HIGH PERFORMANCE RESEARCH COMPUTING

ACES: Introduction to CryoSPARC for Cryo-EM Data Processing in Collaboration with the Laboratory for Biomolecular Structure and Dynamics

High Performance
Research Computing
DIVISION OF RESEARCH

Spring 2026

CryoSPARC on ACES

- CryoSPARC Academic License ID
- Computing Resources and Limitations
- CryoSPARC on the ACES Portal
- Group Data Directories
- Launch a CryoSPARC Interactive Job
- CryoSPARC Live
- CryoSPARC Interactive Tutorial

CryoSPARC Academic License ID

- CryoSPARC provides a personal Academic License ID free of charge for TAMU staff and students
- A CryoSPARC Academic License ID is required to launch the CryoSPARC ACES portal app
- Use your academic email address for the Academic License
  - https://cryosparc.com/download

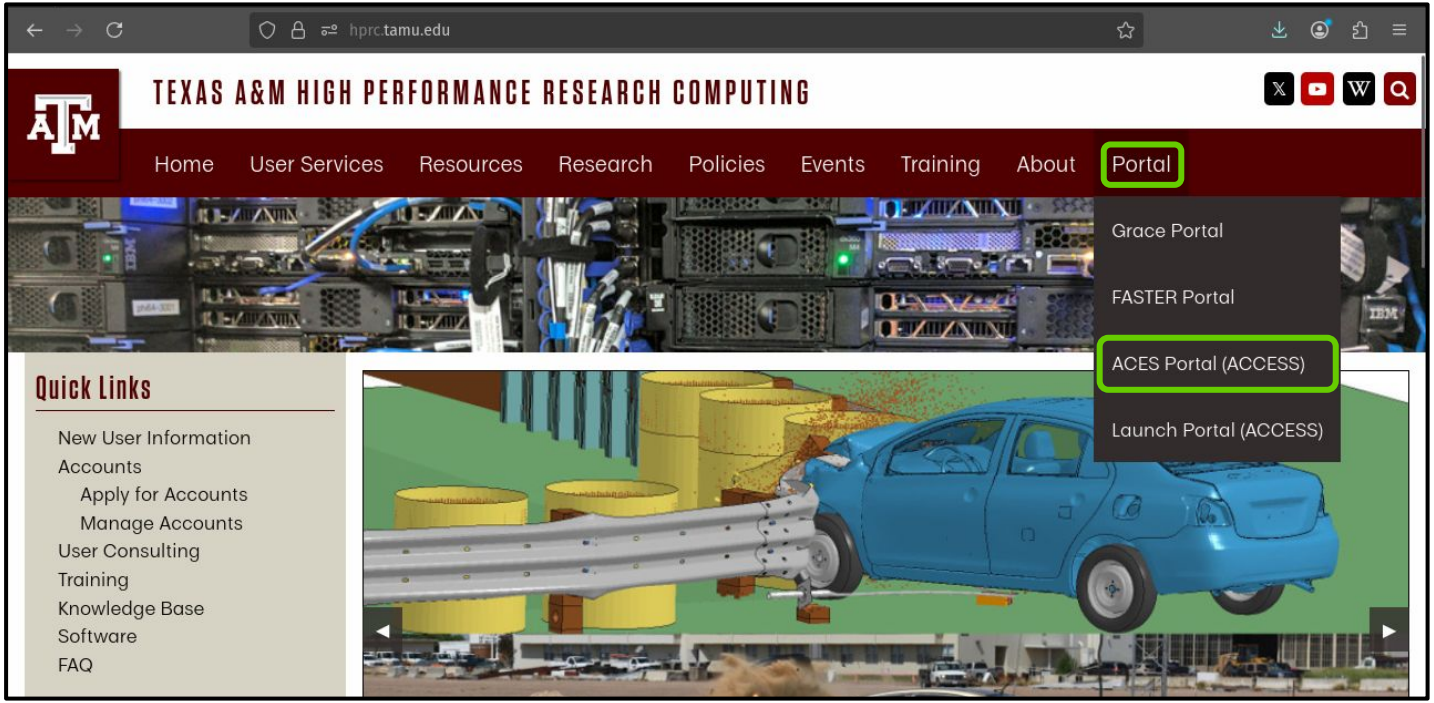
Resources for Running CryoSPARC

- CryoSPARC is available as an Interactive App on the ACES Portal
  - https://portal-aces.hprc.tamu.edu
- ACES hardware overview (can change since ACES is a composable resource cluster)
  - 30 x H100 GPUs (2 x H100 GPUs per node)
  - 6 x A30 GPUs (6 x A30 GPUs per node)
  - 70 x CPU only nodes
  - 10 x other specialized nodes not supported by CryoSPARC
- Specify enough time to allow your processing to complete
- If you launch a job for 24 hours and you finish your work in 12 hours, delete your portal app job to make GPUs resources available for other jobs

