



Cryo-EM Research Center

Intro to the Cryo-EM HPC Cluster Resource

Jennifer Scheuren and Matt Larson



Introduction to HPC

1. About the Cryo-EM Cluster
2. Getting started:
 1. How to request an account
 2. Connecting with Open OnDemand
 3. Basics with SBatch scripts or `submit_to_<queue>` commands.
3. Getting data to/from the HPC Cluster with Globus
4. Examples
5. Policies
6. Help and more information

Where to get HPC help

- Jennifer (jfscheuren@wisc.edu)
 - HPC Administrator for CEMRC
- Matt (mrlarson2@wisc.edu)
 - Sys admin for the CEMRC/MCCET facilities

Email to jfscheuren@wisc.edu and
CC: cryoem@biochem.wisc.edu



HPC Administrator



Computer Scientist/System Administrator

Slurm

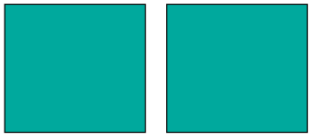
- “Simple Linux Utility for Resource Management”
- Open-source job scheduling and cluster management tool
- Highly customizable – Control resources, jobs and users
- **Cluster** – set of computers for high-performance computing
- **Head node** – computer from which users can submit jobs
- **Compute nodes** – computers that jobs will be assigned by the scheduler. Users do not log in directly.
- **Partition (or Queue)** – a pool of nodes from some part of the cluster
 - Ex. “GPU”, “A5000”, “A100” and “CPU” (what hardware is available in each queue in the cryoemcluster.biochem.wisc.edu)



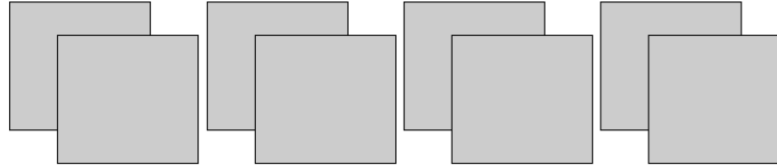
cryoemcluster.biochem.wisc.edu

Users Login/Submit Jobs from a Central Node

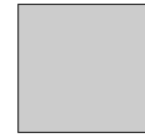
2x nodes have A100
for machine learning tasks



8 nodes will be high-powered 4x A5000 GPU, 15TB nVME local storage



4 nodes will be CPU-only
256 Core total



200 TB nVME-based scratch on
Ceph Cluster for persistent, fast,
cluster data use.



Cryo-EM HTC Cluster

Comparing different compute nodes

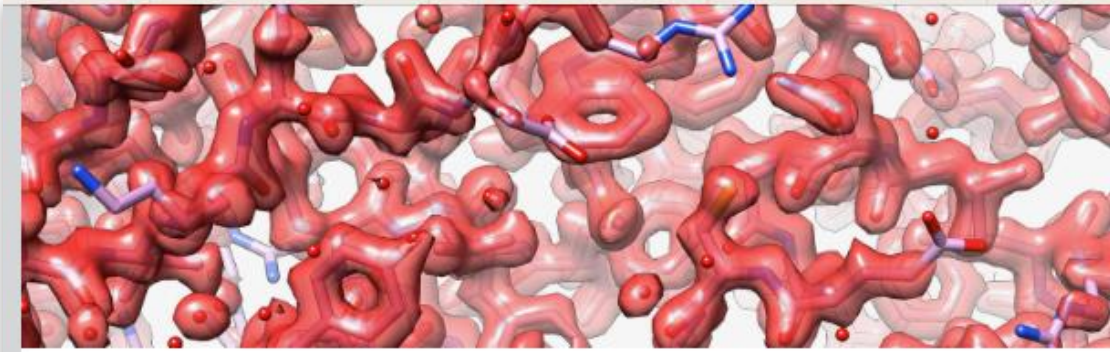
Compute node	GPU	Memory	CPU
a100	4x Nvidia a100s	512 GB	2x AMD 7443 48 cores
a5000	4x Nvidia a5000s	512GB	1x AMD EPYC 64 cores
cpu	none	256 GB	1x AMD EPYC 64 cores

- Use gpu nodes for jobs that can support gpu processing.
- Use cpu nodes for jobs that cannot support gpu processing.

Getting started: request an account

https://explore.wisc.edu/cryoem_hpc_access_request

- You will be added to an allowed access group, and a network directory with quota will be created for use on the HPC Cluster.
- Afterwards you be contacted to you let you know you can now login.



First Name

Last Name

Email Address*

This field is required

Institution

Department

Biochemistry

Provide the name of the Principal Investigator (PI) for your lab group.

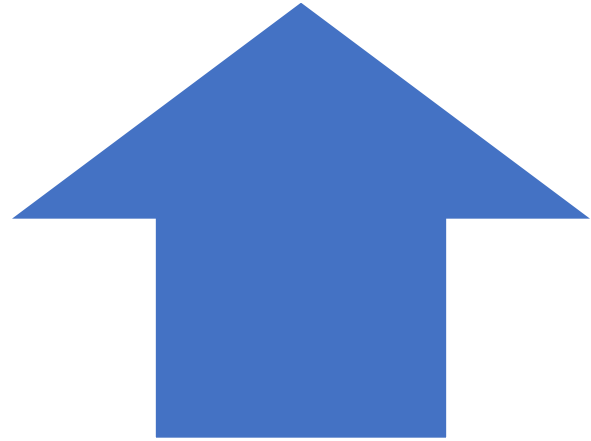
If available, provide your NetID at UW-Madison

Have you or your lab collected data at the UW-Madison Cryo-EM Research Center or Midwest Center for Cryo-Electron Tomography?

☐ Yes

☐ No

Two ways to connect!



SSH to cryoemcluster.biochem.wisc.edu
(using X11 forwarding for graphical apps)



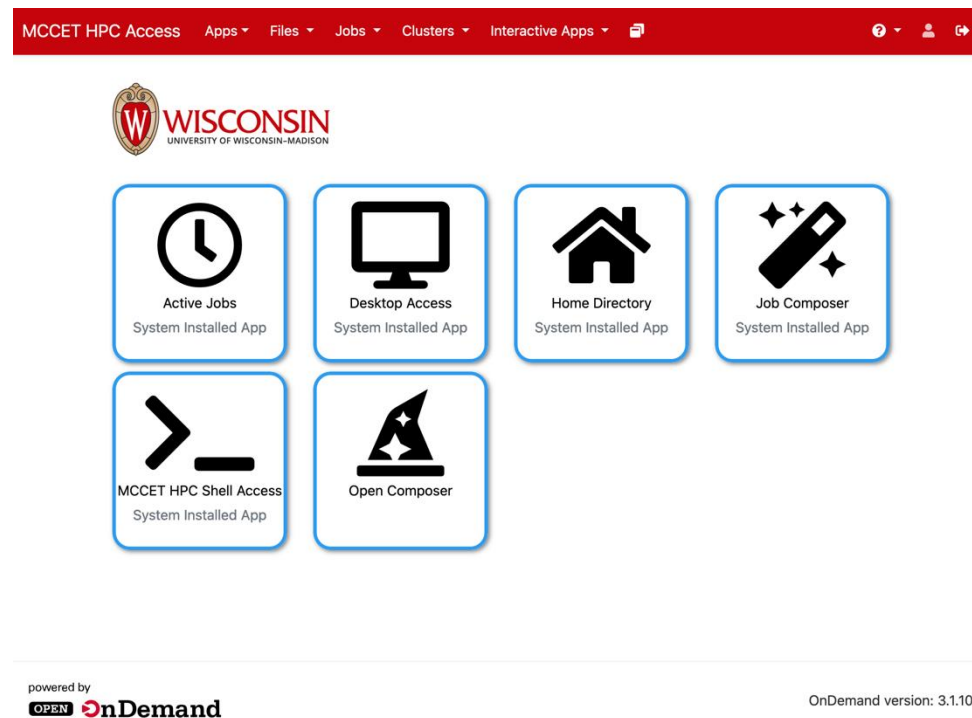
Open OnDemand web portal at
<https://ondemandcryo.biochem.wisc.edu>



Provides cluster access via web browser.

