

Using Containers on ACES for Simulations, Bioinformatics and AI/ML

Richard Lawrence and Joshua Winchell

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Outline

- Overview of Containers on ACES
- Getting Started
- Containerized Scientific Applications
 - Genomics
 - AI/ML
 - Molecular Dynamics

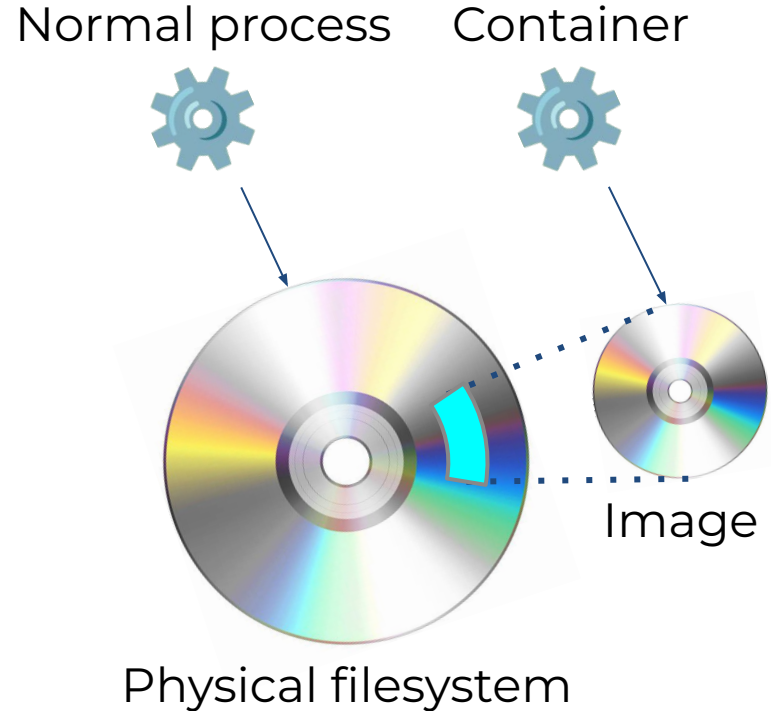


Overview of Containers



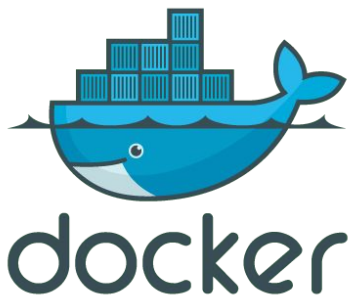
What Are Containers?

- A container is a process (⚙️) that has its own **view** of local resources:
 - **Filesystem**
 - User IDs
 - Network etc.
- Example: this container (⚙️ on the right) sees the **image** instead of the physical filesystem



Container Runtimes on ACES

ACES offers a wide variety of Container Runtimes



Docker



*rootless



Singularity



Charliecloud



*rootless installations do not support all features of the runtime

Singularity on ACES

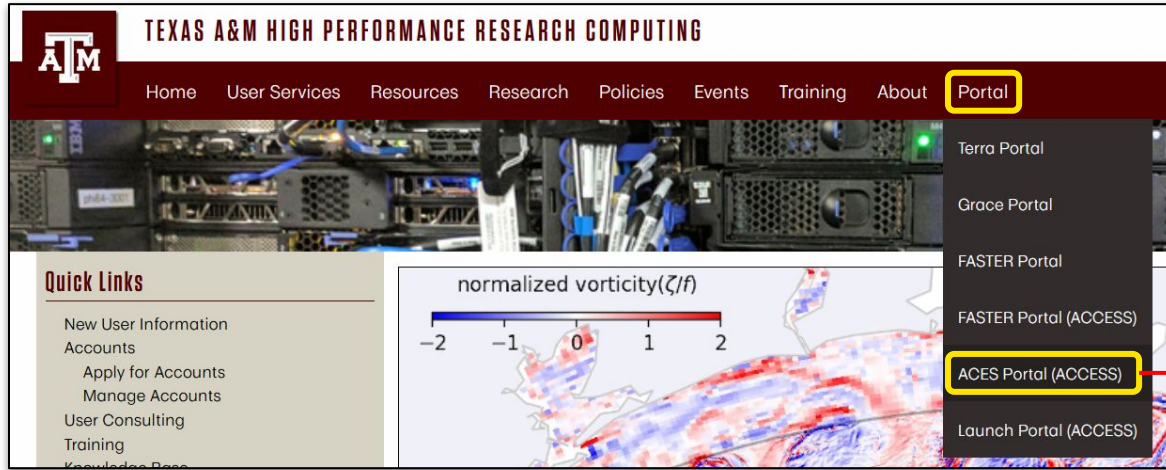
- Singularity is available on Compute nodes
 - Singularity activities are too cpu-intensive for login nodes.
- Singularity images can be large on disk. Be aware of your storage quota. (`/scratch` > `/home`)
- Some container activities may be too I/O-intense for the shared network filesystem. Be courteous to others and use a local filesystem for large image operations.