Resource Limitations

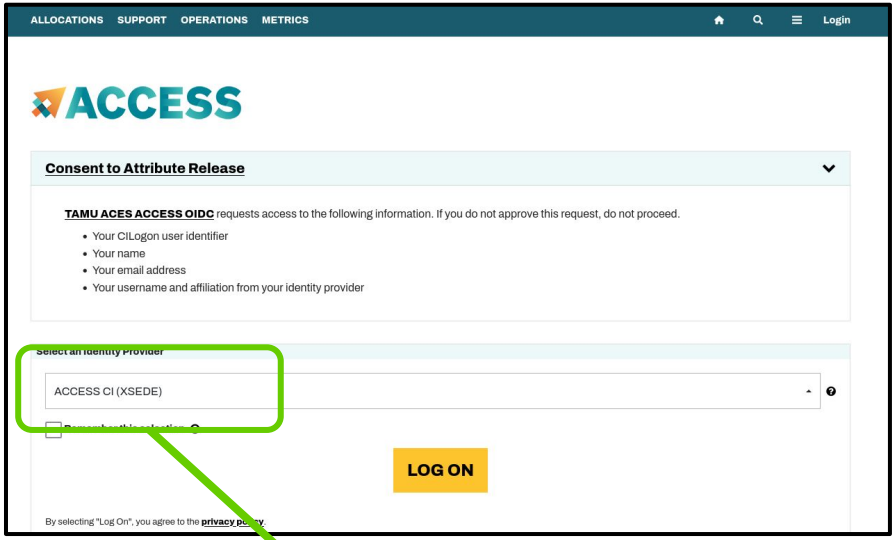
- Can only launch one CryoSPARC portal session at a time
  - can run multiple CryoSPARC jobs within a portal session
- CPUs
  - Some CryoSPARC tasks, such as importing images, do not require a GPU
- GPUs
  - The GPU queue can get busy at times and it may take over an hour for your job to launch
  - Cancel your pending job if you will be away from your computer for a long time and it hasn't started yet
  - CryoSPARC does not support PVC GPUs
- Submitted jobs can have delayed start times due to unavailability of GPUs or scheduled system maintenance

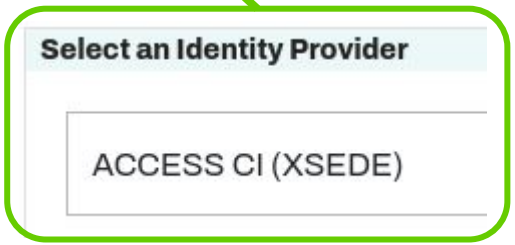
Accessing the HPRC ACES Portal



HPRC webpage: hprc.tamu.edu

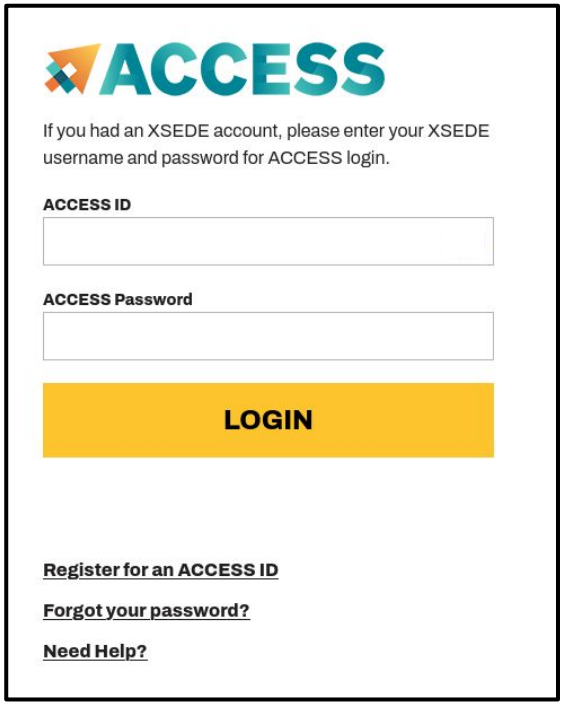
Accessing ACES via the Portal (ACCESS)





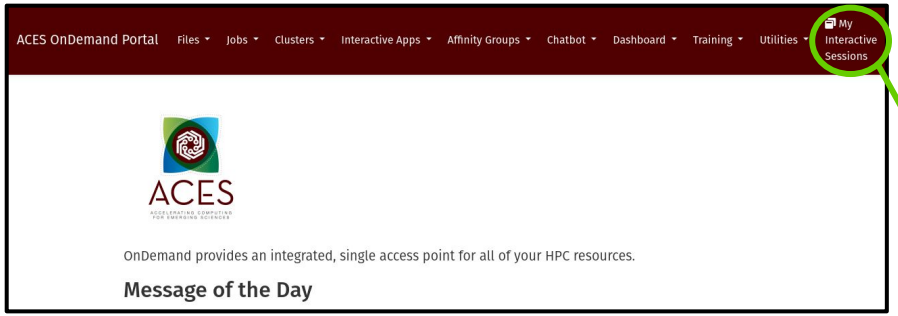
Select the Identity Provider appropriate for your account. ACCESS CI (XSEDE) or search for your institution whichever you used during registration.