- Home directory access
- Active jobs
- Shell access
- Interactive Desktop
- Open composer

Go to <https://ondemandcryo.biochem.wisc.edu>
Login with your NetID (*Let's Try this Now!*)



Alternatively, login via ssh

- Login via SSH:

```
`ssh -YC netid@wisc.edu@cryoemcluster.biochem.wisc.edu`
```

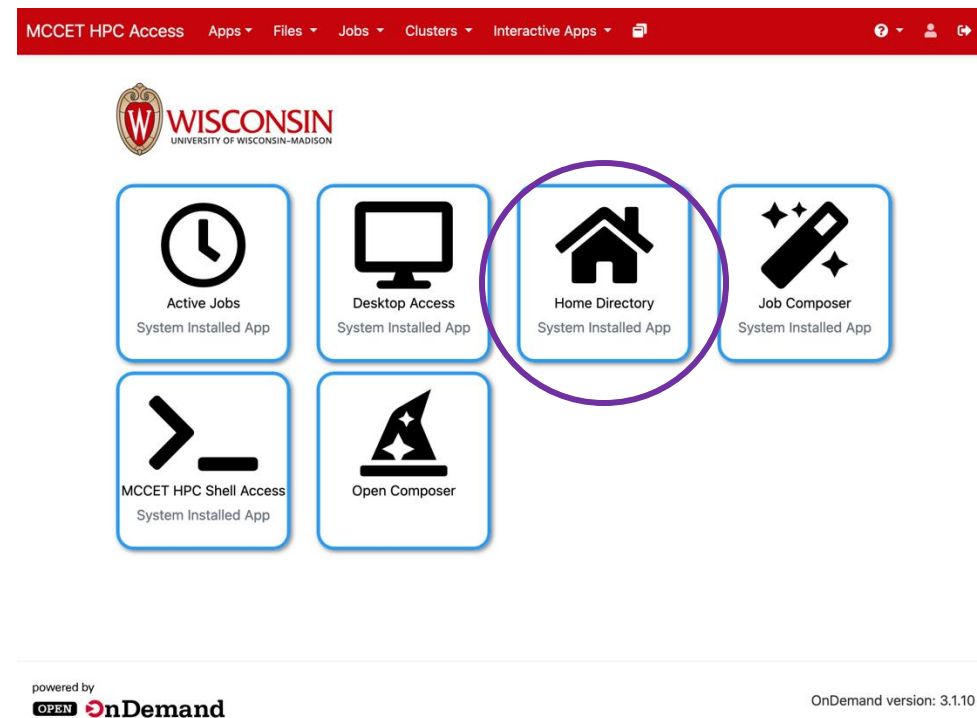
- The (-Y) and (-C) options with SSH enable X11 forwarding, with compression for best performance.
- You need to be on the Biochemistry VPN first.



Provides cluster access via web browser.

- Home directory access
- Active jobs
- Shell access
- Interactive Desktop
- Open composer

Go to <https://ondemandcryo.biochem.wisc.edu>



Home Directory

- View contents of your home directory, and transfer files.
- *But.. use Globus for larger data transfers.*

MCCET HPC Access Apps Files Jobs Clusters Interactive Apps

Open in Terminal Refresh New File New Directory Upload Download Copy/Move Delete

Home Directory

/mnt / hpc_users / home / mrlarson2@ad.wisc.edu /

Change directory

Copy path

☐ Show Owner/Mode ☐ Show Dotfiles Filter:

Showing 12 of 47 rows - 0 rows selected

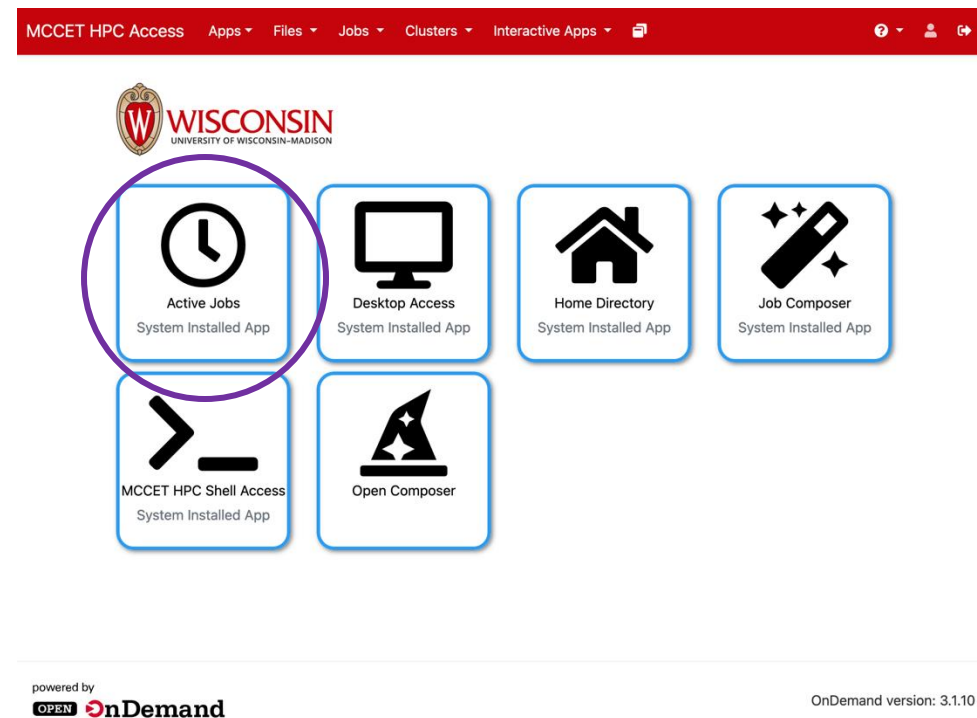
	Type	Name		Size	Modified at
<input type="checkbox"/>	Folder	day1.old		-	9/23/2024 2:22:02 PM
<input type="checkbox"/>	Folder	Desktop		-	10/17/2024 10:55:51 AM
<input type="checkbox"/>	Folder	info		-	4/9/2024 4:02:27 PM
<input type="checkbox"/>	Folder	ondemand		-	10/25/2024 4:32:07 PM
<input type="checkbox"/>	Folder	pipeline		-	4/9/2024 4:38:33 PM
<input type="checkbox"/>	Folder	save		-	2/4/2025 9:17:22 PM



Provides cluster access via web browser.

- Home directory access
- **Active jobs**
- Shell access
- Interactive Desktop
- Open composer

Go to <https://ondemandcryo.biochem.wisc.edu>



Active Jobs

- Show running, queued, completed, and failed jobs.
- Manage running jobs.

All Jobs ▾All Clusters ▾

Active Jobs

Show 50 ▾ entriesFilter:

	ID	Name	User	Account	Time Used	Queue	Status	Cluster	Actions
>	373693	sleep	hpcadmin	admins	00:00:46	cpu	Completed	MCCET HPC	
>	373697	sleep	hpcadmin	admins	00:00:00	cpu	Queued	MCCET HPC	
>	373696	sleep	hpcadmin	admins	00:00:23	cpu	Running	MCCET HPC	
>	373695	sleep	hpcadmin	admins	00:00:29	cpu	Running	MCCET HPC	
>	373694	sleep	hpcadmin	admins	00:00:34	cpu	Running	MCCET HPC	
▾	373692	sys/dashboard/ sys/bc_desktop/ desktop_cpu	jfscheuren@ad.wisc.edu	mccet	00:03:46	ood_cpu	Running	MCCET HPC	

