# Intro to Cryo-EM / Cryo-ET High Performance Computing Cluster

The UW-Madison Cryo-EM Research Center and Midwest Center for Cryo Electron Tomography have a dedicated computing cluster resource, which can accelerate your data processing. New cluster users should apply for an account at:

https://explore.wisc.edu/cryoem\_hpc\_access\_request

# Connecting to the Cryo-EM HPC Cluster

Option #1) SSH

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

Option #2) Open OnDemand portal

https://ondemandcryo.biochem.wisc.edu

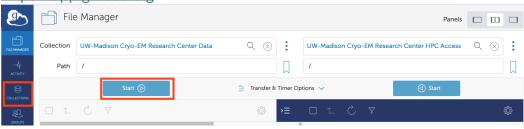


#### **Linux Commands**

ls	Directory listing
ls -l	Formatted listing with information
cd <dir></dir>	Change to directory <dir></dir>
cd	Change to your home directory (/mnt/hpc_users/home/)
pwd	Show current directory
mkdir <dir></dir>	Make a directory <dir></dir>
rm <file></file>	Remove file
mv <file1> <file2></file2></file1>	Move a file to a new location
sinfo	Give current status of the SLURM queue(s)
squeue	List current submitted and running jobs.
scancel <id></id>	Cancel a job id
	,
submit_to_a5000.sh	Submit a job to NVIDIA A5000 queue (requests node /w 4 GPU)
submit_to_a100.sh	Submit a job to NVIDIA A100 queue (higher memory GPU cards)
submit_to_cpu.sh	Submit a job to CPU-only systems, no GPU provided.

## Globus File Transfers

https://app.globus.org

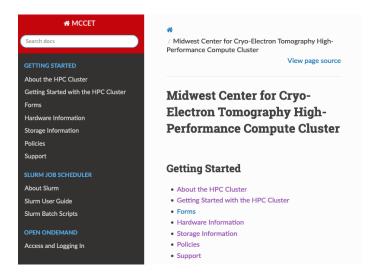


Select your files in the collections you want to transfer, then choose "Start" to begin transferring data to your HPC user home directory, or bringing results back to own storage.

## Documentation available

Learn and get help using SLURM and the HPC cluster.

### https://uwcryoem.github.io/



# Support and Help

Contact jfscheuren@wisc.edu and CC: cryoem@biochem.wisc.edu for email inquiries.

Attend the Office Hours on Thursdays at 9am at the Cryo-EM Office HF Deluca B1131 for questions and help using the HPC cluster.

#### Common Scientific Software

Chimera and ChimeraX	Viewer and visualizations for .mrc data and structures
IMOD, 3dmod, etomo	Image processing, modeling and display programs used
inob, sumou, etomo	for tomographic reconstruction
	9 1
IsoNet	Reconstruct contents of the missing wedge in electron
	tomography
RELION	Single-particle analysis for Cryo-EM and Tomography
	processing workflow in Cryo-ET.
MotionCorr2 / MotionCorr3	Software packages for GPU accelerated motion
	correction of micrographs.
AreTomo	GPU-accelerated software for fiducial-free alignment
	and reconstruction for cryoEM tomography
Dynamo, emClarity, PEET	Subtomogram averaging software packages.
EMAN2	Single-particle analysis for Cryo-EM and for cryo-ET
LITAINZ	- · · · · · · · · · · · · · · · · · · ·
	image processing.