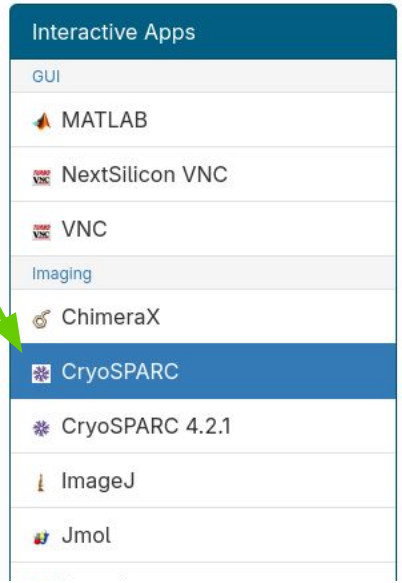
Log-in using your ACCESS credentials.

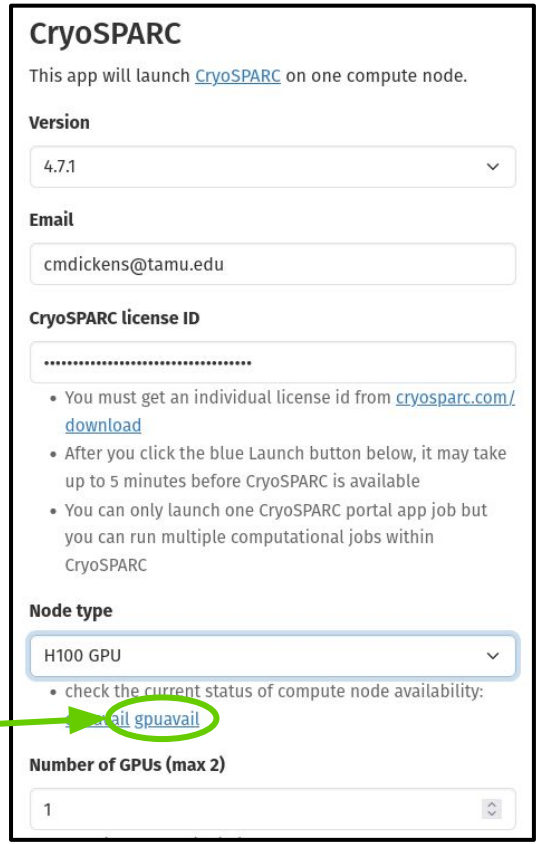


ACES CryoSPARC Interactive App

portal-aces.hprc.tamu.edu







check GPU availability

gpuavail: ACES GPU Configuration & Availability

ACES GPU Availability

This displays the CONFIGURATION of installed GPUs and the status of GPUs readily available for jobs.

GPUs and GPU nodes not in the AVAILABILITY table are busy with other jobs and will be available after jobs have completed.

Output generated: **2026-03-16 14:04:24**

```
$ gpuavail -s type
```

CONFIGURATION	
NODE TYPE	NODE COUNT
gpu:pvc:4	16
gpu:pvc:2	9
gpu:pvc:8	4
gpu:h100:8	2
gpu:h100:4	2
gpu:a30:2	1
gpu:ve:8	1

AVAILABILITY						
NODE COUNT	GPU TYPE	GPU COUNT	GPU AVAIL	CPU AVAIL	GB MEM AVAIL	PARTITION
1	a30	2	**1**	88	438	gpu,gpu_debug
1	pvc	4	**3**	92	481	pvc
4	pvc	8	**8**	96	488	pvc
1	pvc	6	**6**	96	488	pvc
1 (reserved)	pvc	4	**4**	96	488	pvc
8	pvc	2	**2**			
10	pvc	4	**4**			