Running sys/dashboard/sys/bc_desktop/desktop_cpu 373692

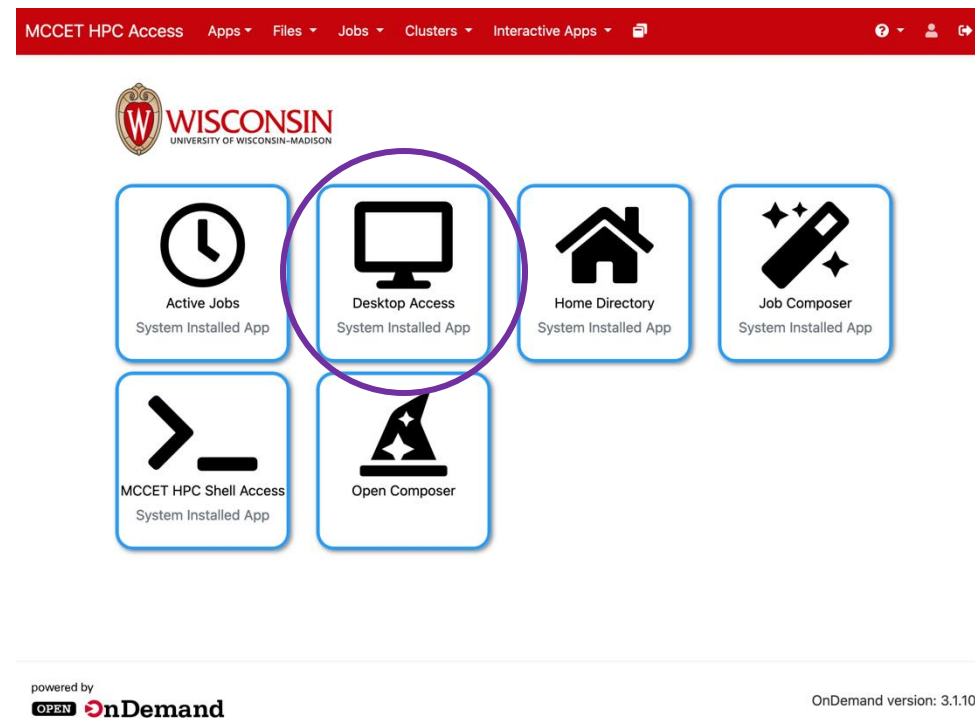
Cluster	MCCET HPC
Job Id	373692
Job Name	sys/dashboard/sys/bc_desktop/desktop_cpu
User	jfscheuren@ad.wisc.edu
Account	mccet
Partition	ood_cpu
State	RUNNING



Provides cluster access via web browser.

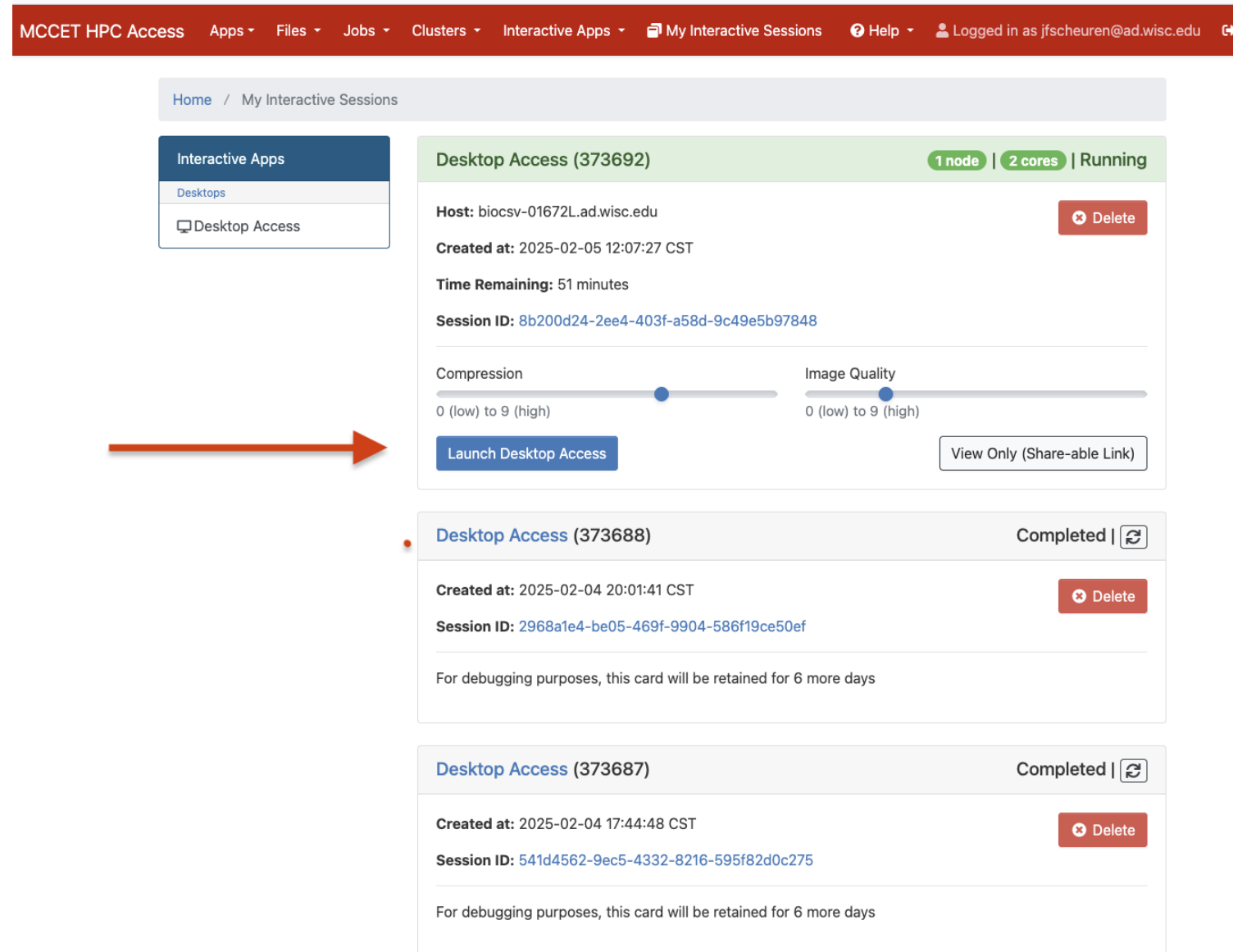
- Home directory access
- Active jobs
- Shell access
- Interactive Desktop
- Open composer

Go to <https://ondemandcryo.biochem.wisc.edu>
Login with your NetID (*Let's Try this Now!*)



