

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

Fall 2025



High Performance Research Computing | hprc.tamu.edu | NSF Award #2112356

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

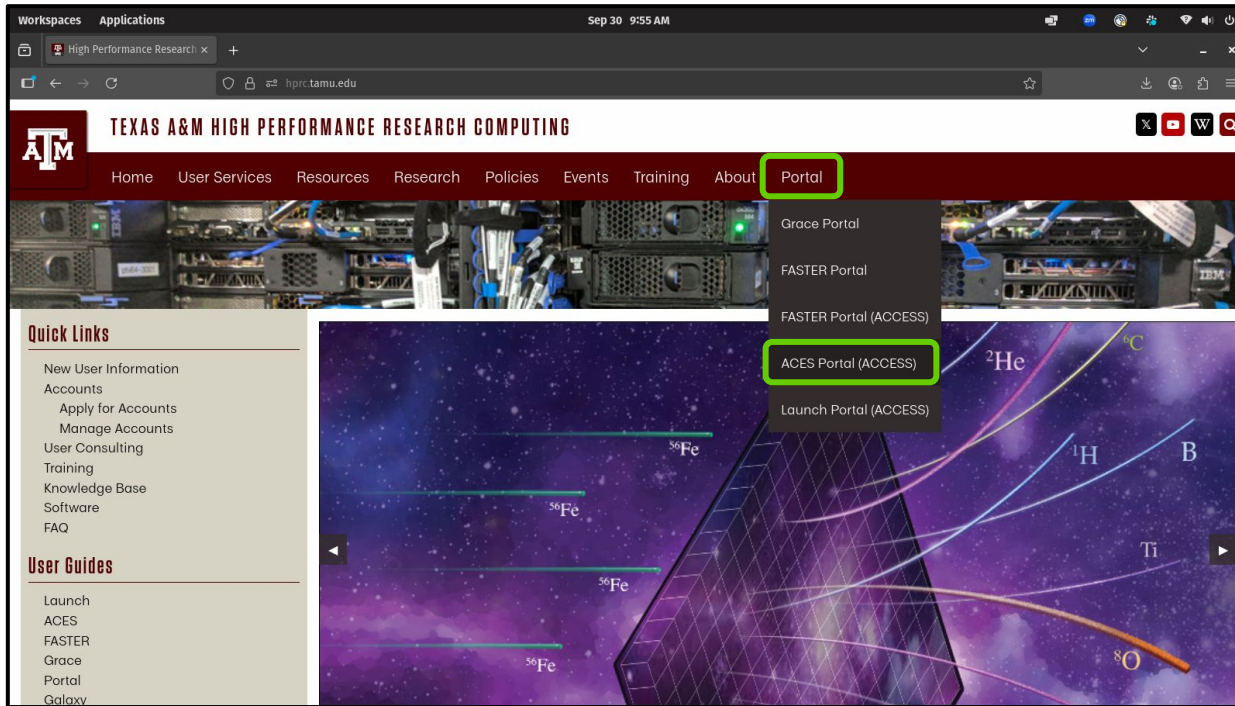
- CryoSPARC is available as an Interactive App on the ACES Portal
 - <https://portal-aces.hprc.tamu.edu>
- ACES hardware overview (can change since ACES is a composable resource cluster)
 - 30 x H100 GPUs (2 x H100 GPUs per node)
 - 6 x A30 GPUs (6 x A30 GPUs per node)
 - 70 x CPU only nodes
 - 10 x 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 a web browser window displaying the Texas A&M High Performance Research Computing (HPRC) website. The browser's address bar shows the URL hprc.tamu.edu. The website's header features the Texas A&M logo and the text "TEXAS A&M HIGH PERFORMANCE RESEARCH COMPUTING". A navigation menu includes 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 visible under the "Portal" link, containing the following options: Grace Portal, FASTER Portal, FASTER Portal (ACCESS), ACES Portal (ACCESS) (highlighted with a green box), and Launch Portal (ACCESS). On the left side of the page, there are sections for "Quick Links" and "User Guides". The "Quick Links" section includes links for New User Information, Accounts, Apply for Accounts, Manage Accounts, User Consulting, Training, Knowledge Base, Software, and FAQ. The "User Guides" section includes links for Launch, ACES, FASTER, Grace, Portal, and Galaxy. The main content area features a large image of a server rack with a space-themed overlay showing particle tracks and labels for ^{56}Fe , ^2He , ^{12}C , ^1H , ^8O , B , and Ti .