Getting Started

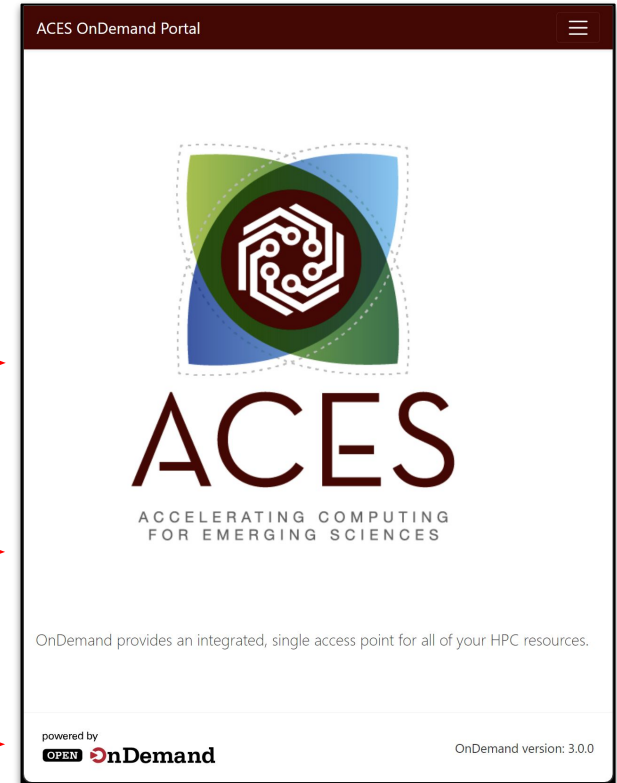


ACES Portal



ACES Portal portal-aces.hprc.tamu.edu
is the web-based user interface for the ACES cluster

Open OnDemand (OOD) is an advanced web-based
graphical interface framework for HPC users



Get a Shell on ACES

Click on “Clusters” menu → _aces Shell Access



Success!

Welcome to the
ACES login node.

```
Last login: Wed Jul 10 16:37:19 2024 from 10.71.1.6
=====
|      Texas A&M University High Performance Research Computing      |
|-----|
| Website:           https://hprc.tamu.edu |
| Consulting:        help@hprc.tamu.edu (preferred) or (979) 845-0219 |
| ACES Documentation: https://hprc.tamu.edu/kb/User-Guides/ACES |
| FASTER Documentation: https://hprc.tamu.edu/kb/User-Guides/FASTER |
| Grace Documentation: https://hprc.tamu.edu/kb/User-Guides/Grace |
| Terra Documentation: https://hprc.tamu.edu/kb/User-Guides/Terra |
| YouTube Channel:   https://www.youtube.com/texasamhprc |
|-----|
=====

*****
*      === IMPORTANT POLICY INFORMATION ===      *
* - Unauthorized use of HPRC resources is prohibited and subject to *
*   criminal prosecution. *
* - Use of HPRC resources in violation of United States export control *
*   laws and regulations is prohibited. Current HPRC staff members are *
*   US citizens and legal residents. *
* - Sharing HPRC account and password information is in violation of *
*   Texas State Law. Any shared accounts will be DISABLED. *
* - Authorized users must also adhere to ALL policies at: *
*   https://hprc.tamu.edu/policies/ *
*****

!! WARNING: THERE ARE ONLY NIGHTLY BACKUPS OF USER HOME DIRECTORIES. !!

Please restrict usage to 8 CORES across ALL login nodes.
Users found in violation of this policy will be SUSPENDED.

To see these messages again, run the motd command.

Your current disk quotas are:
Disk                               Disk Usage    Limit    File Usage    Limit
/home/u.jw123527                   170M          10.0G      632          10000
/scratch/user/u.jw123527           36.5G         1.0T      124995       250000
/scratch/group/p.tra230003.000      4K            1.0T         1          500000
/scratch/group/p.tra220029.000      4K            1.0T         1          500000
/scratch/group/p.sta220004.000      4K            1.0T         1          500000
Type 'showquota' to view these quotas again.
[u.jw123527@aces-login3 ~]$
```



Set Up Your Tutorial Environment

```
cd $SCRATCH  
mkdir s_tutorial  
cd s_tutorial  
pwd
```

```
export TRAINING=/scratch/training/singularity  
cd $TRAINING  
pwd
```