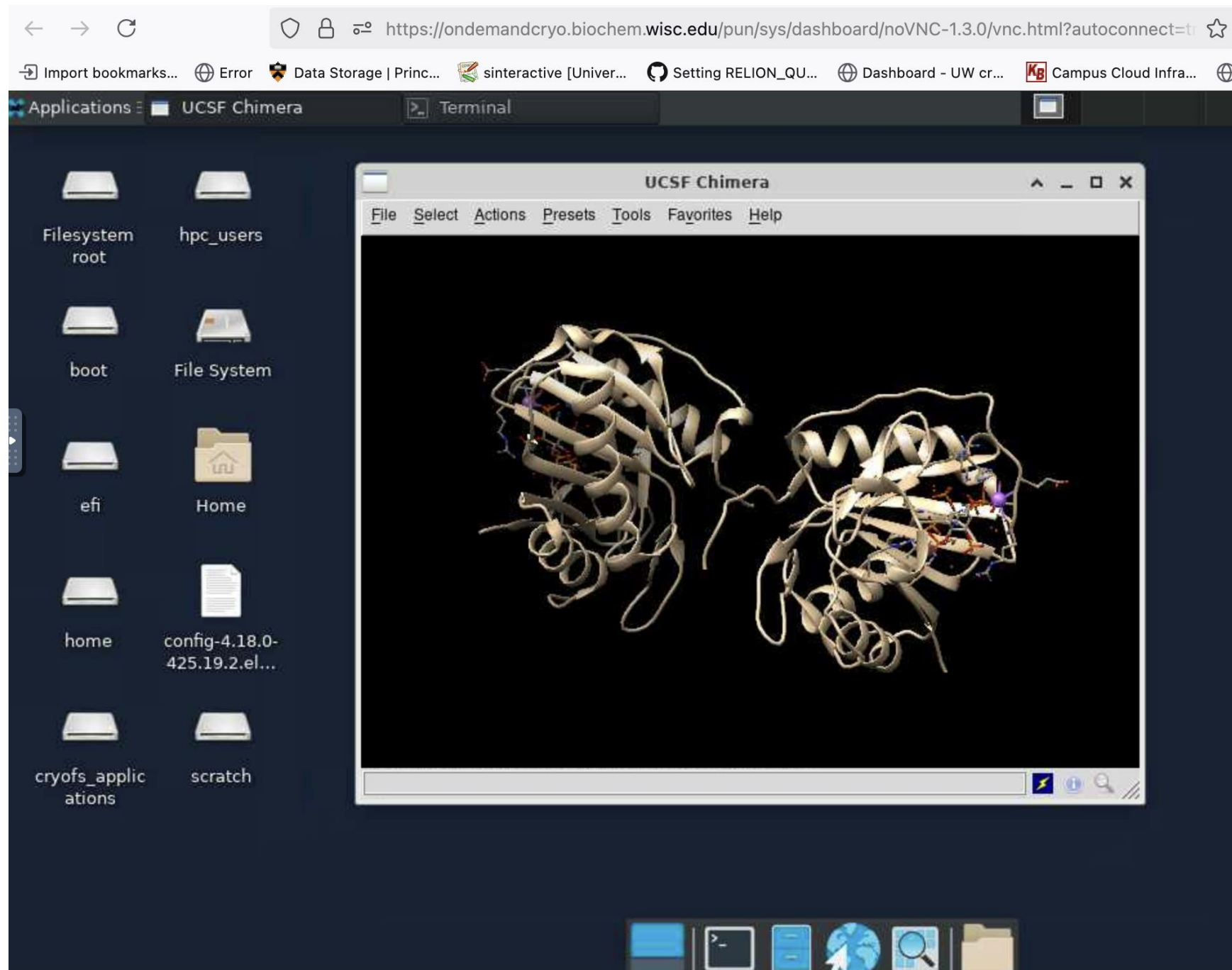
Interactive Desktop Access

- Access the desktop of one of the compute nodes. You can currently select between a machine in the cpu or a5000 queues.

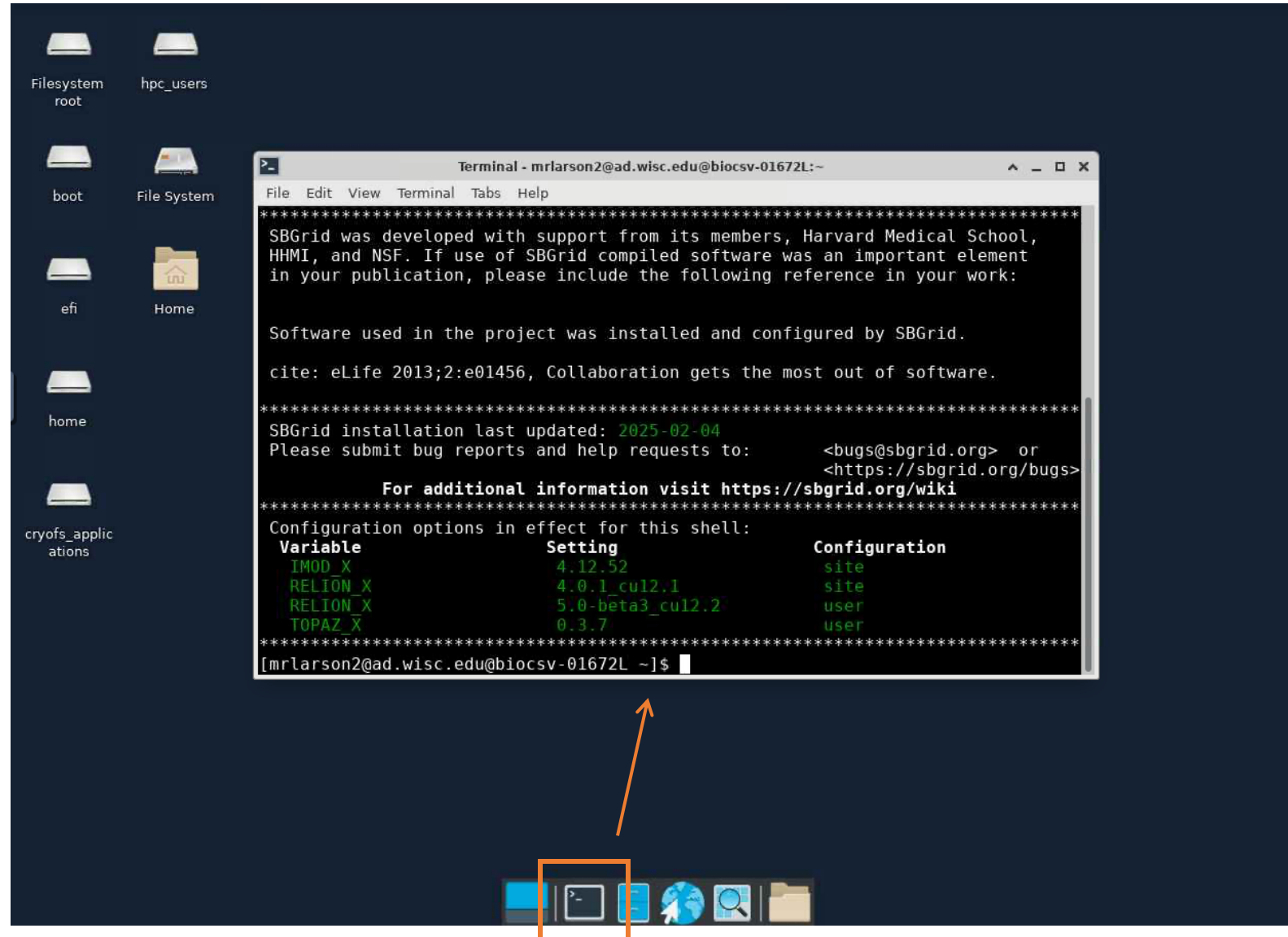


The screenshot displays the MCCET HPC Access web interface. The top navigation bar includes links for MCCET HPC Access, Apps, Files, Jobs, Clusters, Interactive Apps, My Interactive Sessions, Help, and a user login status for jfscheuren@ad.wisc.edu. The main content area is titled 'My Interactive Sessions' and features a sidebar with 'Interactive Apps' and 'Desktops' options. A red arrow points from the 'Desktops' option to the 'Desktop Access (373692)' session card. This card is currently 'Running' and shows details such as Host (biocsv-01672L.ad.wisc.edu), Created at (2025-02-05 12:07:27 CST), Time Remaining (51 minutes), and Session ID (8b200d24-2ee4-403f-a58d-9c49e5b97848). It also includes sliders for Compression and Image Quality, a 'Launch Desktop Access' button, and a 'View Only (Share-able Link)' button. Below this, two other 'Desktop Access' cards are shown, both marked as 'Completed'. The first completed card (373688) was created on 2025-02-04 at 20:01:41 CST and has Session ID 2968a1e4-be05-469f-9904-586f19ce50ef. The second completed card (373687) was created on 2025-02-04 at 17:44:48 CST and has Session ID 541d4562-9ec5-4332-8216-595f82d0c275. Both completed cards include a note: 'For debugging purposes, this card will be retained for 6 more days'.

