

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

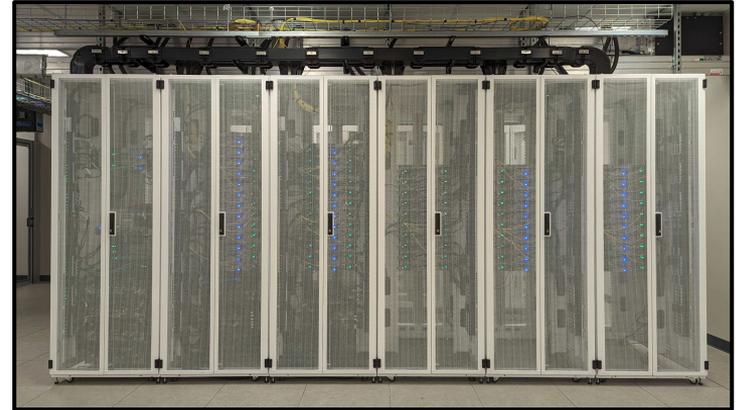
- CryoSPARC Academic License ID
- Computing Resources and Limitations
- CryoSPARC on the ACES Portal
- Group Data Directories
- Launch a CryoSPARC Interactive Job
- CryoSPARC Live
- CryoSPARC Interactive Tutorial

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

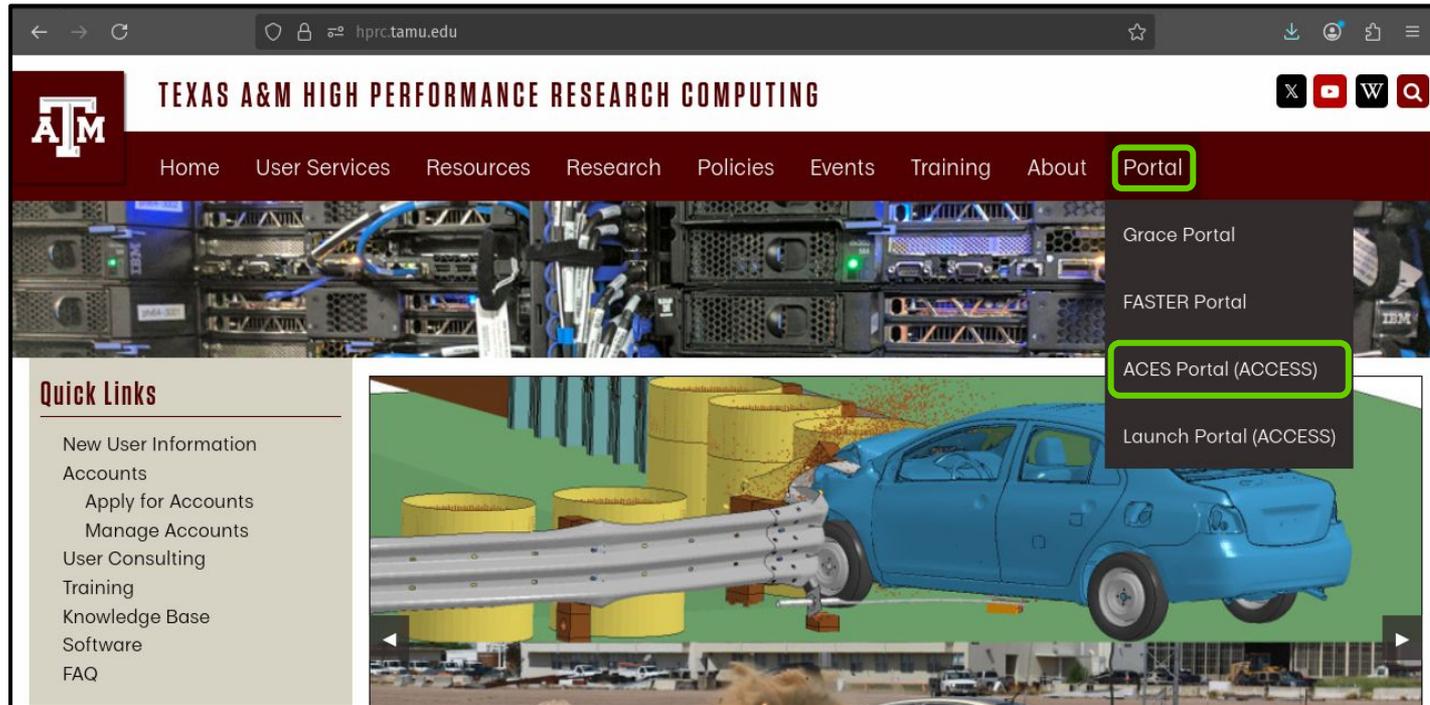
- CryoSPARC is available as an Interactive App on the ACES Portal
 - <https://portal-aces.hprc.tamu.edu>
- ACES hardware overview (can change since ACES is a composable resource cluster)
 - 30 x H100 GPUs (2 x H100 GPUs per node)
 - 6 x A30 GPUs (6 x A30 GPUs per node)
 - 70 x CPU only nodes
 - 10 x 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



