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

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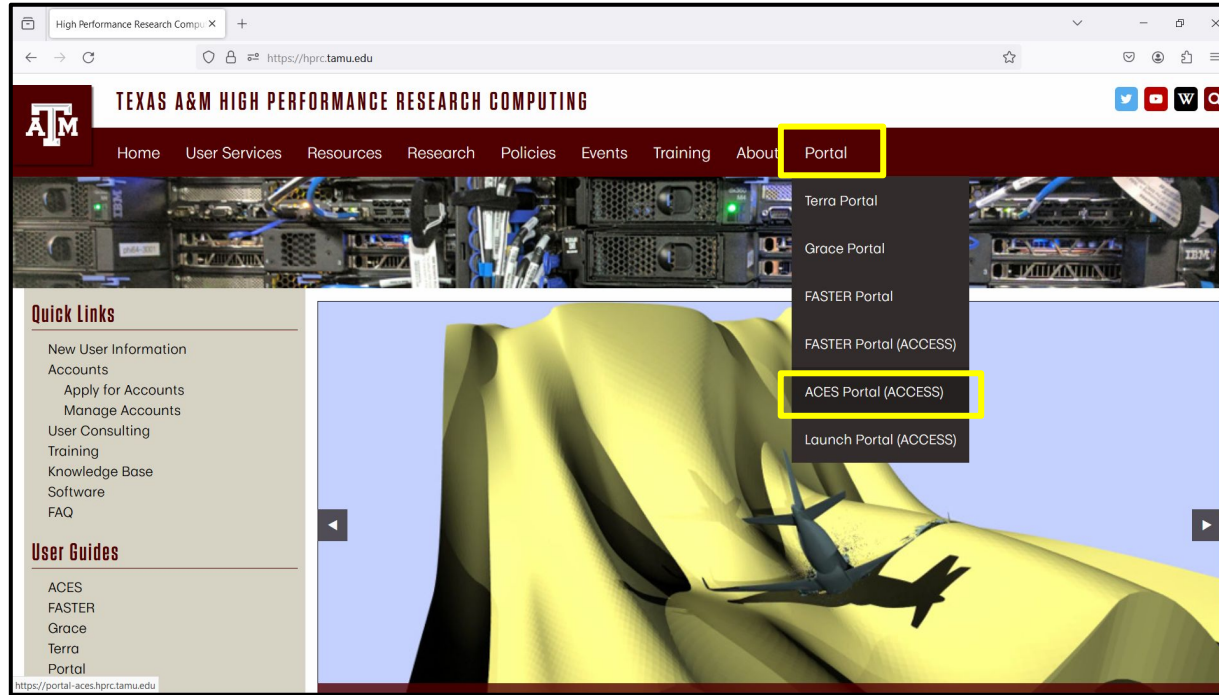
HPRC webpage: hprc.tamu.edu
Apply for an ACCESS ID if you don't already have one

Accessing ACES via the Portal (ACCESS)

Log-in using your ACCESS credentials.

Select the Identity Provider appropriate for your account.

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
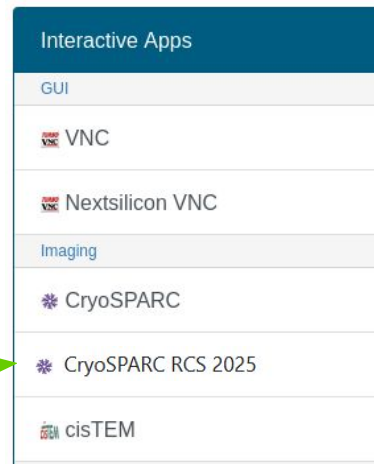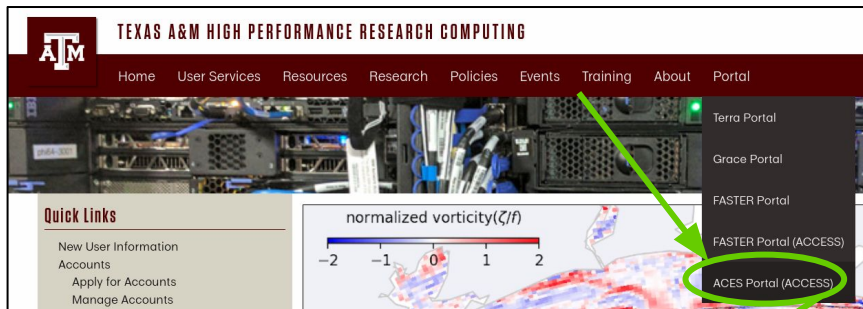
Resource Limitations

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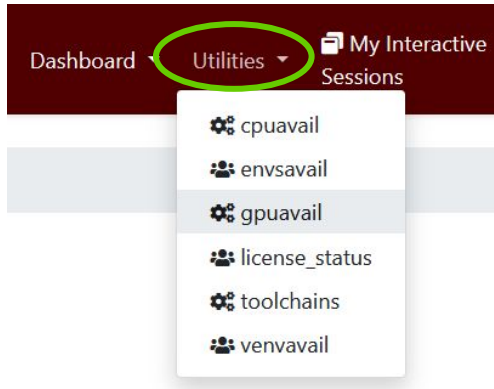
Launch CryoSPARC the first time using **CPU only** in order to initialize the database.

