

# 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 2024



High Performance Research Computing | [hprc.tamu.edu](http://hprc.tamu.edu) | NSF Award #2112356

# CryoSPARC on ACES

- CryoSPARC Academic License ID
- Resources and Limitations
- CryoSPARC on the ACES Portal
- Group data directories
- 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

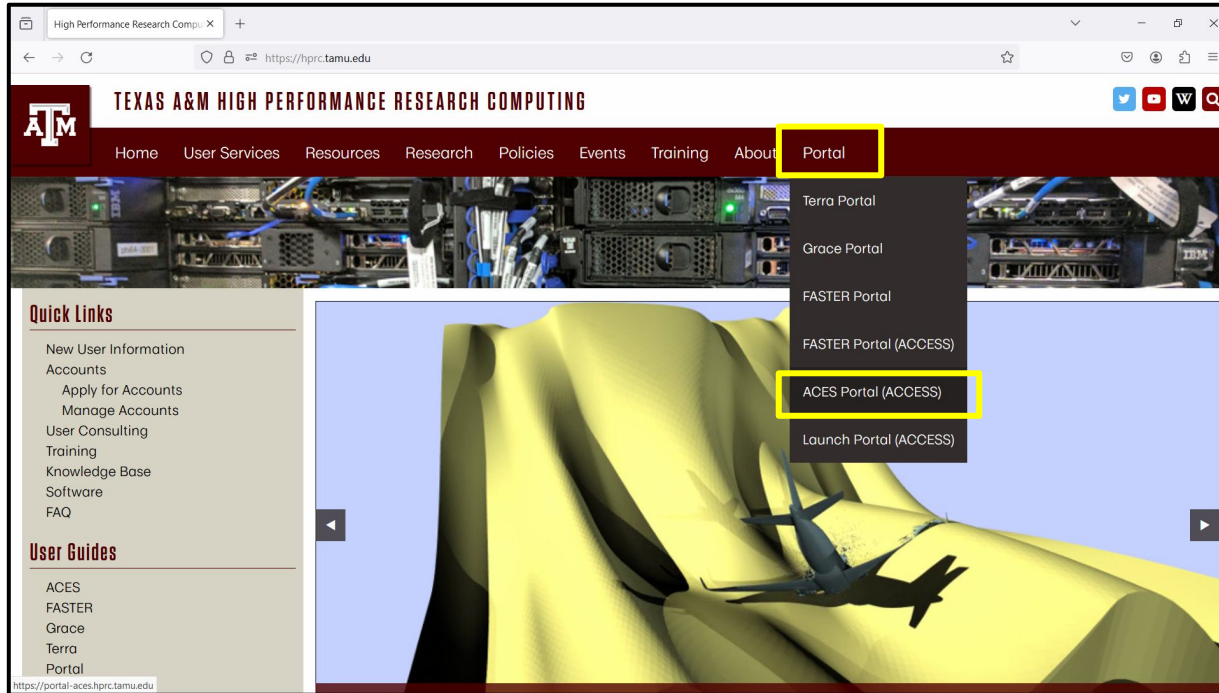
- CryoSPARC is available as an Interactive App on the ACES Portal
  - <https://portal-aces.hprc.tamu.edu>
- ACES hardware overview (can change since ACES is a composable resource cluster)
  - 30 x H100 GPUs (2 x H100 GPUs per node)
  - 6 x A30 GPUs (6 x A30 GPUs per node)
  - 70 x CPU only nodes
  - 10 x other specialized nodes not for 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 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
- 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](https://hprc.tamu.edu)

# Accessing ACES via the Portal (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 CI/Logon user identifier
- Your name
- Your email address
- Your username and affiliation from your identity provider

ACCESS CI (XSEDE)

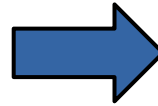
**LOG ON**

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

**Select an Identity Provider**

ACCESS CI (XSEDE)

Select the Identity Provider appropriate for your account.