The screenshot shows the Texas A&M High Performance Research Computing (HPRC) website. The browser address bar displays hprc.tamu.edu. The website header includes the Texas A&M logo and the text "TEXAS A&M HIGH PERFORMANCE RESEARCH COMPUTING". A navigation menu contains links for Home, User Services, Resources, Research, Policies, Events, Training, About, and Portal. The "Portal" link is highlighted with a green box. A dropdown menu is open under "Portal", listing "Grace Portal", "FASTER Portal", "ACES Portal (ACCESS)", and "Launch Portal (ACCESS)". The "ACES Portal (ACCESS)" link is highlighted with a green box. On the left side, there is a "Quick Links" section with a list of links: New User Information, Accounts, Apply for Accounts, Manage Accounts, User Consulting, Training, Knowledge Base, Software, and FAQ. The main content area features a large image of server racks and a 3D simulation of a blue car crashing into a guardrail.

HPRC webpage: hprc.tamu.edu

Accessing ACES via the Portal (ACCESS)

ALLOCATIONS SUPPORT OPERATIONS METRICS

ACCESS

Consent to Attribute Release

TAMU ACES ACCESS OIDC requests access to the following information. If you do not approve this request, do not proceed.

- Your CILogon user identifier
- Your name
- Your email address
- Your username and affiliation from your identity provider

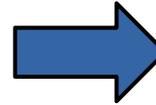
Select an Identity Provider

ACCESS CI (XSEDE)

LOG ON

By selecting "Log On", you agree to the [privacy policy](#).

Log-in using your ACCESS credentials.



ACCESS

If you had an XSEDE account, please enter your XSEDE username and password for ACCESS login.

ACCESS ID

ACCESS Password

LOGIN

[Register for an ACCESS ID](#)

[Forgot your password?](#)

[Need Help?](#)

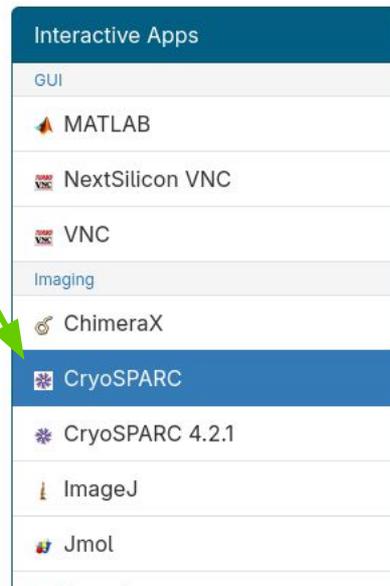
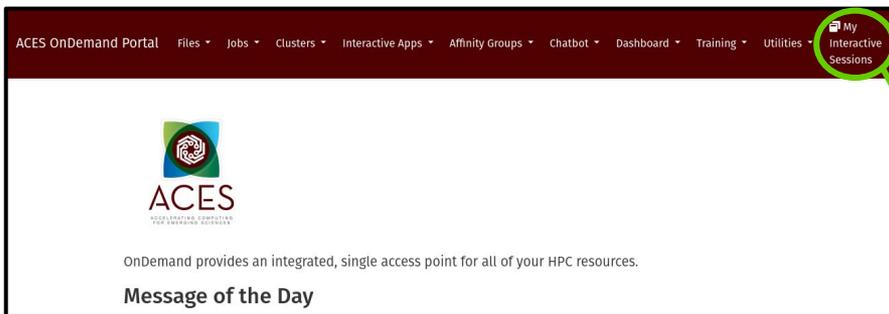
Select an Identity Provider

