

HIGH PERFORMANCE RESEARCH COMPUTING

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

May 14, 2025

Michael Dickens



High Performance
Research Computing

DIVISION OF RESEARCH



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

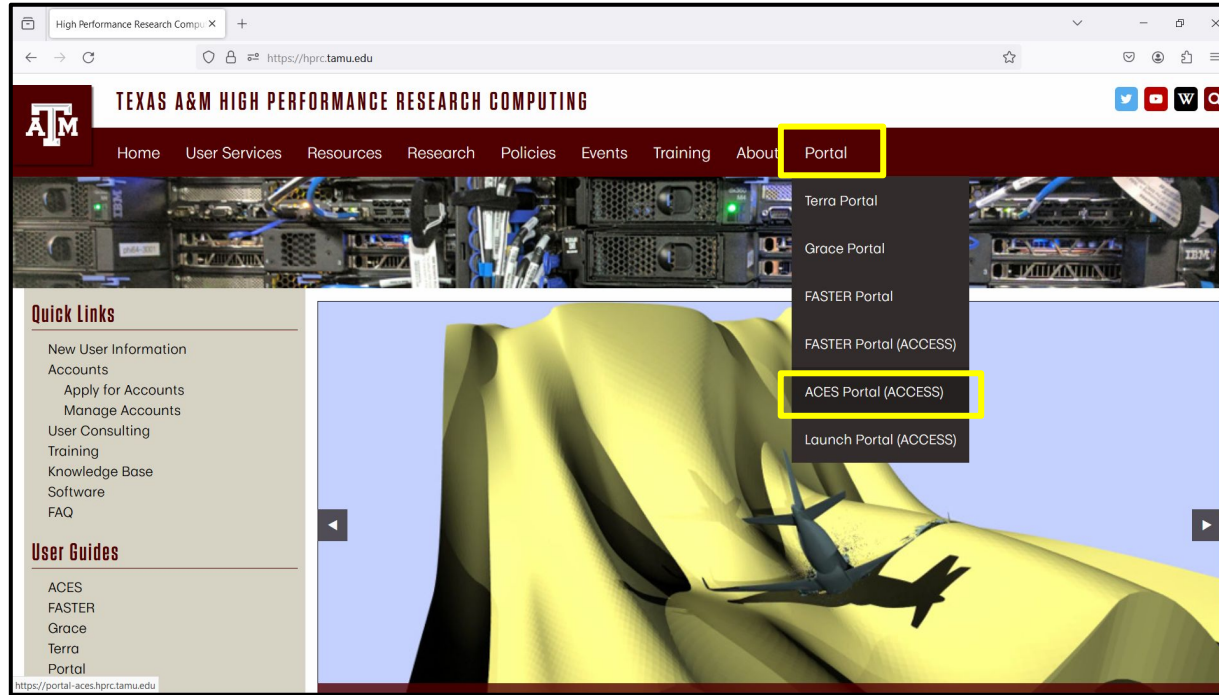
CryoSPARC on ACES

- CryoSPARC Academic License ID
- CryoSPARC on the ACES Portal
- Resources and Limitations
- 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>

Accessing the HPRC ACES Portal



HPRC webpage: hprc.tamu.edu
[Apply](#) for an ACCESS ID if you don't already have one

Accessing ACES via the Portal (ACCESS)

ALLOCATIONS SUPPORT OPERATIONS METRICS

Home Search Menu Login



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

ACCESS CI (XSEDE)

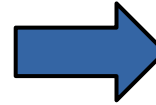
LOG ON

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?](#)

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 (2-8 x H100 GPUs per node)
 - 2 x A30 GPUs (2 x A30 GPUs per node)
 - 59 x CPU only nodes
 - 31 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

