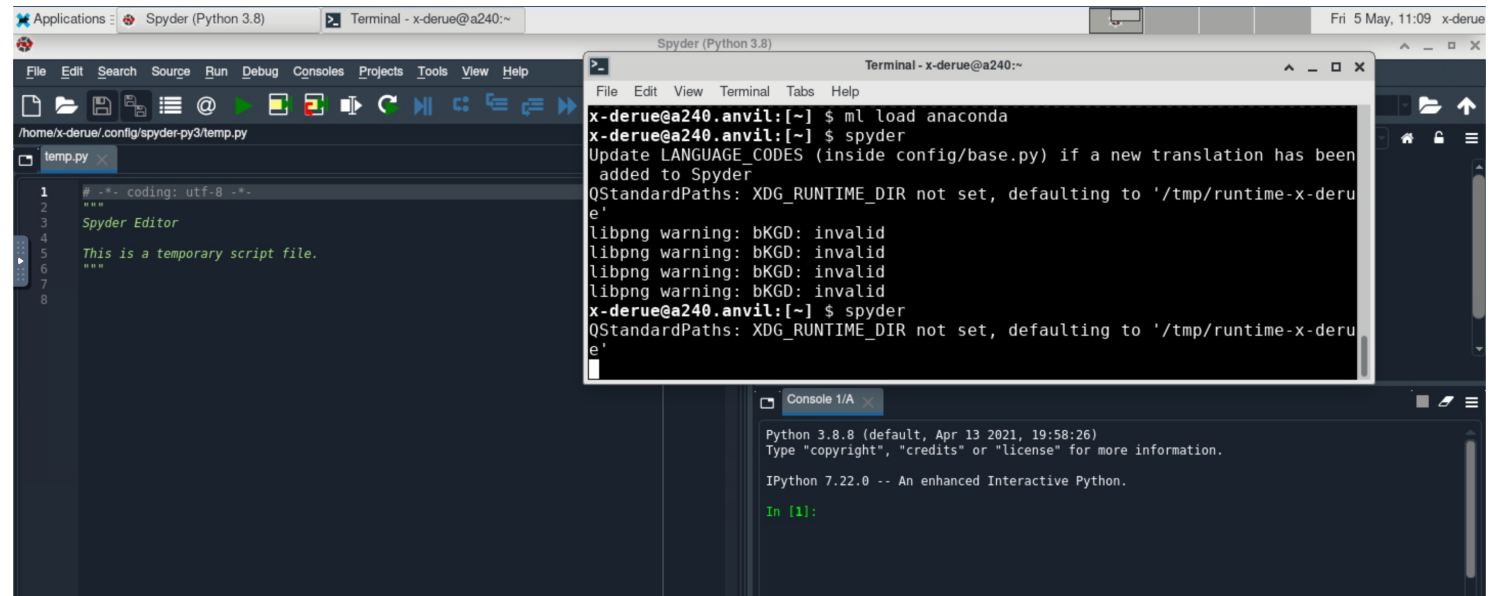
x-derue@a240.anvil: [~] $
```


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!