Example Desktop: Chimera



Open a terminal in the OOD desktop



Getting started commands: sinfo

```
jfscheuren — hpcadmin@biocsv-01625L:~ — ssh hpcadmin@128.104.135.90 — 100x24
[hpcadmin@biocsv-01625L ~]$ sinfo
PARTITION AVAIL  TIMELIMIT  NODES  STATE NODELIST
a100      up     infinite    2    idle biocsv-01624L,biocsv-01625L
a5000     up     infinite    2    resv biocsv-01666L,biocsv-01667L
a5000     up     infinite    1    mix  biocsv-01668L
a5000     up     infinite    5    idle biocsv-01661L,biocsv-01662L,biocsv-01663L,biocsv-01664L,biocsv-01665L
cpu*      up     infinite    4    idle biocsv-01669L,biocsv-01670L,biocsv-01671L,biocsv-01672L
gpu       up     infinite    2    resv biocsv-01666L,biocsv-01667L
gpu       up     infinite    1    mix  biocsv-01668L
gpu       up     infinite    7    idle biocsv-01624L,biocsv-01625L,biocsv-01661L,biocsv-01662L,biocsv-01663L,biocsv-01664L,biocsv-01665L
[hpcadmin@biocsv-01625L ~]$
```

Displays partitions and state of the nodes

- See which nodes are busy – “STATE” column

Getting started commands: queue

```
jfscheuren — hpcadmin@biocsv-01625L:~ — ssh hpcadmin@128.104.135.90 — 100x24
[hpcadmin@biocsv-01625L ~]$ queue
```

JOBID	PARTITION	NAME	USER	ST	TIME	NODES	NODELIST(REASON)
831	a100	run_subm	hpcadmin	PD	0:00	1	(Resources)
829	a100	run_subm	hpcadmin	R	0:12	1	biocsv-01624L
830	a100	run_subm	hpcadmin	R	0:09	1	biocsv-01625L

```
[hpcadmin@biocsv-01625L ~]$
```

Displays pending and currently running jobs

Sbatch and Srun

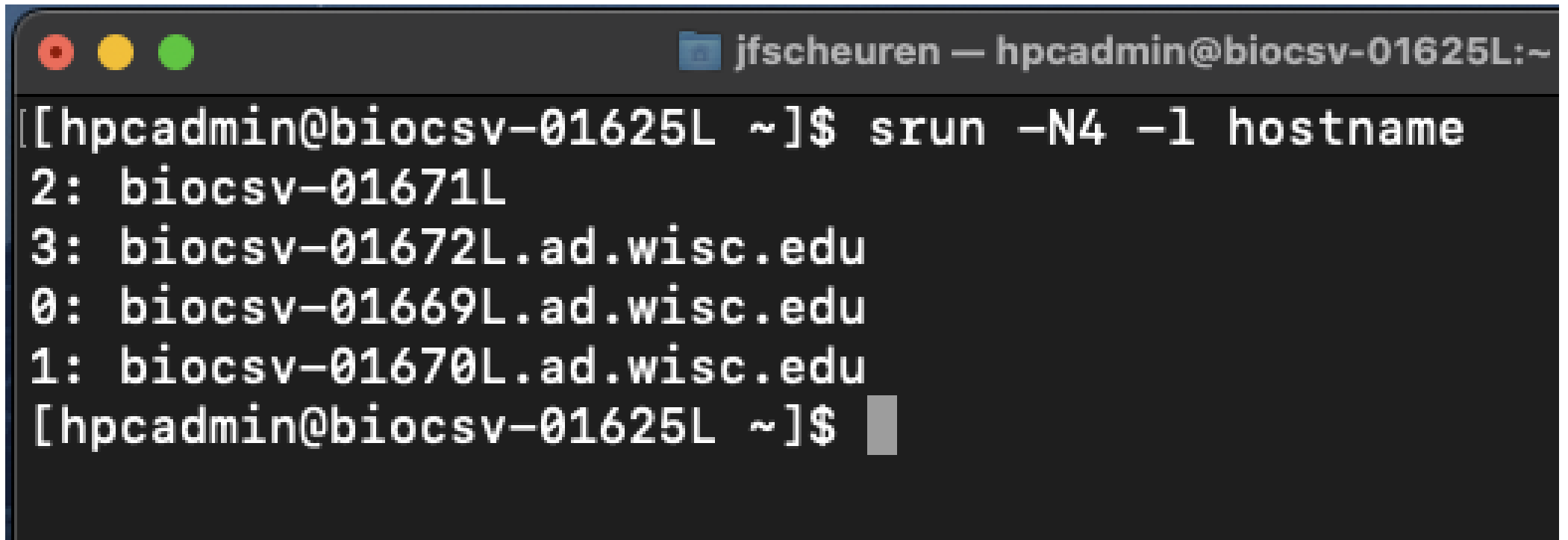
- Sbatch – submits a batch script with configuration and task commands to Slurm
- Srun – runs job interactively from command line (if you close terminal session the job will be cancelled)
- Srun – in sbatch scripts creates 'job steps' - srun jobs can be run in parallel using multiple srun commands with an "&" after the command

Job Profiles

- Each job can specify the resources it will require:
 - Partition to run on
 - Number of compute nodes to reserve
 - CPU count per node
 - CPU features
 - GPU count
 - GPU features (minimum size, etc)
 - Minimum free local space
 - Runtime required
- In SLURM, these are defined by the “Sbatch” script. (#SBATCH lines)

Run a simple command

- `srun -N4 -l hostname.` ← runs the `hostname` command on 4 different nodes

A terminal window with a dark background and light text. The title bar at the top shows three colored window control buttons (red, yellow, green) on the left and a text label 'jfscheuren — hpcadmin@biocsv-01625L:~' on the right. The terminal content shows a command prompt '[hpcadmin@biocsv-01625L ~]\$' followed by the command 'srun -N4 -l hostname'. Below the command, four lines of output are displayed: '2: biocsv-01671L', '3: biocsv-01672L.ad.wisc.edu', '0: biocsv-01669L.ad.wisc.edu', and '1: biocsv-01670L.ad.wisc.edu'. The prompt '[hpcadmin@biocsv-01625L ~]\$' appears again at the bottom, followed by a grey cursor block.

```
jfscheuren — hpcadmin@biocsv-01625L:~  
[hpcadmin@biocsv-01625L ~]$ srun -N4 -l hostname  
2: biocsv-01671L  
3: biocsv-01672L.ad.wisc.edu  
0: biocsv-01669L.ad.wisc.edu  
1: biocsv-01670L.ad.wisc.edu  
[hpcadmin@biocsv-01625L ~]$
```


Sbatch example

```
#!/bin/bash

#SBATCH --partition=cpu      ## specify which partition (group of nodes) to run on
#SBATCH --nodes=1           ## specify how many nodes to use
#SBATCH --cpus-per-task=1   ## number of cpus per task
#SBATCH --mem=100M          ## amount of memory to be allocated from node
#SBATCH --time=1:00:00     ## allowed runtime

srun hostname               ## command to be run
```

~

Building jobs with Open OnDemand: Open Composer

- View and submit jobs
- Works better than built-in Job Composer

[Top](#) [Application ▾](#) [History](#) [Open OnDemand](#)

slurm

This application generates an arbitrary job script in Slurm.

Script Location*
[Select Path](#)

Script Name*

Job Name

Partition

Number of cores (1 - 48)

Maximum run time hours (0 - 24)

Maximum run minutes (0 - 59)

Array Job (start index)

Array Job (last index)

Script Contents

```
#!/usr/bin/env bash
#SBATCH -p a100
#SBATCH -n 1
#SBATCH -t 1:0:00
```

Each job executed from an array job is assigned a task ID, which can be referenced in the shell script via the environment variable SLURM_ARRAY_TASK_ID.

[Submit](#)