HPRC webpage: hprc.tamu.edu

Accessing ACES via the Portal (ACCESS)

ALLOCATIONS SUPPORT OPERATIONS METRICS Login

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.

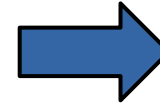
- Your CILogon user identifier
- Your name
- Your email address
- Your username and affiliation from your identity provider

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.

gpuavail: ACES GPU Configuration & Availability

ACES OnDemand Portal / ACES GPU 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: 2025-07-15 09:22:45

```
$ gpuavail
```

CONFIGURATION		AVAILABILITY						
NODE TYPE	NODE COUNT	NODE NAME	GPU TYPE	GPU COUNT	GPU AVAIL	CPU AVAIL	GB MEM AVAIL	PARTITION
gpu:pvc:4	16	ac049	h100	4	1	32	16	gpu
gpu:pvc:2	9	ac098	h100	2	2	96	488	gpu_debug
gpu:pvc:8	4	ac087	pvc	2	2	96	488	pvc
gpu:h100:4	3	ac078	pvc	4	4	96	488	pvc
gpu:h100:8	2	ac089	pvc	4	4	96	488	pvc
gpu:h100:2	1	ac086	pvc	2	2	96	488	pvc
gpu:a30:2	1	ac032	pvc	8	8	96	488	pvc
gpu:ve:8	1	ac095	pvc	2	2	96	488	pvc
gpu:pvc:6	1	ac083	pvc	2	2	96	488	pvc

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

Launch a CryoSPARC Interactive Job

Input your License ID

Select a GPU Node type and count

Click the blue Launch button

CryoSPARC

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

Version

4.7.1

CryoSPARC license id (required)

.....

- 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

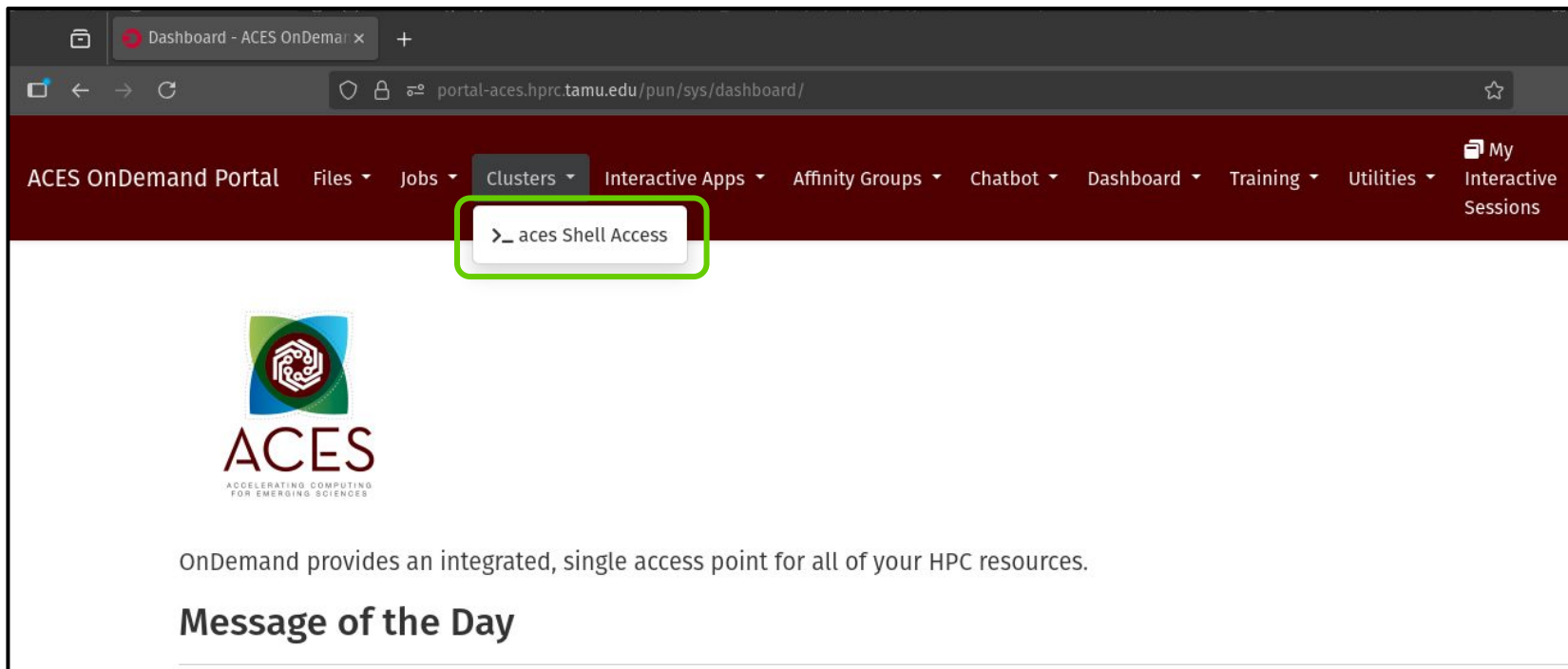
- check the current status of compute node availability: [cpuavail](#) [gpuavail](#)