CryoSPARC does not support PVC GPUs

https://hprc.tamu.edu/kb/Software/useful-tools/gpuavail

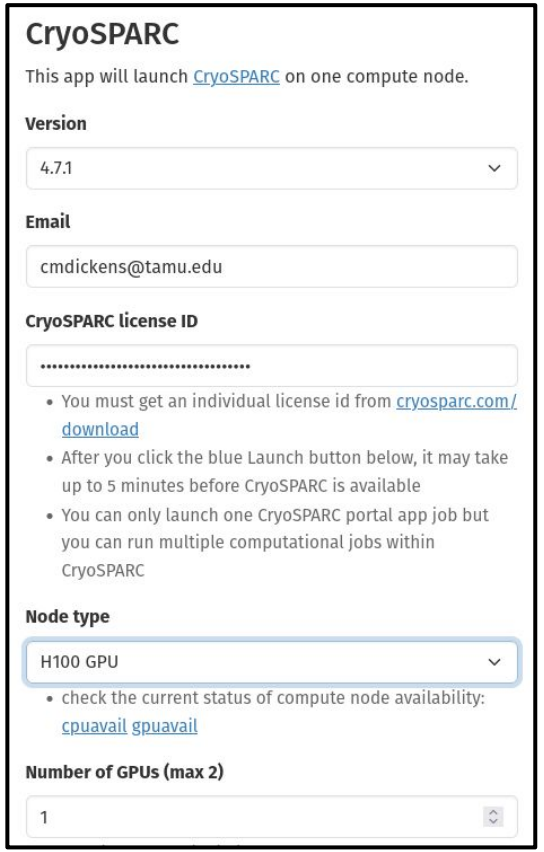
Launch a CryoSPARC Interactive Job

Input your Email and License ID

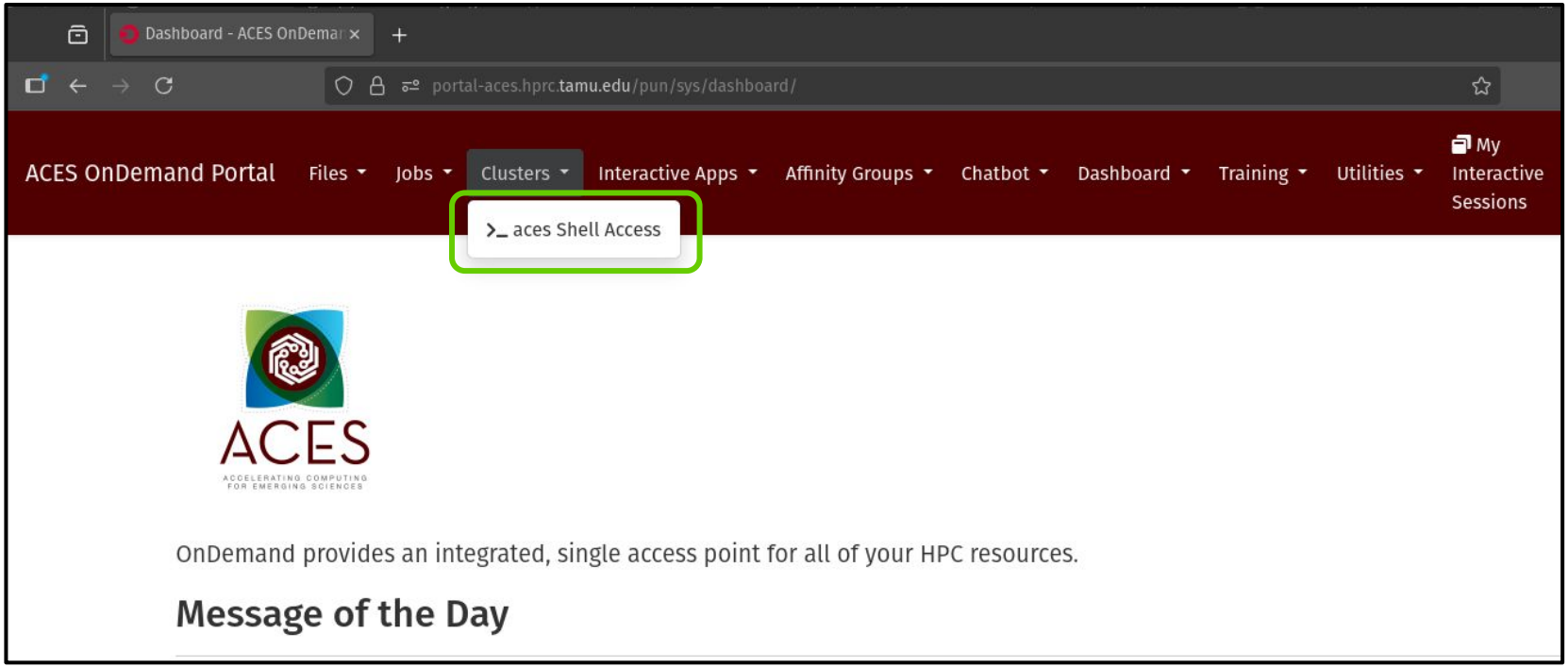
Select a GPU Node type

Number of GPUs = 1

Click the blue Launch button



Shell Access via the ACES Portal



ACES Command Line

Use the "aces Shell Access" to create directories for use with CryoSPARC projects

```
[userid@aces-login ~]$ cd $SCRATCH

[userid@aces-login userid]$ mkdir -p cryosparc_projects/cryosparc_live/first_run/data

[userid@aces-login userid]$
```

the -p option is used to create directories within a directory that does not yet exist