Set Up Your Singularity Environment

- Get to a compute node from the login node
`srun --time=120 --mem=4G --pty bash -i`
- Return to your tutorial directory (if necessary)
`cd $SCRATCH/s_tutorial`
- Set your singularity cache directory for temporary files
`export SINGULARITY_CACHEDIR=$TMPDIR`
- Connect to the internet for fetching images
`module load WebProxy`



Your First Singularity Container

- Singularity can fetch an image *and* launch a shell in one line.
`singularity shell --help`

Activity:

- Fetch an image and launch a shell from it
`singularity shell docker://almalinux:8`
`cat /etc/redhat-release`
`exit`

Compare:

- The ACES compute nodes also have Red Hat linux installed.
`cat /etc/redhat-release`

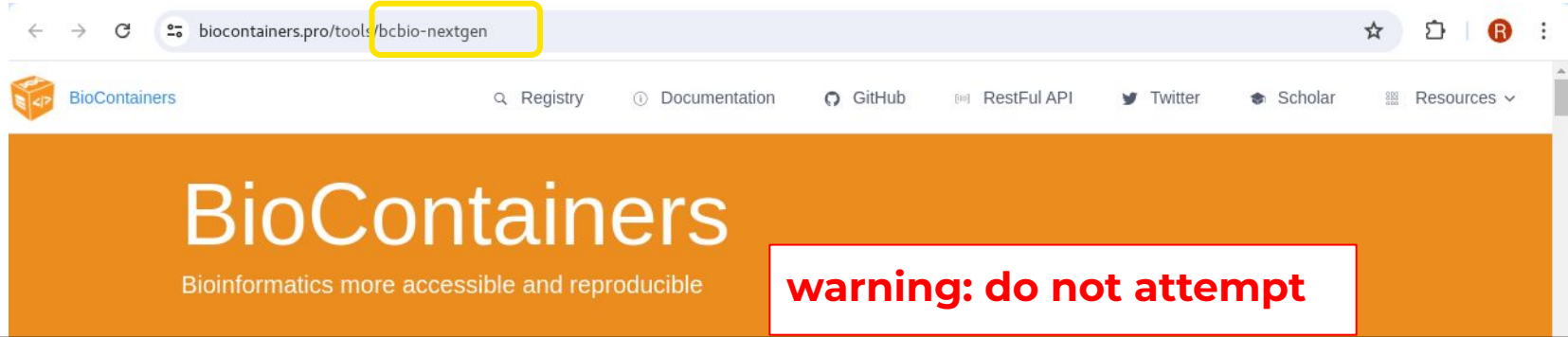









Containerized Scientific Applications



Biocontainers Registry Example



```
singularity pull docker://quay.io/biocontainers/bcbio-nextgen:1.2.9--pyh5e36f6f_3
```

Readme Packages and Containers Similar Tools						
Type	Version	Last Update	Size	Full Tag	Security	
	1.2.9	2022-05-08	279.28M	<code>docker pull quay.io/biocontainers/bcbio-nextgen:1.2.9--pyh5e36f6f_3</code>		
	1.2.9	2021-12-15	296.45M	<code>docker pull quay.io/biocontainers/bcbio-nextgen:1.2.9--pyh5e36f6f_1</code>		

Biocontainers Exercise

- Image file: bcbio-nextgen-1.2.8.sif
From `docker://quay.io/biocontainers/bcbio-nextgen`
Located at: `/scratch/training/singularity`

Activity:

- From the login node:
`srun --mem=4G --time=60 --pty bash -i`
- From the compute node:
`cd /scratch/training/singularity or cd $TRAINING`
- (all on one line)
`singularity exec bcbio-nextgen-1.2.8.sif python -c "import pysam; print(pysam.__version__)"`

Singularity with NVIDIA GPU

- Containers should be built with CUDA version compatible with local GPUs (CUDA \geq 11)
- Just add the `--nv` flag to your singularity command

Many repositories on Docker Hub have GPU-ready images. Search for images with “gpu” in tags

The nvidia cloud also provides GPU-ready images. See:
<https://hprc.tamu.edu/kb/Software/Singularity/Examples/#nvidia-gpu-cloud>



NVIDIA Container Registry Example

NVIDIA NGC | CATALOG Welcome Guest ▾

Catalog > Containers > PyTorch

PyTorch

PyTorch Accelerated with NVIDIA

23.09-py3 Get Container ▾ Deploy to Vertex AI

Copy the latest tag's image path below:

```
nvcr.io/nvidia/pytorch:23.09-py3
```

warning: do not attempt

```
singularity pull docker://nvcr.io/nvidia/pytorch:23.09-py3
```

PyTorch

PyTorch is an optimized tensor library for deep learning, designed to run on NVIDIA GPUs. It is done with a tape-based system and provides a high level of flexibility and speed of functionality. NGC Containers are the easiest way to get started with PyTorch. The PyTorch NGC Container has all dependencies included, providing an easy place to start developing common applications, such as computational AI, natural language processing (NLP), recommenders, and computer vision.