Log-in using your ACCESS credentials.



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

**ACCESS ID**

**ACCESS Password**

**LOGIN**

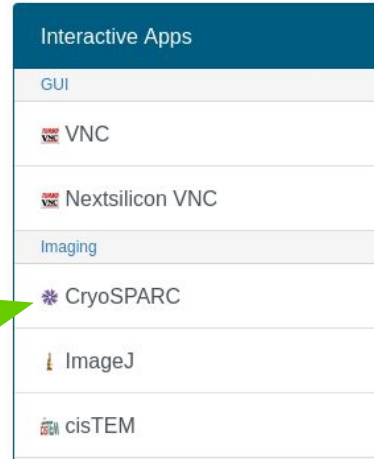
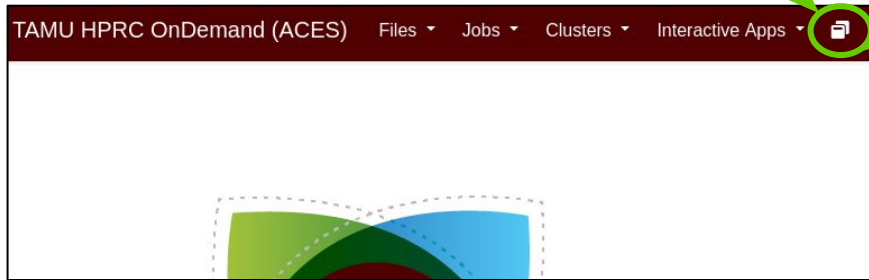
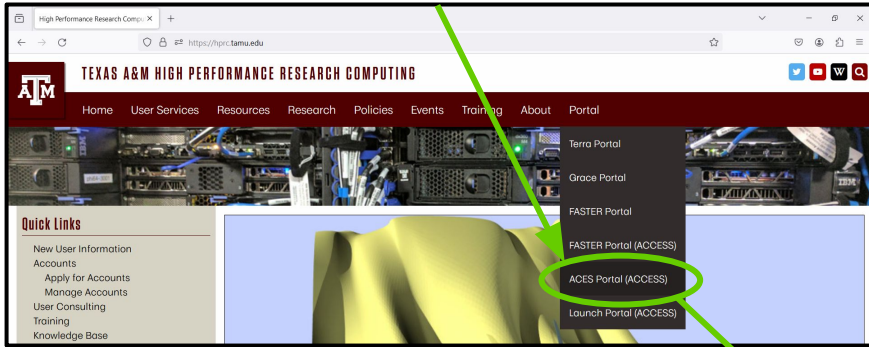
[Register for an ACCESS ID](#)

[Forgot your password?](#)

[Need Help?](#)

# ACES CryoSPARC Portal App

[portal-aces.hprc.tamu.edu](https://portal-aces.hprc.tamu.edu)



**CryoSPARC**

This app will launch CryoSPARC on one ACES cluster compute node.

Version  
4.2.1

CryoSPARC license id (required)

- You must get an individual license id from [cryosparc.com/download](https://cryosparc.com/download)
- After you click the blue Launch button below, it may take up to 5 minutes before CryoSPARC is available
- Use the following to login to your CryoSPARC session:
  - username: **admin@cryo.edu**
  - password: **admin**
- You can only launch one CryoSPARC portal app job but you can run multiple computational jobs within CryoSPARC