Group Data Directories

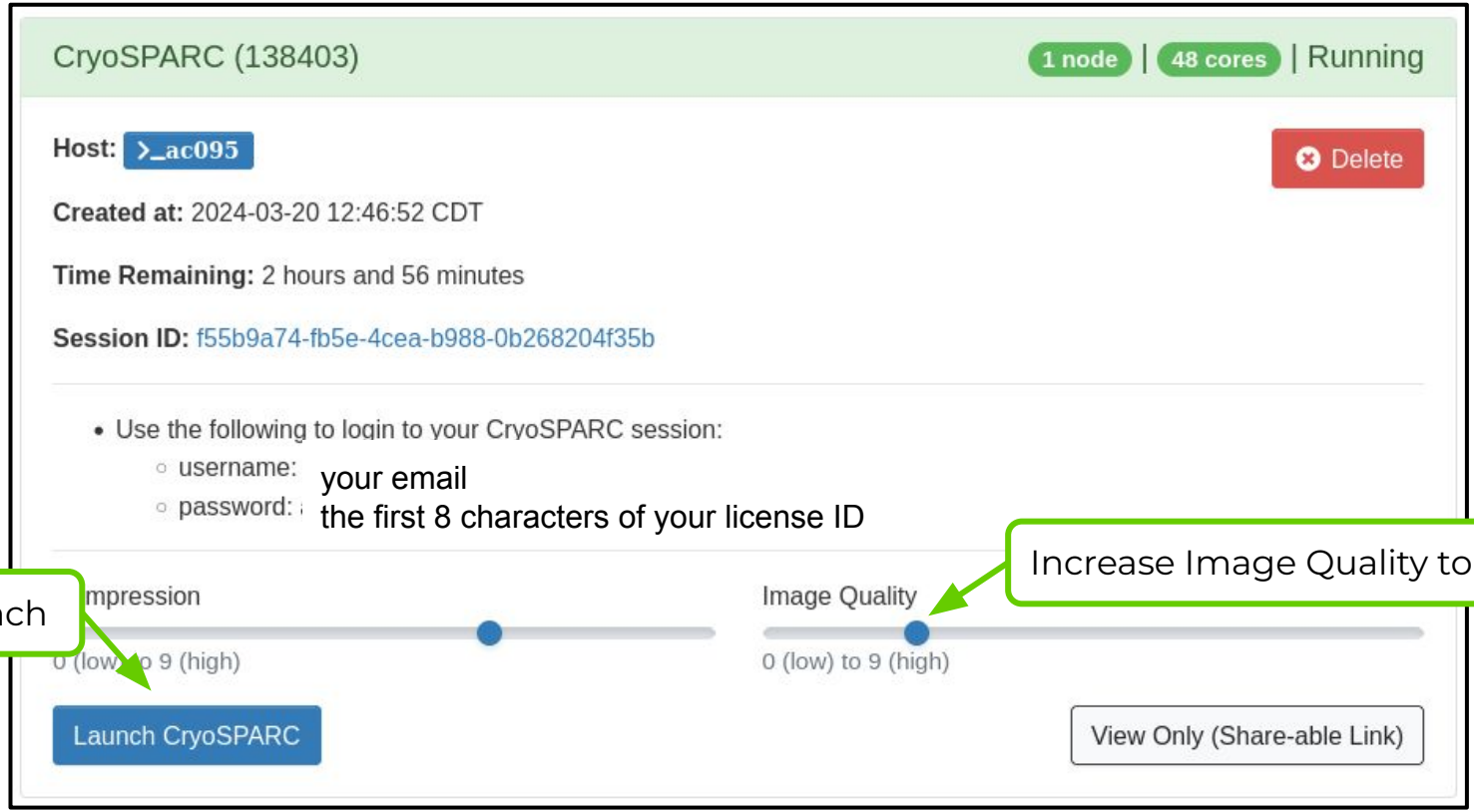
- Group data directories can be used to share input files and to have a group work space
- Each PI receives a 5TB group directory that the PI's researchers can access for reading and writing files