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   ❌ 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**

Increase Image Quality to 9

Click Launch

Compression   Image Quality
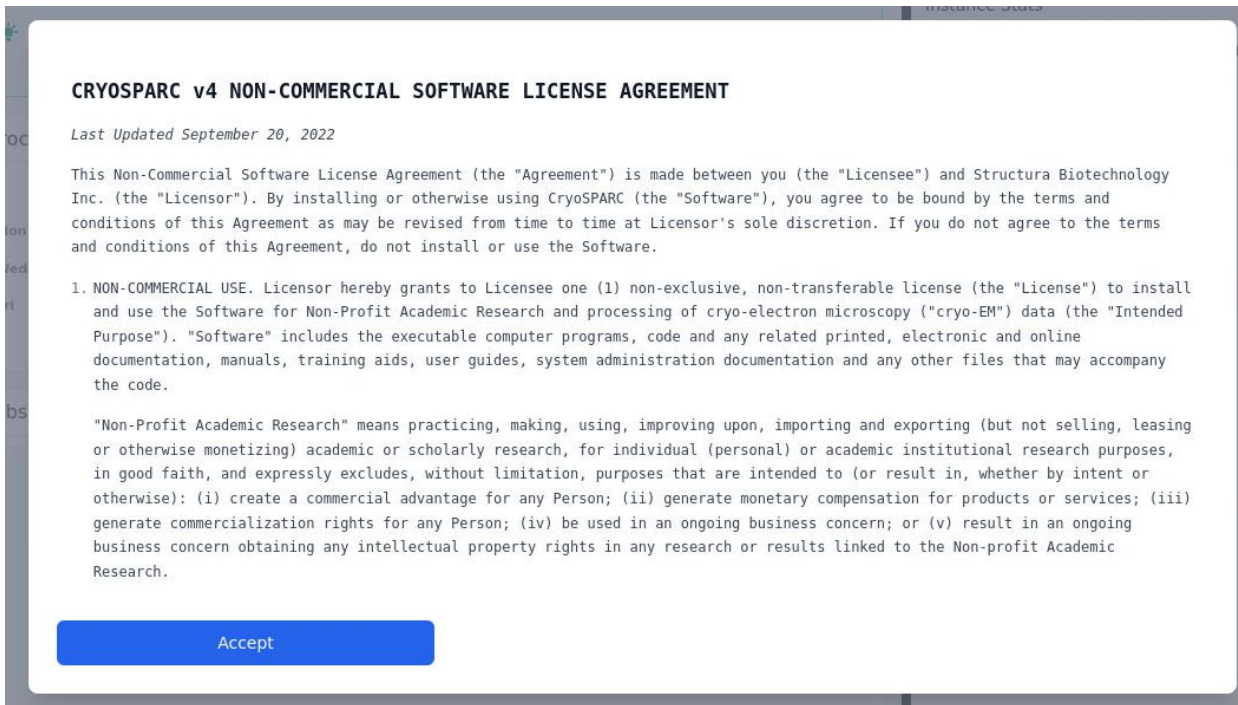
0 (low) to 9 (high)   0 (low) to 9 (high)

Launch CryoSPARC   View Only (Share-able Link)

Read and Accept the License

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
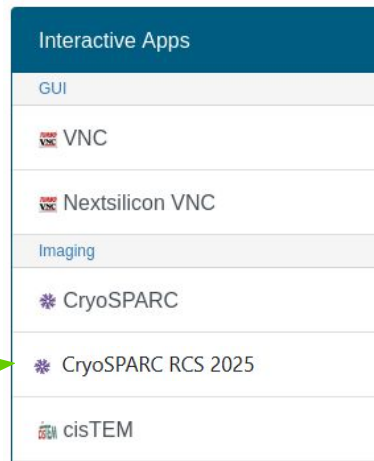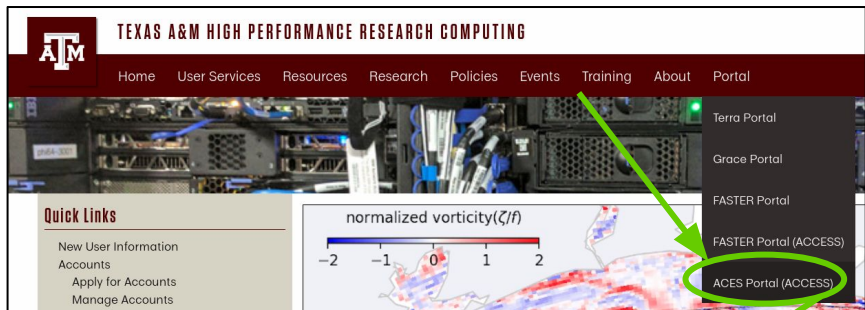
CryoSPARC

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

Version

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 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:
  - /junjiez
  - /scratch/group/davislab

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