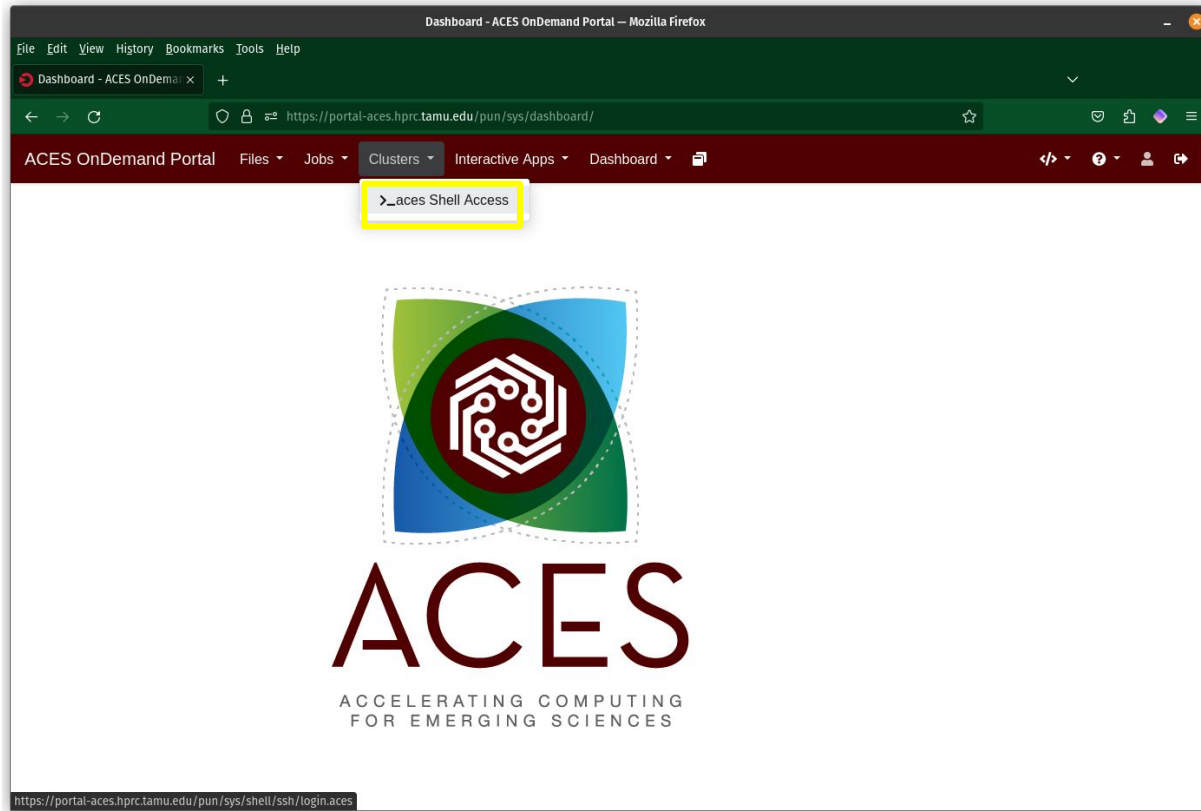
Number of hours (max 168)  
3

Node type  
CPU only

Launch CryoSPARC the first time using **CPU only** in order to initialize the database.



# Shell Access via the ACES Portal



# Display GPU Availability on ACES

See GPU configuration and current availability using the ACES portal shell access

- <https://portal-aces.hprc.tamu.edu>
- select "Clusters" then ">\_aces Shell Access"
- at the command line prompt, enter **gpuavail**
- the CONFIGURATION will change frequently since ACES is a composable resource cluster

Based on this output, there are 9 compute nodes on ACES that have exactly 2 x H100 GPUs attached to each

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

## gpuavail

### CONFIGURATION

NODE TYPE	NODE COUNT
gpu:h100:2	9
gpu:pvc:4	9
gpu:h100:4	4
gpu:a30:2	2

### AVAILABILITY

NODE NAME	GPU TYPE	GPU COUNT	GPU AVAIL	CPU AVAIL	GB MEM AVAIL
ac027	h100	4	1	72	248
ac048	h100	2	2	96	488
ac049	h100	2	1	88	408
ac050	h100	2	2	96	488
ac064	a30	2	2	96	488