```
x-derue@a240.anvil:~$ ml load anaconda
x-derue@a240.anvil:~$ spyder
Update LANGUAGE_CODES (inside config/base.py) if a new translation has been
added to Spyder
QStandardPaths: XDG_RUNTIME_DIR not set, defaulting to '/tmp/runtime-x-deru
e'
libpng warning: bKGD: invalid
libpng warning: bKGD: invalid
libpng warning: bKGD: invalid
libpng warning: bKGD: invalid
x-derue@a240.anvil:~$ spyder
QStandardPaths: XDG_RUNTIME_DIR not set, defaulting to '/tmp/runtime-x-deru
e'
```

The screenshot shows a terminal window with the above commands and output. In the background, a Spyder Python 3.8 application window is open, displaying a file editor with a temporary script file containing the text: `1 # -*- coding: utf-8 -*-`, `2 """`, `3 Spyder Editor`, `4`, `5 This is a temporary script file.`, `6 """`, `7`, `8`.

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

Jupyter Notebook

This app will launch a Jupyter Notebook server on a node.

Allocation

asc170016 (75102.6 SUs remaining)

Queue (partition)

shared

- GPU-only allocations MUST use the 'gpu' queue
- CPU-only allocations MAY NOT use the 'gpu' queue

Wall Time in Hours

1

Number of hours you are requesting for your job.

Cores

1

Number of cores (up to 128) for a shared job. Non-shared jobs will have exclusive nodes and be charged at 128 cores per node requested

Use Jupyter Lab instead of Jupyter Notebook

I would like to receive an email when the session starts

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.

Jupyter Notebook

This app will launch a Jupyter Notebook server on a node.

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Use Jupyter Lab instead of Jupyter Notebook