ACES Maintenance

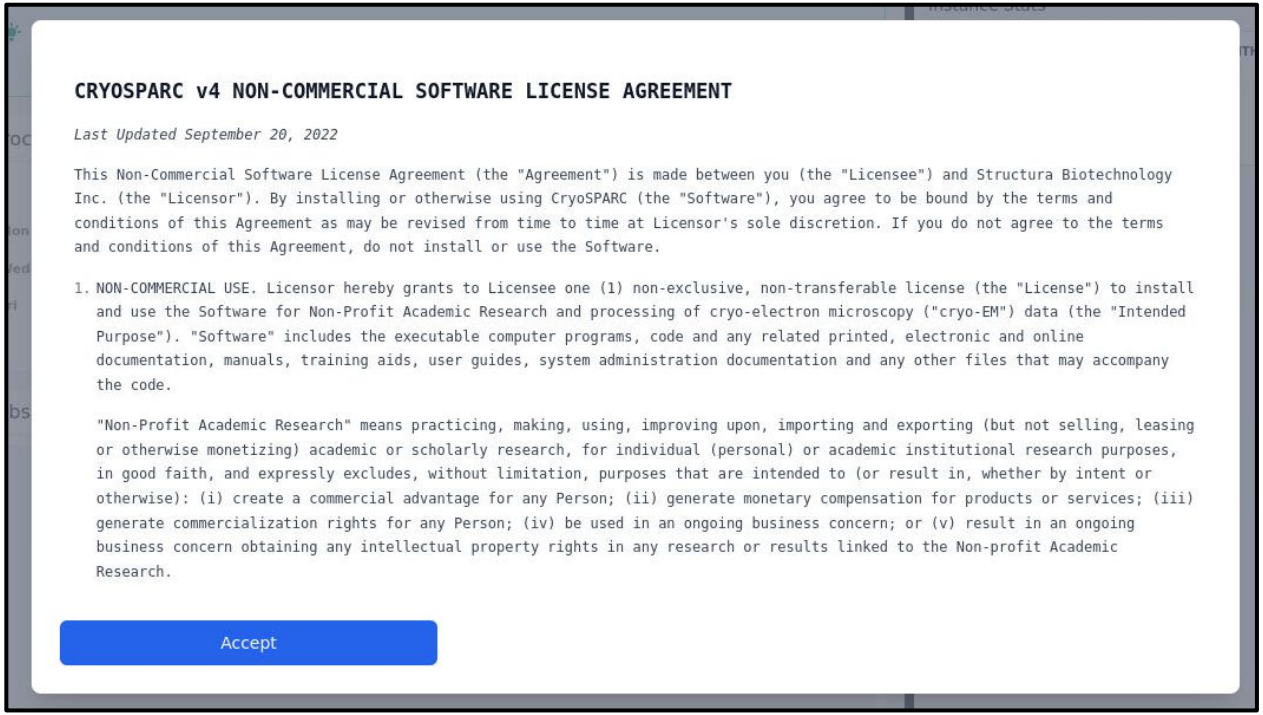
- ACES will be offline during routinely scheduled maintenances which may occur a few times each year
- Submitted jobs will remain PENDING and not run if the job script wall time overlaps with the maintenance start time
- When maintenance is complete, scheduled jobs will automatically begin running based on priority
- Use the **`maintenance`** command to see if a maintenance is scheduled and to display the time until the start of the maintenance

```
[userid@aces-login ~]$ maintenance

 The scheduled 35 hour ACES maintenance will start in:

  3 days    21 hours    32 minutes

Scheduled jobs will not start if they overlap with this maintenance window.
```

ACES CryoSPARC Running Job



Read and Accept the License



CRYOSPARC v4 NON-COMMERCIAL SOFTWARE LICENSE AGREEMENT

Last Updated September 20, 2022

This Non-Commercial Software License Agreement (the "Agreement") is made between you (the "Licensee") and Structura Biotechnology Inc. (the "Licensor"). By installing or otherwise using CryoSPARC (the "Software"), you agree to be bound by the terms and conditions of this Agreement as may be revised from time to time at Licensor's sole discretion. If you do not agree to the terms and conditions of this Agreement, do not install or use the Software.

1. NON-COMMERCIAL USE. Licensor hereby grants to Licensee one (1) non-exclusive, non-transferable license (the "License") to install and use the Software for Non-Profit Academic Research and processing of cryo-electron microscopy ("cryo-EM") data (the "Intended Purpose"). "Software" includes the executable computer programs, code and any related printed, electronic and online documentation, manuals, training aids, user guides, system administration documentation and any other files that may accompany the code.