# 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

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

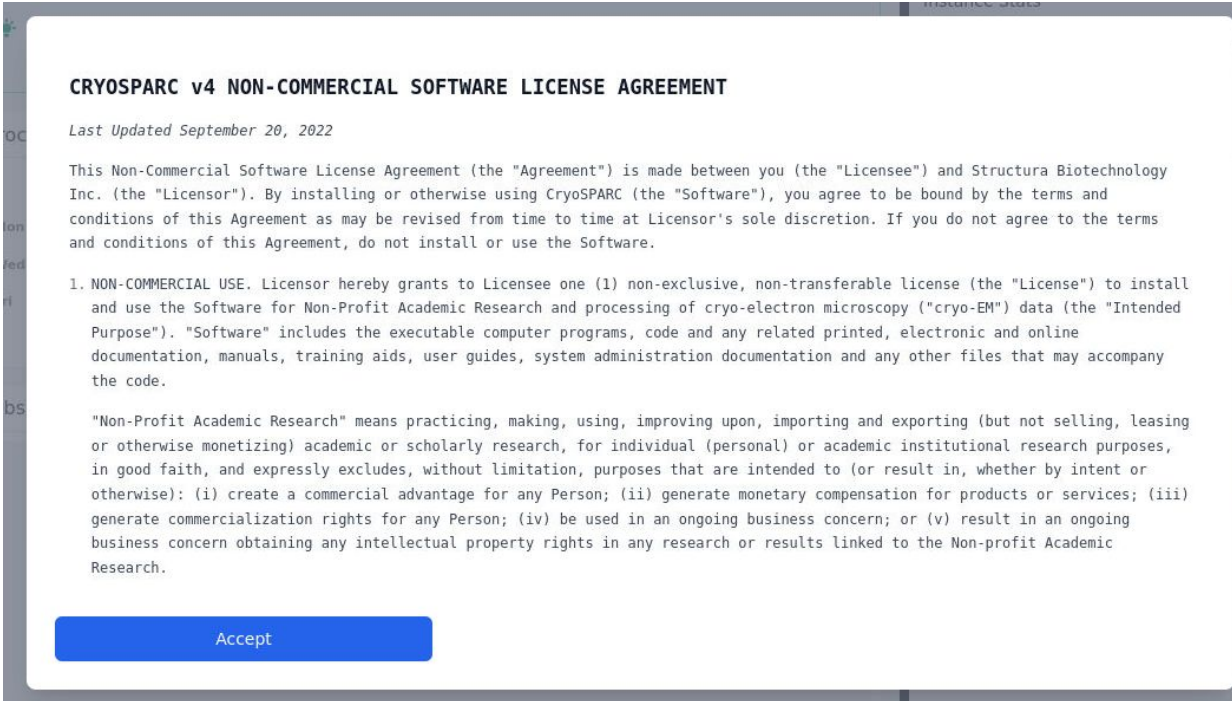
Impression 0 (low) to 9 (high)

Image Quality 0 (low) to 9 (high)

Click Launch Increase Image Quality to 9

Launch CryoSPARC View Only (Share-able Link)

# 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

then exit and start a new CryoSPARC job this time with a GPU

# ACES CryoSPARC Portal App

[portal-aces.hprc.tamu.edu](http://portal-aces.hprc.tamu.edu)

## CryoSPARC

This app will launch **CryoSPARC** on one **ACES** cluster compute node.

Version

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CryoSPARC license id (required)

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Number of hours (max 96)

3

Node type

H100 GPU

Number of GPUs

1

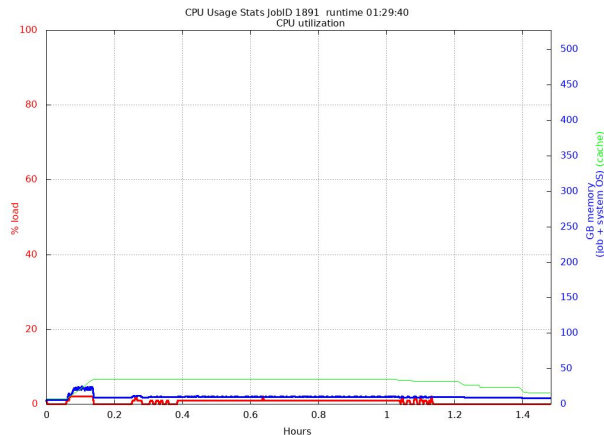
Delete your CryoSPARC "CPU only" job and launch a new CryoSPARC job using 1 x H100 GPU for the interactive tutorial