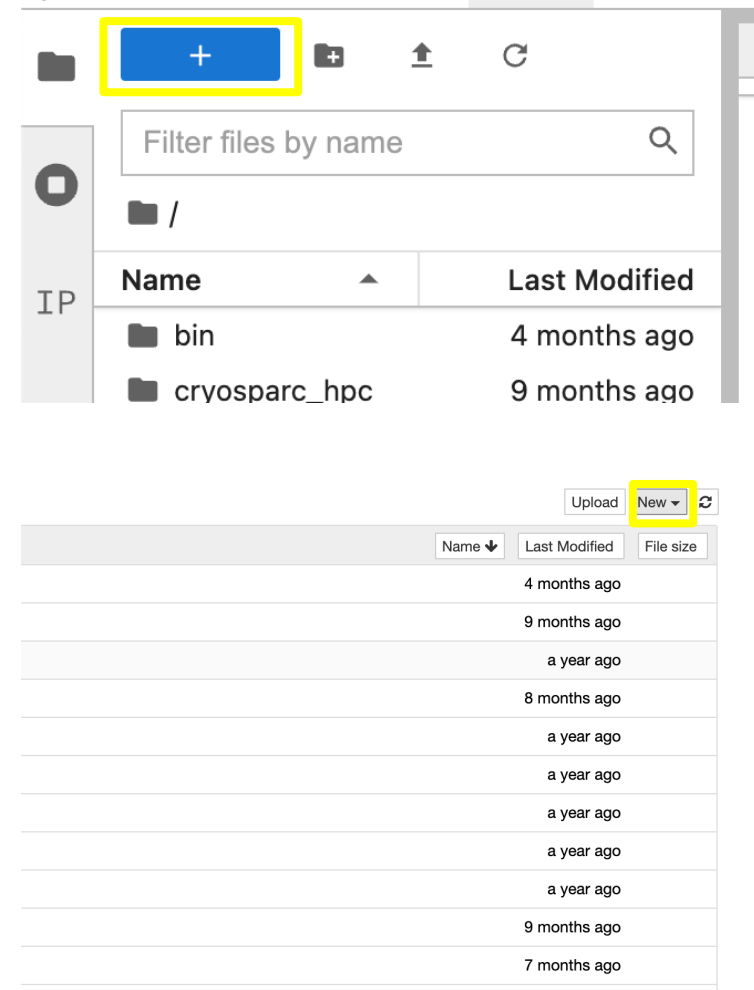
I would like to receive an email when the session starts

<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)

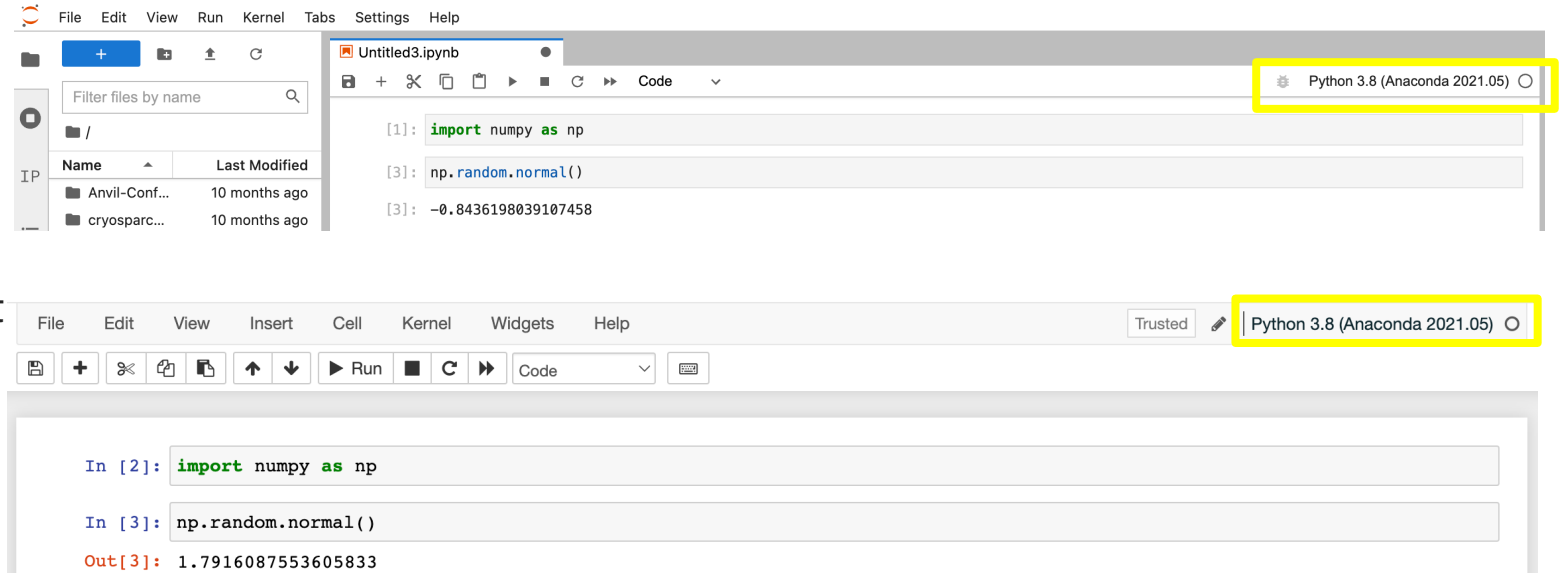


Using Open OnDemand: Applications

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



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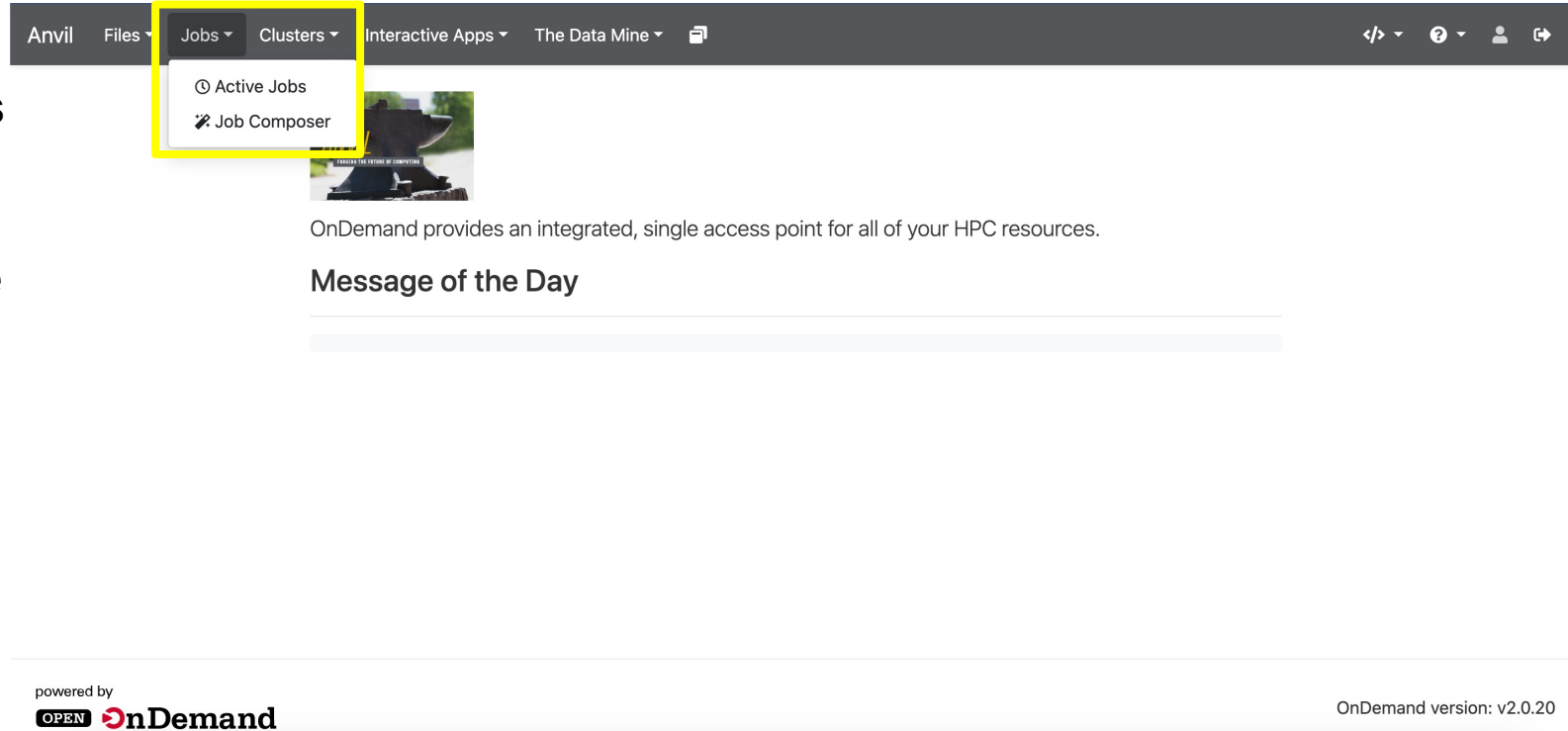
Using Open OnDemand: Job Composer

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



The screenshot shows the Open OnDemand web interface. The top navigation bar includes 'Anvil', 'Files', 'Jobs', 'Clusters', 'Interactive Apps', and 'The Data Mine'. The 'Jobs' menu is open, showing 'Active Jobs' and 'Job Composer'. Below the navigation bar, there is a section titled 'Message of the Day' with a description: 'OnDemand provides an integrated, single access point for all of your HPC resources.' At the bottom of the page, it says 'powered by OPEN OnDemand' and 'OnDemand version: v2.0.20'.

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

Active Jobs Your Jobs ▾ All Clusters ▾

Show entries Filter:

ID	Name	User	Account	Time Used	Queue	Status	Cluster	Actions
> 1677958	OnDemand/Jupyter	x-derue	asc170016	00:07:09	shared	Running	Anvil	
▼ 1677957	OnDemand/Jupyter	x-derue	asc170016	00:07:16	shared	Running	Anvil	

Running OnDemand/Jupyter 1677957

Cluster	Anvil
Job Id	1677957
Job Name	OnDemand/Jupyter
User	x-derue
Account	asc170016
Partition	shared
State	RUNNING
Reason	None
Total Nodes	1
Node List	a240
Total CPUs	1
Time Limit	1:00:00
Time Used	7:31
Memory	1918M

Output Location:

```
/home/x-derue/ondemand/data/sys/dashboard/batch_connect/sys/jupyter/output/d86cc533-1e77-4480-b17f-aeded1f525b1
```

Open in File Manager Open in Terminal Delete

5/5/23 | 40

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

The screenshot shows the Anvil Job Composer interface. At the top, there is a navigation bar with 'Anvil / Job Composer Jobs Templates'. Below this, the 'Jobs' section is visible. It includes a '+ New Job' button and a 'Create Template' button. A toolbar contains 'Edit Files', 'Job Options', 'Open Terminal', 'Submit', 'Stop', and 'Delete' buttons. A search bar and a 'Show 25 entries' dropdown are also present. The main area displays a table with columns for 'Created', 'Name', 'ID', 'Cluster', and 'Status'. One job is listed: 'May 5, 2023 11:37am (default) Simple Sequential Job' on the 'Anvil' cluster, with a status of 'Not Submitted'. At the bottom, it shows 'Showing 1 to 1 of 1 entries' and pagination controls for 'Previous', '1', and 'Next'.

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”

The screenshot shows the Open OnDemand Job Composer interface. At the top, there is a navigation bar with "Anvil / Job Composer Jobs Templates". Below this is a "Jobs" section. A dropdown menu is open, showing options: "Create a new job from the default template", "From Default Template", "From Specified Path", and "From Selected Job". To the right of the dropdown are buttons for "Open Terminal", "Submit", "Stop", and "Delete". There is also a "Create Template" button. Below the dropdown is a search bar. The main part of the interface is a table with columns: "Created", "Name", "ID", "Cluster", and "Status". The table contains one entry: "May 5, 2023 11:37am", "(default) Simple Sequential Job", "Anvil", and "Not Submitted". At the bottom, there is a pagination bar showing "Showing 1 to 1 of 1 entries" and "Previous 1 Next".

Using Open OnDemand: Job Composer

A Widget For Talking to the Scheduler

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

Anvil / Job Composer Jobs Templates

Job Options

Name

Cluster

Specify job script

Files larger than 65KB are omitted for the job script field

Account

Account is an optional field. If not set, the account may be auto-set by the submit filter.

Job array specification

Job arrays are optional. e.g. 1-10

Using Open OnDemand: Job Composer

A Widget For Talking to the Scheduler

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

Job Details

Job Name:
(default) Simple Sequential Job

Submit to:
Anvil

Account:
asc170016

Script location:
/home/x-derue/ondemand/data/sys/myjobs/projects/default/1

Script name:
main_job.sh

Folder Contents:
main_job.sh

Submit Script

main_job.sh

Script contents:

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

echo "Hello World"
```