MCCET UW-Madison

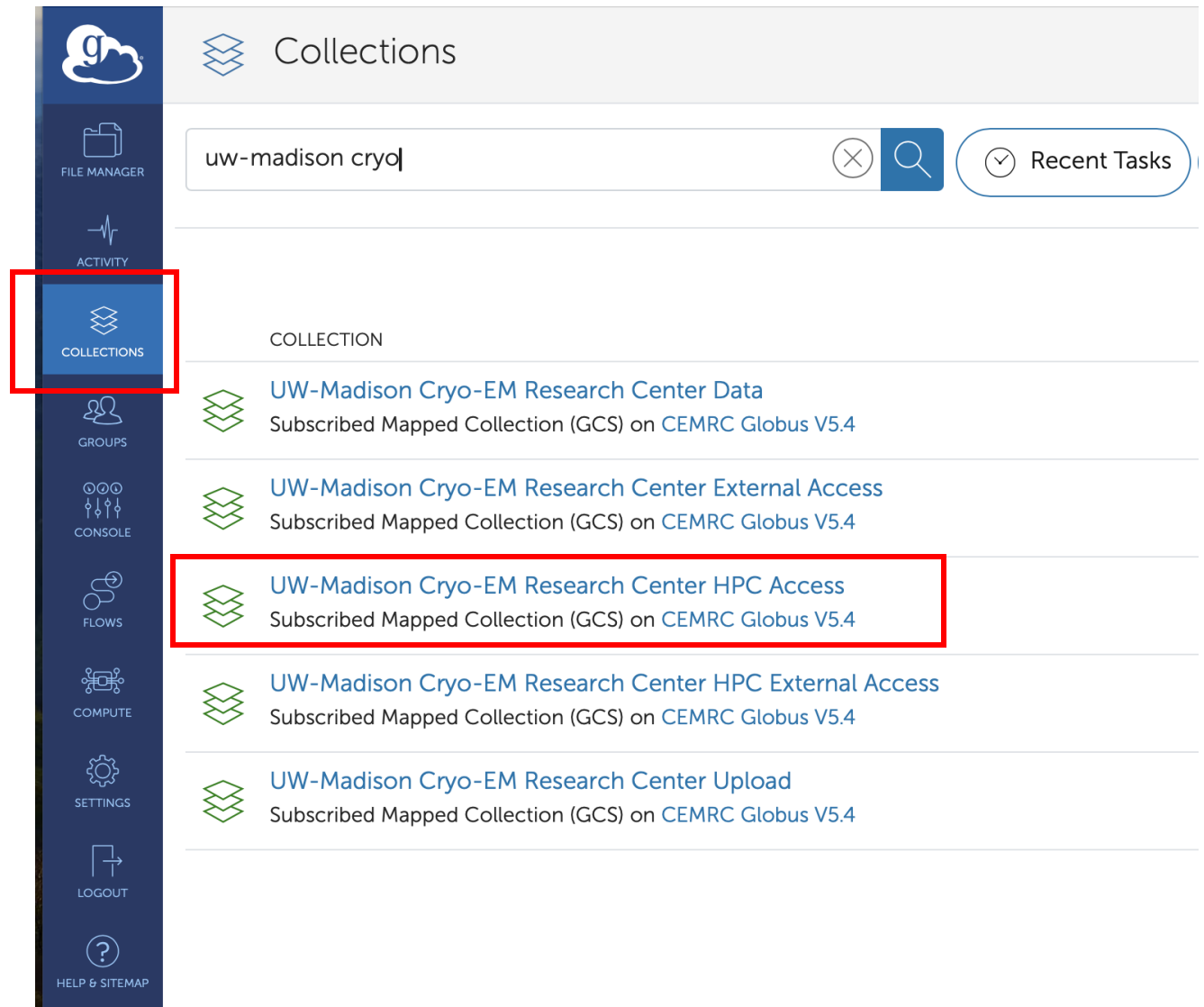
Open Composer version: 1.2.0

Finding on Globus

Go to <https://app.globus.org> to use the Globus tool for moving data between facility and research group collections

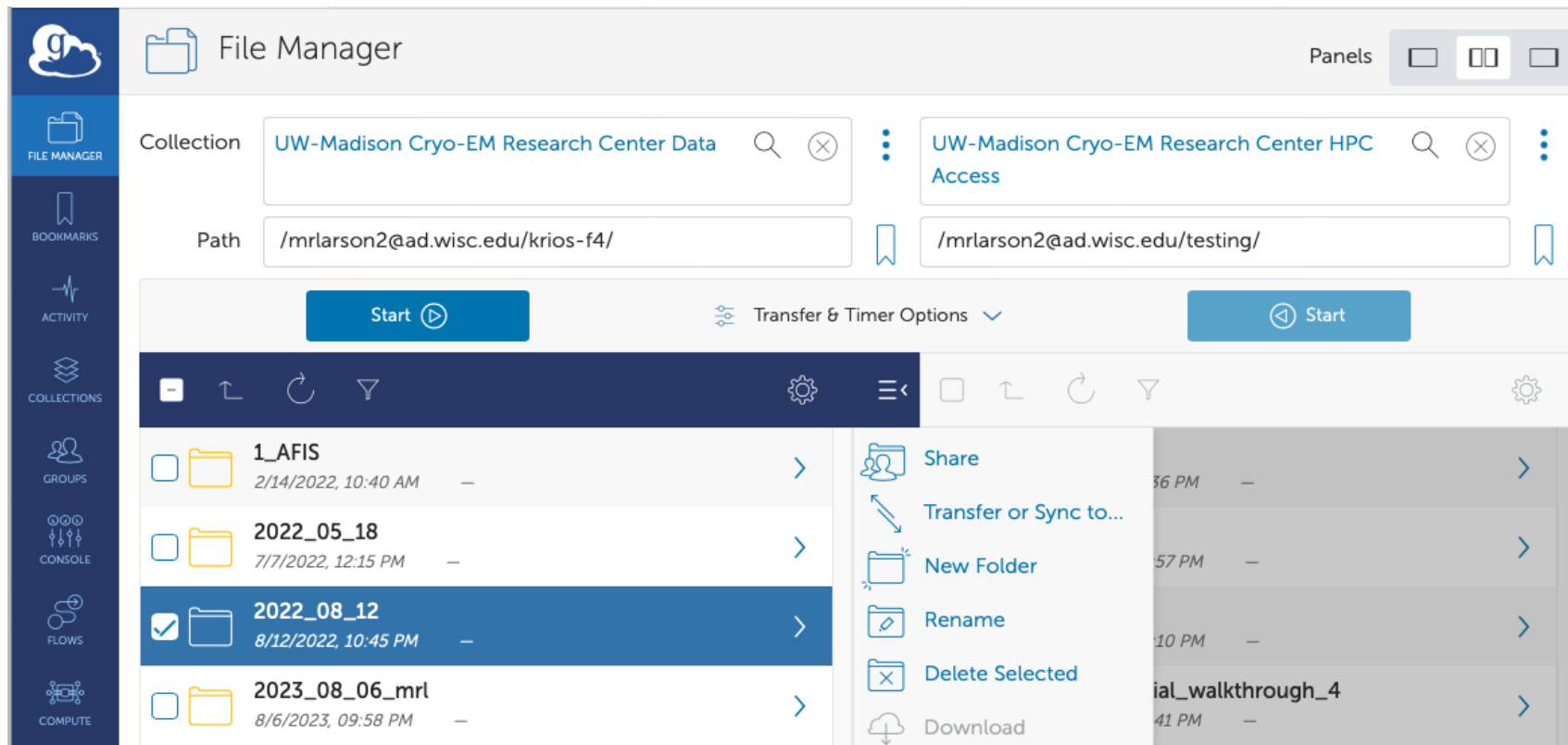
This will go directly to your home directory on the cluster.

You can setup a second collection with Cryo-EM Center Data or Wright lab collections to copy data.



Examples: transfer via Globus

- Choose a dataset and set destination to the HPC cluster, Start!



See also “UW-Madison Wright” for transfers to/from cryofs_wright data.

Getting started: submitting an AreTomo job

submit_to_a5000.sh AreTomo -InMrc 1138_G1__L4_TS_001_aligned.st -OutMrc test/tomogram.mrc -VolZ 1350 -AlignZ 1200 -OutBin 6 -DarkTol 0.1 -FlipVol 1 -Kv 300 -PixSize 1.4 -Wbp 1 -AngFile angles.txt -Patch 4 4 -TiltAxis 89.9

Submits a job via the pre-built Sbatch script from **/mnt/hpc_users/share/sbatch/a5000_gpu_sbatch.sh**

Outputs are “Submitted batch job 833” after job starts, and then you can follow output of the jobs via “slurm.out” and “slurm.err” and the results in the “test/” output folder.

tail -f slurm_<id>.out to follow the standard output.

ssh -YC netid@wisc.edu@cryoemcluster.biochem.wisc.edu

`cd $HOME`

`tar -xvf /mnt/hpc_users/share/resources/HPC_sample_data.tar`

`cd HPC_sample_data/AreTomo_2023_07_13/Evaluation/1138_G1_L4_TS_001/`

> Examine the command for AreTomo

`cat Example_Command.sh`

> Submit your job!

`submit_to_gpu.sh ./Example_Command.sh`

> Check what is running!