# CryoSPARC Visualization of Resource Utilization

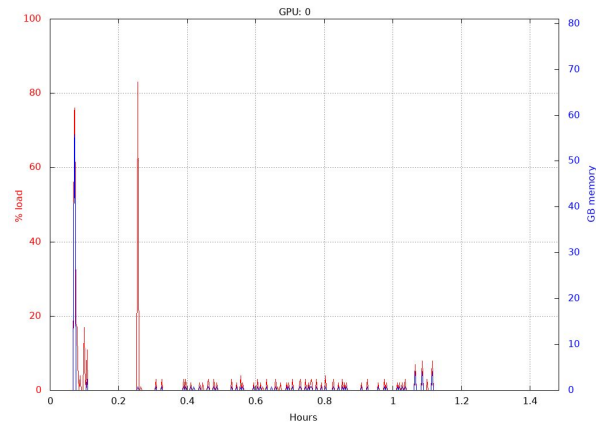
# Review CPU and GPU usage for a Job

The **jobstats** utility automatically runs for each CryoSPARC portal job and monitors CPU and GPU resource usage and creates a graph for each.

- CPU stats monitors all cores regardless of how many were configured for the job
  - CryoSPARC jobs use a fraction of total cores and memory if selecting one of many GPUs on a compute node to allow users to request the other GPUs on the compute node
- GPU stats will create a graph for each GPU that was configured for the job



stats\_cpu.1891.png



stats\_gpu.1891.png

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



# Review CPU and GPU usage for a CryoSPARC Job

1. At the bottom of the CryoSPARC portal app, access the CryoSPARC data root directory
2. Click 'output'
3. Click 'Modified at' to sort newest session on top
4. Click the Name of the session you want to view based on the date
5. Click the .png image files to view the CPU and GPU usage stats
  - a. CPU usage stats are for the entire GPU node so it will include any other jobs running on that node
  - b. GPU stats are exclusive to your job

- 1.
- 2.
- 3.
- 4.
- 5.

The screenshot shows the CryoSPARC portal interface. At the top, there is a blue 'Launch' button. Below it, a note states: '\* The CryoSPARC session data for this session can be accessed under the **data root directory**.' Below the note is a table with columns 'Type' and 'Name'. The first row shows a folder icon and the name 'output'. Below the table, there is a 'Modified at' dropdown menu showing the date and time '4/5/2023 2:30:43 PM'. Below that is another table with columns 'Type' and 'Name'. The first row shows a folder icon and the name '03634bca-8f96-43c5-acc4-d779d1e8eeb7'. Below the table, there is a list of files: 'stats\_cpu.7954633.png' and 'stats\_gpu.7954633.png'.

# Group Data Directories

- Group data directories can be used to share input files or to have a group work space
- Send a request to the HPRC helpdesk to create a group
  - [help@hprc.tamu.edu](mailto:help@hprc.tamu.edu)
  - provide a group name and usernames of members
  - group directories have their own disk quotas separate from individual users
- You will need to mount your group directory when launching the CryoSPARC portal app

Optional group directory to mount

- You must already be a member of the group
- Example values:
  - /junjiez
  - /scratch/group/davislab



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<https://hprc.tamu.edu>

HPRC Helpdesk:

help@hprc.tamu.edu

Phone: 979-845-0219

*Take our short course survey!*



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HPRC Survey

[https://u.tamu.edu/hprc\\_shortcourse\\_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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