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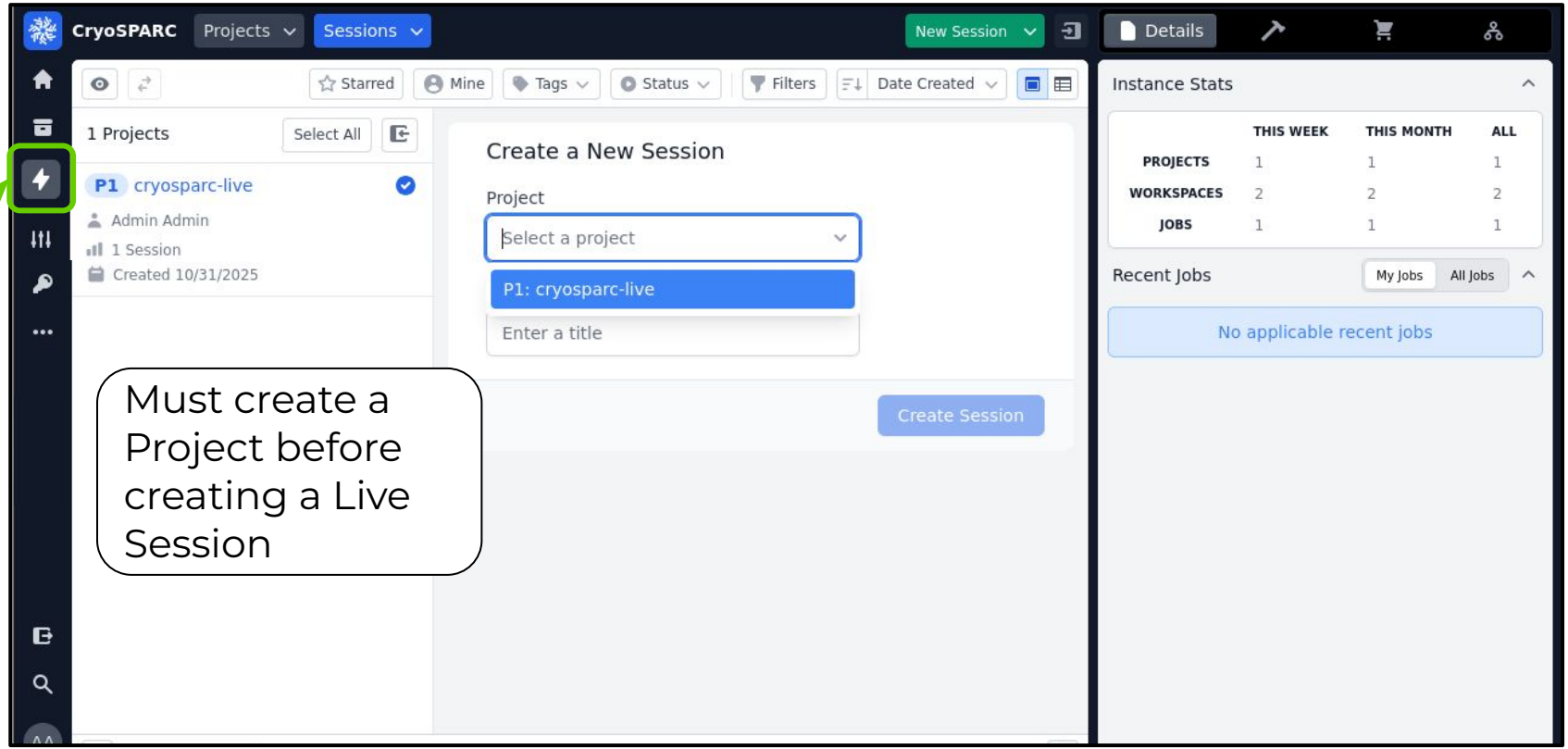
Accept

CryoSPARC Live

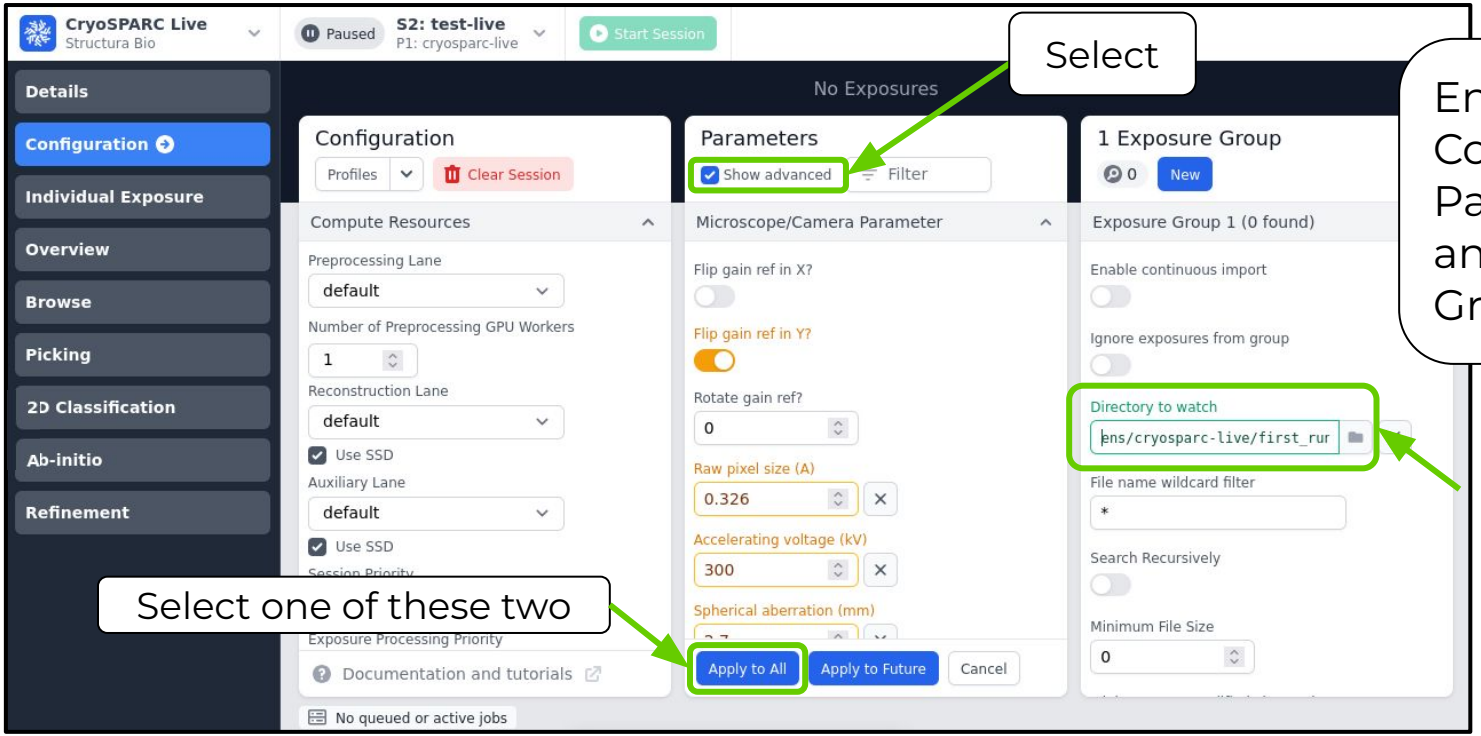
- A CryoSPARC Live session can be configured and saved in preparation for processing image files as they become available
- Mounting an ACES directory on your workstation is not supported. Use Globus Connect Personal to copy files to ACES as they become available
  - Configure Globus Connect Personal with a directory on ACES that CryoSPARC will watch and process files as they are uploaded
  - https://hprc.tamu.edu/kb/Software/Globus
- Launch CryoSPARC with enough time to cover the duration of image generation and processing