`squeue`

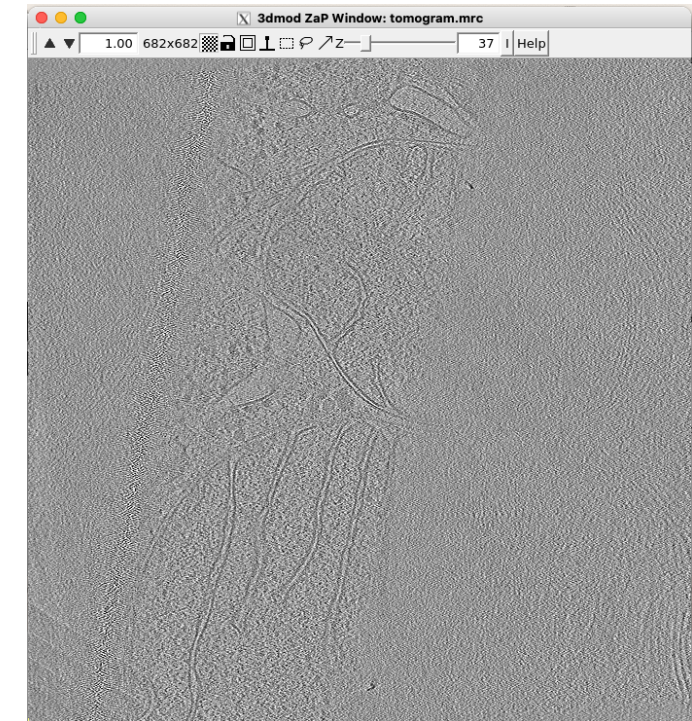
JOBID	PARTITION	NAME	USER	ST	TIME	NODES	NODELIST(REASON)
845	gpu	gpu_sbat	mlarson	R	9:18	1	biocsv-01668L

`sinfo`

> See output of the job and view the results...

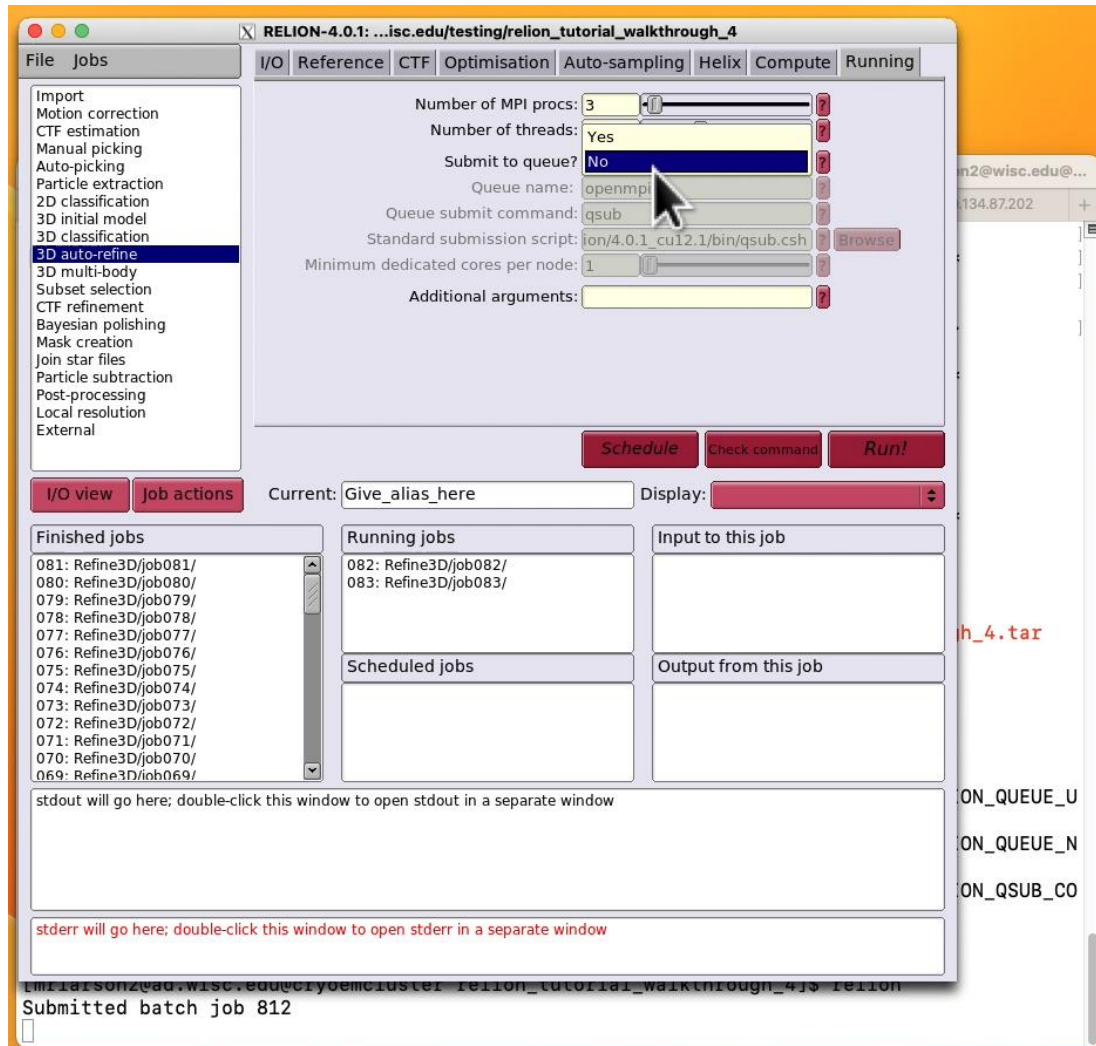
`tail -f slurm_<jobid>.out`

`3dmod output/tomogram.mrc`



Demo /w AreTomo

RELION -> SLURM



Enable “**Submit to queue**” to provide SLURM specific options command + queue.

Needs a “Standard submission script” :

/mnt/hpc_users/share/sbatch/relion_template_**gpu**.sh

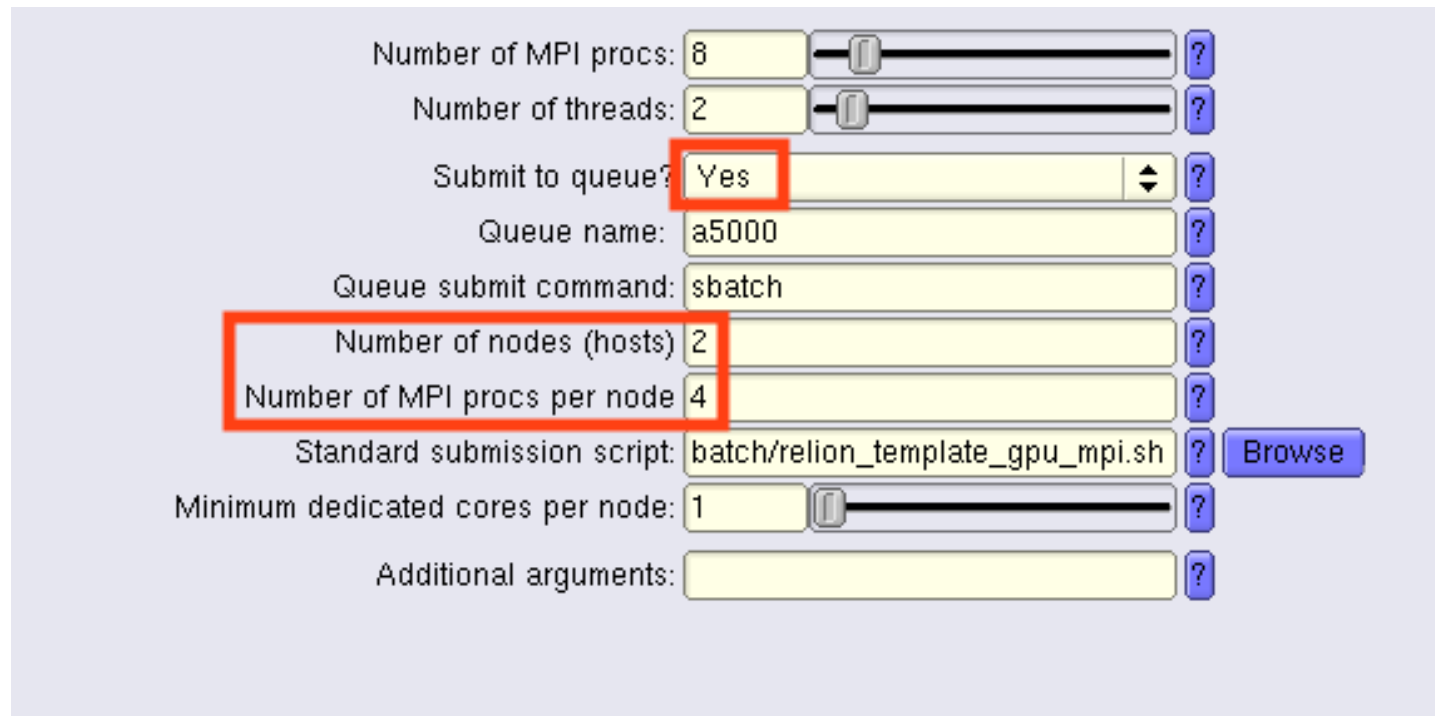
or

/mnt/hpc_users/share/sbatch/relion_template_**cpu**.sh

RELION

RELION – using multiple nodes (MPI)