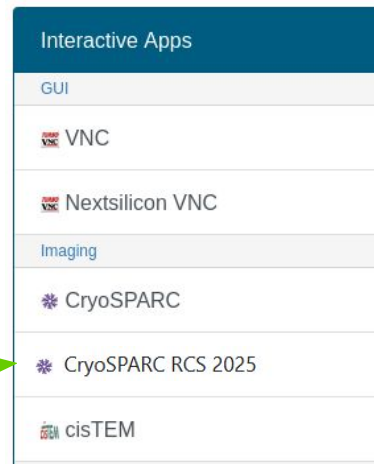
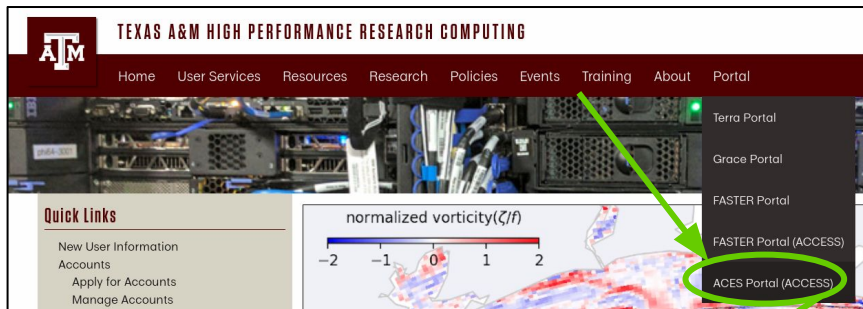


Resource Limitations

- Each user can only launch one CryoSPARC portal session at a time
 - you 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
- If your portal job is about to end and you need more time to finish processing, send an email to our helpdesk to request a time extension

ACES CryoSPARC Portal App

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
- 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

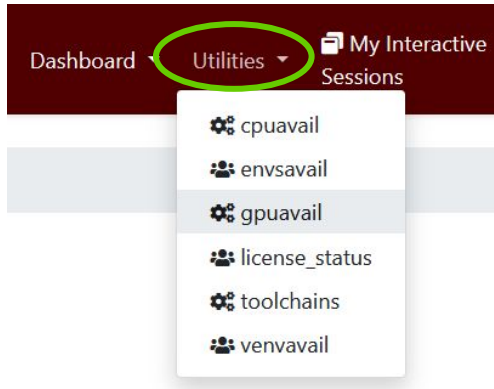
Node type
CPU only

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

Display GPU Availability on ACES

See GPU configuration and current availability using the gpuavail utility

The CONFIGURATION will change frequently since ACES is a composable resource cluster



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: 2025-05-14 09:52:10

```
$ gpuavail
```

CONFIGURATION		AVAILABILITY					
NODE TYPE	NODE COUNT	NODE NAME	GPU TYPE	GPU COUNT	GPU AVAIL	CPU AVAIL	GB MEM AVAIL
gpu.pvc:4	16	ac041	h100	8	2	80	150
gpu.pvc:2	9	ac045	h100	8	5	84	38
gpu.pvc:8	4	ac011	pvc	4	4	96	488
gpu.h100:4	2	ac094	pvc	2	2	96	488
gpu.h100:8	2	ac081	pvc	4	4	96	488
gpu.ve:8	1	ac087	pvc	2	2	96	488
gpu.a30:2	1	ac039	pvc	4	4	96	488
gpu.pvc:6	1	ac102	pvc	4	4	96	488
gpu.h100:2	1	ac078	pvc	4	4	96	488

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

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

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**

Compression

0 (low) to 9 (high)

Image Quality

0 (low) to 9 (high)