CryoSPARC Live



Must create a Project before creating a Live Session

CryoSPARC Live Session



Click the green "Start Session" button when you are ready to start the Live Session

End CryoSPARC Session when finished working

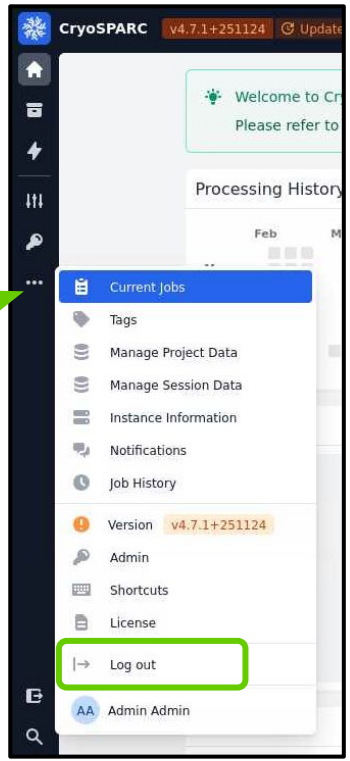
Make sure all processing is complete

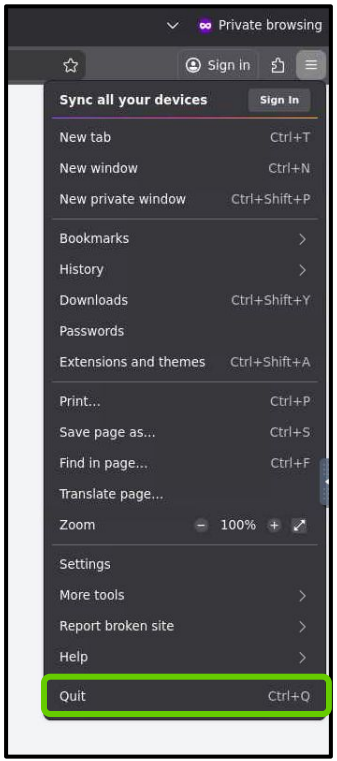
Pause any Live sessions

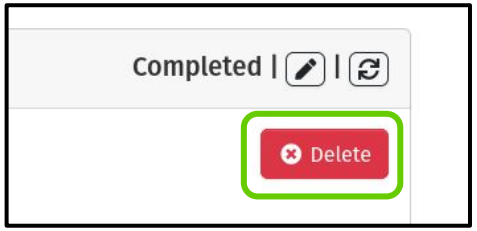
Log out of CryoSPARC

Quit the Firefox Browser

Delete the Portal session







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Help us help you. Please include details in your request for support, such as, Cluster (ACES, FASTER, Grace, Launch), NetID (UserID), Job information (JobID(s), Location of your jobfile, input/output files, Application, Module(s) loaded, Error messages, etc), and Steps you have taken, so we can reproduce the problem.

CryoSPARC Tutorial
presented by:

Gaya Yadav, PhD

Cryo-EM Technical Director at the Laboratory for Biomolecular Structure and Dynamics