Number of GPUs (max 2)

1

- Selecting 1 GPU will set max cores 48 and max memory 244GB

Shell Access via the ACES Portal



The screenshot shows a web browser window with the address bar displaying `portal-aces.hprc.tamu.edu/pun/sys/dashboard/`. The page features a dark red navigation bar with the following items: **ACES OnDemand Portal**, **Files**, **Jobs**, **Clusters** (highlighted with a green box), **Interactive Apps**, **Affinity Groups**, **Chatbot**, **Dashboard**, **Training**, **Utilities**, and **My Interactive Sessions**. A dropdown menu for the **Clusters** item is open, showing a link labeled `>_ acs Shell Access`, which is also highlighted with a green box. Below the navigation bar, the ACES logo is displayed, consisting of a stylized circuit icon and the text **ACES** with the tagline ACCELERATING COMPUTING FOR EMERGING SCIENCES. Below the logo, the text reads: **OnDemand provides an integrated, single access point for all of your HPC resources.** and **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

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: **admin@cryo.edu**
- password: **admin**

Compression0 (low) to 9 (high)

Image Quality0 (low) to 9 (high)

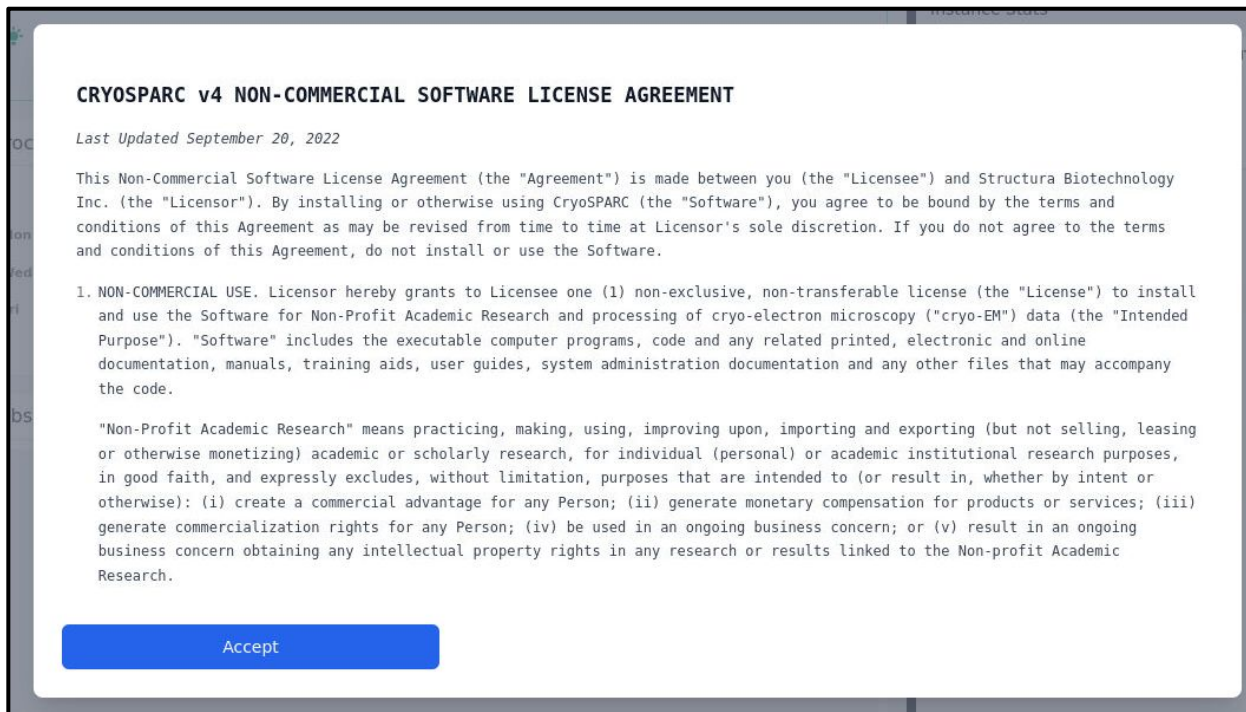
Launch CryoSPARC

View Only (Share-able Link)