ACCESS CI (XSEDE)

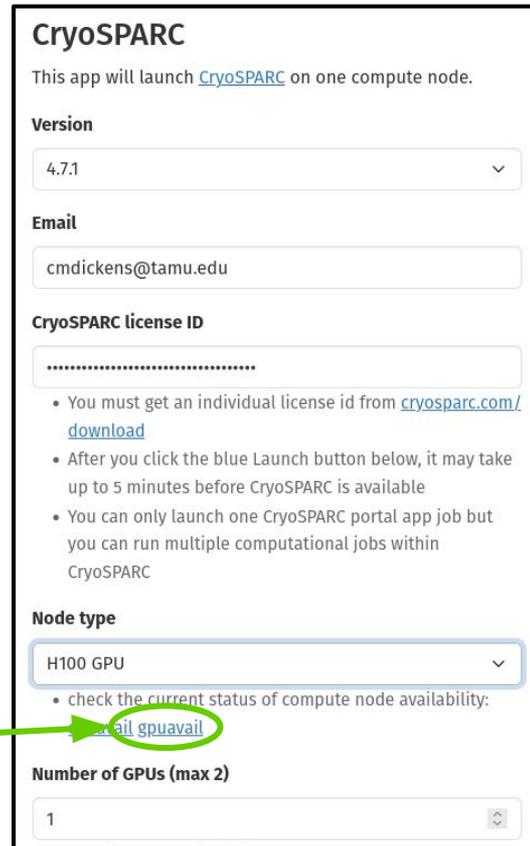
Select the Identity Provider appropriate for your account. ACCESS CI (XSEDE) or search for your institution whichever you used during registration.

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		AVAILABILITY						
NODE TYPE	NODE COUNT	NODE COUNT	GPU TYPE	GPU COUNT	GPU AVAIL	CPU AVAIL	GB MEM AVAIL	PARTITION
gpu:pvc:4	16	1	a30	2	1	88	438	gpu,gpu_debug
gpu:pvc:2	9	1	pvc	4	3	92	481	pvc
gpu:pvc:8	4	4	pvc	8	8	96	488	pvc
gpu:h100:8	2	1	pvc	6	6	96	488	pvc
gpu:h100:4	2	1 (reserved)	pvc	4	4	96	488	pvc
gpu:a30:2	1	8	pvc	2	2			
gpu:ve:8	1	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

CryoSPARC

This app will launch [CryoSPARC](#) on one compute node.

Version

4.7.1

Email

cmdickens@tamu.edu

CryoSPARC license ID

.....

- You must get an individual license id from [cryosparc.com/download](#)
- After you click the blue Launch button below, it may take up to 5 minutes before CryoSPARC is available
- You can only launch one CryoSPARC portal app job but you can run multiple computational jobs within CryoSPARC