[Open Editor](#) [Open Terminal](#) [Open Dir](#)

Using Open OnDemand: Job Composer

A Widget For Talking to the Scheduler

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

```
Save /home/x-derue/ondemand/data/sys/myjobs/projects/default/1/main_job.sh
1 #!/bin/bash
2 # JOB HEADERS HERE
3
4 echo "Going to sleep for 30 seconds, but when I wake up, I'll greet you!"
5 sleep 30
6 echo "Hello from Open OnDemand!"
7
```

Using Open OnDemand: Job Composer

A Widget For Talking to the Scheduler

- 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”

Jobs

The screenshot displays the 'Jobs' management interface in Open OnDemand. It features a top navigation bar with buttons for '+ New Job', 'Edit Files', 'Job Options', 'Open Terminal', 'Submit Job', 'Submit', 'Stop', and 'Delete'. A 'Create Template' button is also present. Below the navigation, there are controls for 'Show 25 entries' and a search field. The main area contains a table with columns for 'Created', 'Name', 'ID', 'Cluster', and 'Status'. A single job entry is shown with a status change from 'Not Submitted' to 'Running'. The job details are: Created: May 5, 2023 11:37am; Name: (default) Simple Sequential Job; ID: 1677976; Cluster: Anvil; Status: Running. Navigation buttons for 'Previous', '1', and 'Next' are visible at the bottom of the table.

Created	Name	ID	Cluster	Status
May 5, 2023 11:37am	(default) Simple Sequential Job	1677976	Anvil	Running

Using Open OnDemand: Job Composer

A Widget For Talking to the Scheduler

- 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:

```
Save /home/x-derue/ondemand/data/sys/myjobs/projects/default/1/slurm-1677976.out
1 Going to sleep for 30 seconds, but when I wake up, I'll greet you!
2 Hello from Open OnDemand!
3
```

Job Details

1677976

Job Name:
(default) Simple Sequential Job

Submit to:
Anvil

Account:
asc170016

Script location:
/home/x-derue/ondemand/data/sys/myjobs/projects/default/1

Script name:
main_job.sh

Folder Contents:
main_job.sh
slurm-1677976.out

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Conclusions

Conclusions

- 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

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Questions?

THANK YOU

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

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