Click Launch

Increase Image Quality to 9

Read and Accept the License



The image shows a screenshot of a web browser window displaying the "CRYOSPARC v4 NON-COMMERCIAL SOFTWARE LICENSE AGREEMENT". The window has a grey border and a white background. The title bar at the top is partially visible, showing "CRYOSPARC v4 NON-COMMERCIAL SOFTWARE LICENSE AGREEMENT". The main content area is white and contains the following text:

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.

"Non-Profit Academic Research" means practicing, making, using, improving upon, importing and exporting (but not selling, leasing or otherwise monetizing) academic or scholarly research, for individual (personal) or academic institutional research purposes, in good faith, and expressly excludes, without limitation, purposes that are intended to (or result in, whether by intent or otherwise): (i) create a commercial advantage for any Person; (ii) generate monetary compensation for products or services; (iii) generate commercialization rights for any Person; (iv) be used in an ongoing business concern; or (v) result in an ongoing business concern obtaining any intellectual property rights in any research or results linked to the Non-profit Academic Research.

At the bottom of the window, there is a blue button with the text "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

CryoSPARC Projects Sessions New Session Details

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
JOBS	1	1	1

Recent Jobs My Jobs All Jobs

No applicable recent jobs

localhost:62946/browse/P*-S*

Must create a
Project before
creating a Live
Session

CryoSPARC Live Session

The screenshot shows the CryoSPARC Live web interface. On the left is a sidebar with navigation links: Details, Configuration (highlighted in blue), Individual Exposure, Overview, Browse, Picking, 2D Classification, Ab-initio, and Refinement. The main area is divided into three panels: Configuration, Parameters, and Exposure Groups. The Configuration panel shows settings for Preprocessing Lane (default), Number of Preprocessing GPU Workers (1), Reconstruction Lane (default), and checkboxes for Use SSD. The Parameters panel has a 'Show advanced' checkbox checked, and various microscope parameters like Flip gain, Rotate gain, Raw pixel size (0.326), Accelerating voltage (300 kV), and Spherical aberration. The Exposure Groups panel shows '1 Exposure Group' with a 'New' button and fields for 'Directory to watch' (set to /ens/cryosparc-live/first_rur) and 'File name wildcard filter' (*). Annotations include a green box around the 'Start Session' button at the top, a green box around the 'Show advanced' checkbox, a green box around the 'Apply to All' button, and a green box around the 'Directory to watch' field. A 'Select' callout points to the 'Start Session' button, and another 'Select' callout points to the 'Apply to All' button. A third callout points to the 'Directory to watch' field.

Configuration

Profiles

Compute Resources

Preprocessing Lane: default

Number of Preprocessing GPU Workers: 1

Reconstruction Lane: default

☒ Use SSD

Auxiliary Lane: default

☒ Use SSD

Session Priority: 0

Exposure Processing Priority

[Documentation and tutorials](#)

Parameters

☒ Show advanced

Microscope/Camera Parameter

Flip gain ref in X? ☐

Flip gain ref in Y? ☒

Rotate gain ref? 0

Raw pixel size (Å) 0.326

Accelerating voltage (kV) 300

Spherical aberration (mm)

1 Exposure Group

0

Exposure Group 1 (0 found)

Enable continuous import ☐

Ignore exposures from group ☐

Directory to watch: /ens/cryosparc-live/first_rur

File name wildcard filter: *

Search Recursively ☐

Minimum File Size: 0

Enter values for Configuration, Parameters and Exposure Group

Select an already existing directory for image files

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



**HIGH PERFORMANCE
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<https://hprc.tamu.edu>

HPRC Helpdesk:

help@hprc.tamu.edu

Phone: 979-845-0219

Take our short course survey!



HPRC Survey

https://u.tamu.edu/hprc_shortcourse_survey

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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