Node type

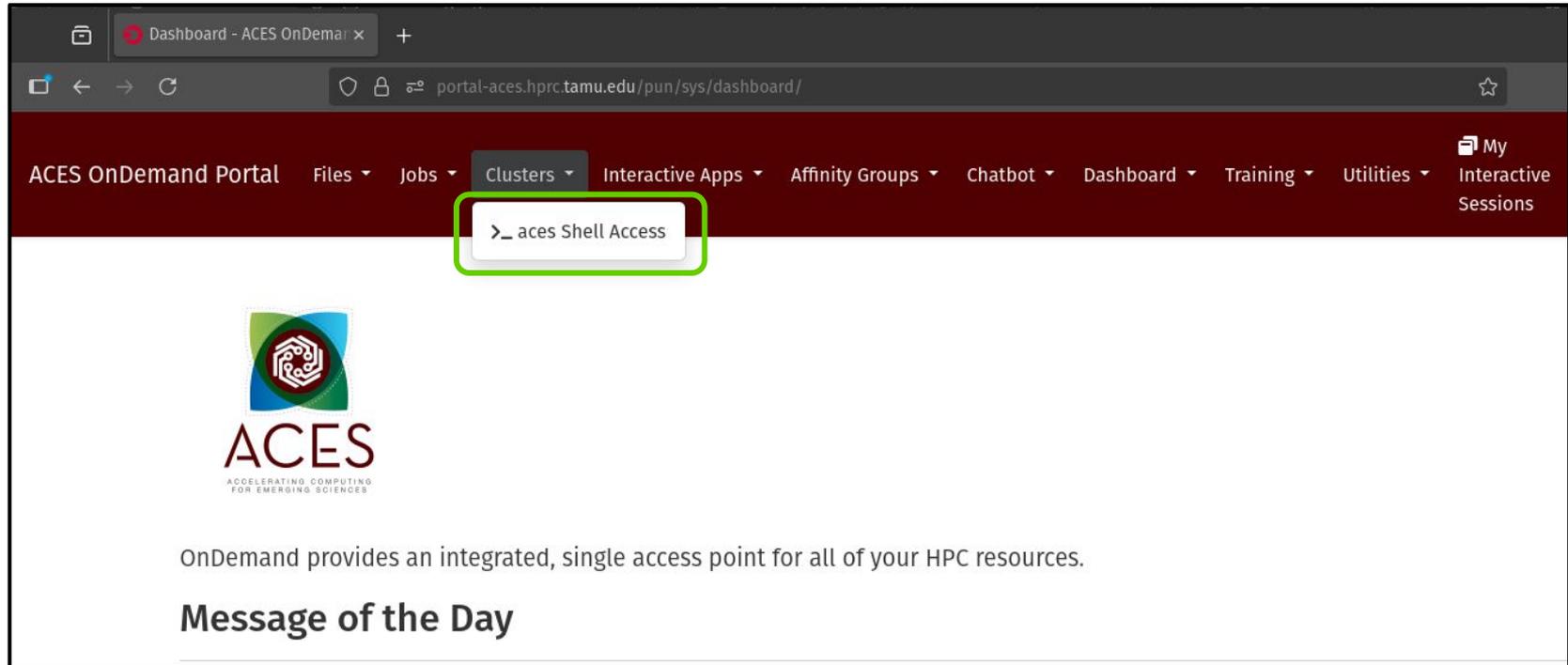
H100 GPU

- check the current status of compute node availability: [cpuavail](#) [gpuavail](#)

Number of GPUs (max 2)

1

Shell Access via the ACES Portal



The screenshot shows a web browser window with the URL `portal-aces.hprc.tamu.edu/pun/sys/dashboard/`. The navigation bar includes links for 'ACES OnDemand Portal', 'Files', 'Jobs', 'Clusters', 'Interactive Apps', 'Affinity Groups', 'Chatbot', 'Dashboard', 'Training', 'Utilities', and 'My Interactive Sessions'. The 'Clusters' menu is expanded, and the option '>_ aces Shell Access' is highlighted with a green box. Below the navigation bar, the ACES logo is displayed with the tagline 'ACCELERATING COMPUTING FOR EMERGING SCIENCES'. A message states: 'OnDemand provides an integrated, single access point for all of your HPC resources.' Below this is a section titled 'Message of the Day'.

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

CryoSPARC (138403) 1 node | 48 cores | Running

Host: >_ac095 Delete

Created at: 2024-03-20 12:46:52 CDT

Time Remaining: 2 hours and 56 minutes

Session ID: f55b9a74-fb5e-4cea-b988-0b268204f35b

- Use the following to login to your CryoSPARC session:
 - username: your email
 - password: the first 8 characters of your license ID

Impression 0 (low) to 9 (high)

Image Quality 0 (low) to 9 (high)

Launch CryoSPARC View Only (Share-able Link)