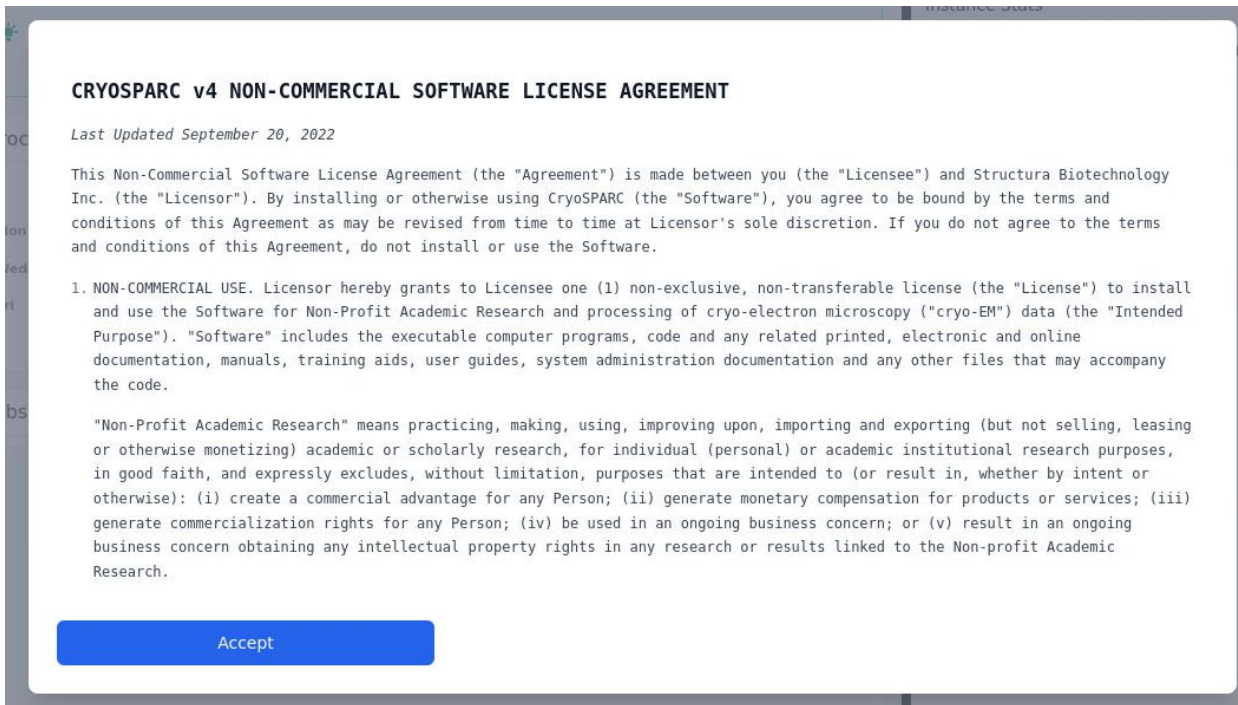
Click Launch

Launch CryoSPARC

View Only (Share-able Link)

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.

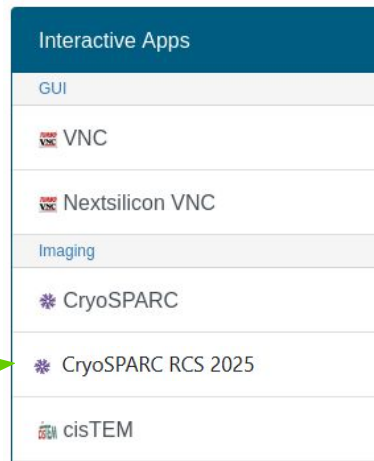
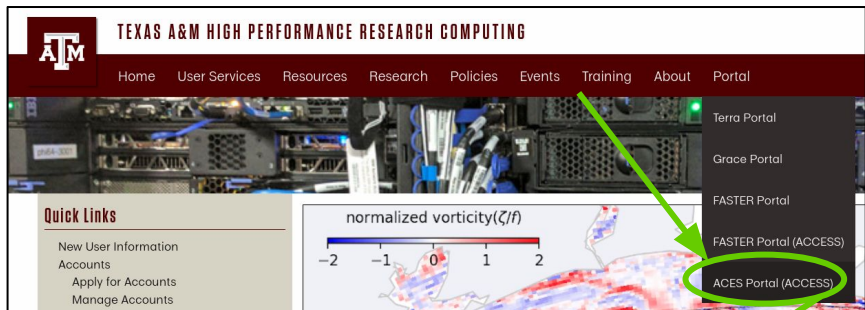
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Accept

wait a few minutes, then logout using the CryoSPARC menu

ACES CryoSPARC Portal App

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



CryoSPARC

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

Version

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Number of hours (max 96)

3

Node type

H100 GPU

Number of GPUs

1

Group Data Directories

- Group data directories can be used to share input files or to have a group work space
- All users automatically receive a 5TB \$PROJECT directory
- Contact the HPRC helpdesk to request a shared group directory
- 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:
 - /junjez
 - /scratch/group/davislab



**HIGH PERFORMANCE
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TEXAS A&M UNIVERSITY

<https://hprc.tamu.edu>

HPRC Helpdesk:

help@hprc.tamu.edu

Phone: 979-845-0219

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