- Some jobs can be split among multiple nodes for faster processing
- Use the `relion_template_gpu_mpi.sh` or the `relion_template_cpu_mpi.sh` submission script
- Set number of nodes to < 8 for a5000 jobs. Set number of nodes to 2 for a100 jobs. Set number of nodes to < 4 for cpu jobs.



The screenshot displays the RELION submission configuration interface. The following fields are visible:

- Number of MPI procs: 8 (with a slider)
- Number of threads: 2 (with a slider)
- Submit to queue? Yes (highlighted with a red box)
- Queue name: a5000
- Queue submit command: sbatch
- Number of nodes (hosts) 2 (highlighted with a red box)
- Number of MPI procs per node 4 (highlighted with a red box)
- Standard submission script: batch/relion_template_gpu_mpi.sh (with a "Browse" button)
- Minimum dedicated cores per node: 1 (with a slider)
- Additional arguments: (empty field)

Each field has a blue question mark icon to its right.

Command-line example: AlphaFold job

AlphaFold requires a FASTA input (T1083.fasta):

```
>T1083
```

```
GAMGSEIEHIEEAIANAKTKADHERLVAHYEEEAKRLEKKSEEYQELAKVYKKITDVYPNIRSYMVLHYQNLTRRYKE  
AAEENRALAKLHHELAIVED
```

Submit via an Sbatch wrapper script:

```
submit_to_a5000.sh /mnt/hpc_users/share/bin/alphafold-monomer.sh T1083.fasta
```

Policies

- Start jobs from the login node, but do not run significant processing on login node. Using significant resources on the login node will result in a warning and repeat offense will result in a locked account. Jobs running on the login node will be stopped.
- Large datasets should be removed from the cluster storage when jobs are complete. Cluster space will be audited periodically and users with old data will be contacted for transferring off storage.
- Each account is limited to 5TB quota in the shared network storage.

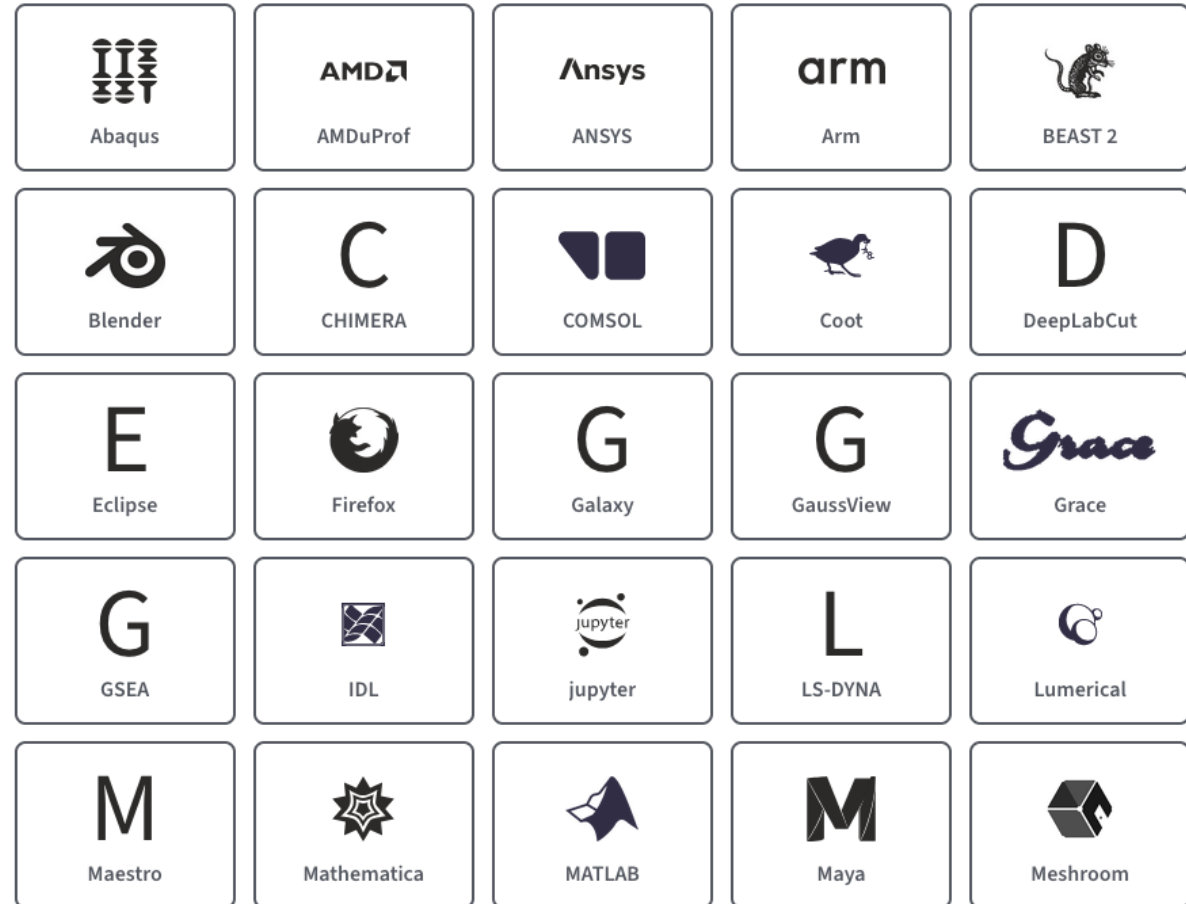
Other integrated OOD applications to consider

- <https://openondemand.org/run-open-ondemand#enabled-applications>
- Some of these other integrated applications might be useful to test on the HPC cluster.
- Applications available via SBGrid can always be used directly whether connecting via SSH or Open OnDemand.
- Some graphical applications may work better via the Open OnDemand Desktop (ex. Chimera, IMOD, and Napari).

FIND SOFTWARE:

All

Popular



Thank you!



**Cryo Electron Microscopy
Research Center**
DEPARTMENT OF BIOCHEMISTRY
UNIVERSITY OF WISCONSIN-MADISON

**Supported by the Department of Biochemistry at UW-Madison and
Morgridge Institute for Research**

- Director Elizabeth Wright
- CEMRC Staff and Wright Lab members
- NIH support for the National Centers for cryo-ET U24 GM139168-01
- Robert Landick, UW2020: WARF Discovery Initiative Award
- VCRGE Office for Research
- UW SMPH and CALS
- DoIT (networking, Globus, and hosting)



CEMRC Contacts: <https://cryoem.wisc.edu> cryoem@biochem.wisc.edu

- Elizabeth Wright (erwright2@wisc.edu)
- Jennifer Scheuren (jfscheuren@wisc.edu) - HPC Administrator
- Matt Larson (mrlarson2@wisc.edu) – CS and SysAdmin

Questions and Discussion

- What additional software should we support on the cluster?
(Cryosparc, Matlab, Jupyter)
- What additional training would be useful?
<https://bcrf.biochem.wisc.edu/all-tutorials/>
- Visit the UW-Madison Cryo-EM documentation for additional information and guidance (<https://uwcryoem.github.io>)