Click Launch

Increase Image Quality to 9



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

1 Projects

Select All

P1 cryosparc-live

Admin Admin

1 Session

Created 10/31/2025

Create a New Session

Project

Select a project

P1: cryosparc-live

Enter a title

Create Session

Instance Stats

	THIS WEEK	THIS MONTH	ALL
PROJECTS	1	1	1
WORKSPACES	2	2	2
JOB	1	1	1

Recent Jobs

My Jobs All Jobs

No applicable recent jobs

Must create a Project before creating a Live Session

CryoSPARC Live Session

The screenshot shows the CryoSPARC Live interface with several key elements highlighted by green boxes and callouts:

- Start Session:** A green button at the top center.
- Configuration:** A panel on the left with a dropdown menu for Profiles and a 'Clear Session' button.
- Parameters:** A central panel with a 'Show advanced' checkbox checked, a 'Filter' input, and various microscope parameters like 'Flip gain ref in X?', 'Raw pixel size (A)', and 'Accelerating voltage (kV)'. At the bottom, there are 'Apply to All', 'Apply to Future', and 'Cancel' buttons.
- Exposure Group:** A panel on the right with a 'New' button and options for 'Enable continuous import' and 'Ignore exposures from group'. It also features a 'Directory to watch' field containing the path '/ens/cryosparc-live/first_rur' and a 'File name wildcard filter' field.

Callouts and annotations include:

- A callout box labeled "Select" with an arrow pointing to the "Show advanced" checkbox in the Parameters panel.
- A callout box labeled "Enter values for Configuration, Parameters and Exposure Group" with an arrow pointing to the "Directory to watch" field in the Exposure Group panel.
- A callout box labeled "Select one of these two" with an arrow pointing to the "Apply to All" button in the Parameters panel.
- A callout box labeled "Select an already existing directory for image files" with an arrow pointing to the "Directory to watch" field in the Exposure Group panel.

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

End CryoSPARC Session when finished working

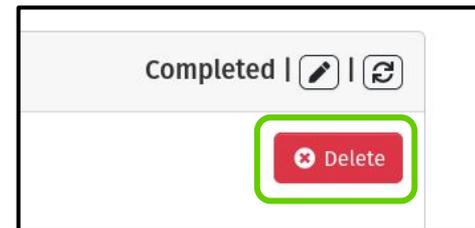
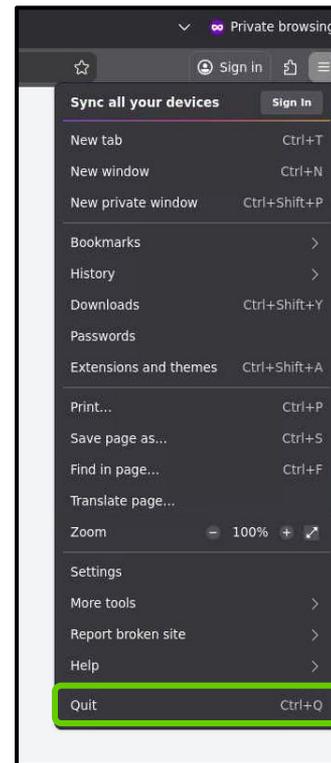
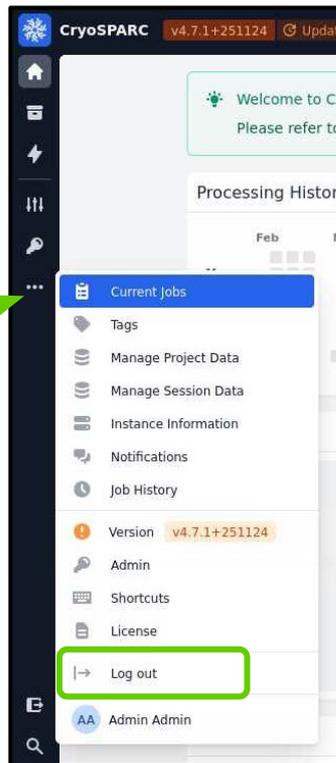
Make sure all processing is complete

Pause any Live sessions

Log out of CryoSPARC

Quit the Firefox Browser

Delete the Portal session





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HPRC Survey

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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:

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