The PyTorch NGC Container is optimized for GPU acceleration, and contains a validated set of libraries that



PyTorch NVIDIA GPU Exercise

- Image file: `pytorch_23.09-py3.sif`
from: `docker://nvcr.io/nvidia/pytorch:23.09-py3`
Located at: `/scratch/training/singularity/`

Activity:

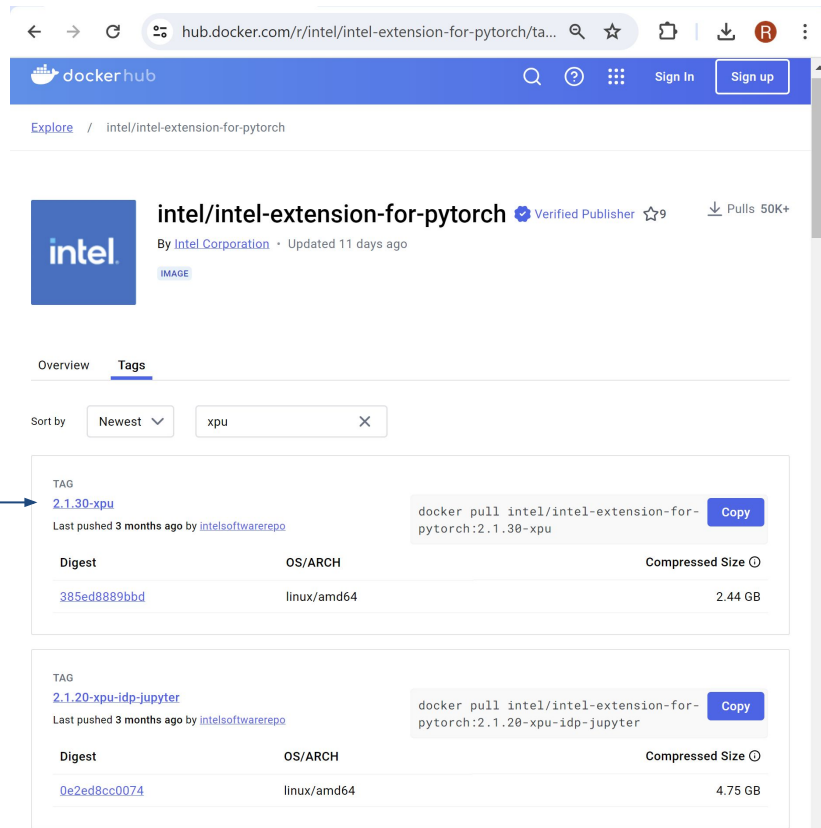
- From the login node: (all on one line) **Following along live? add**
`srn --mem=4G --time=60` **--reservation=workshop_h100**
`--gres=gpu:1 --partition=gpu --pty bash -i`
- On the compute node (if necessary):
`cd /scratch/training/singularity or cd $TRAINING`
- From the compute node: (all on one line)
`singularity exec --nv pytorch_23.09-py3.sif`
`python3 -c "import torch;`
`print(torch.cuda.device_count())"`



PyTorch with Intel GPU

- Containers should be built with OneAPI version compatible with local GPUs
- No additional steps

Many repositories on Docker Hub have GPU-ready images. Search for images with “xpu” in the tag



The screenshot shows the Docker Hub interface for the repository `intel/intel-extension-for-pytorch`. The 'Tags' tab is selected, and a filter for 'xpu' is applied. Two tags are listed:

TAG	Digest	OS/ARCH	Compressed Size
2.1.30-xpu Last pushed 3 months ago by intelsoftwarerepo	385ed8889bbd	linux/amd64	2.44 GB
2.1.20-xpu-idp-jupyter Last pushed 3 months ago by intelsoftwarerepo	0e2ed8cc0074	linux/amd64	4.75 GB

For each tag, a 'docker pull' command is provided in a box, and a 'Copy' button is available. The first command is `docker pull intel/intel-extension-for-pytorch:2.1.30-xpu`.

Learn more about Intel extension for PyTorch at
https://intel.github.io/intel-extension-for-pytorch/xpu/latest/tutorials/getting_started.html



PyTorch Intel GPU Exercise

- Image file: `pytorch_2.1.20-xpu-idp-jupyter.sif`
from: `docker://intel/intel-extension-for-pytorch`
Located at: `/scratch/training/singularity/`

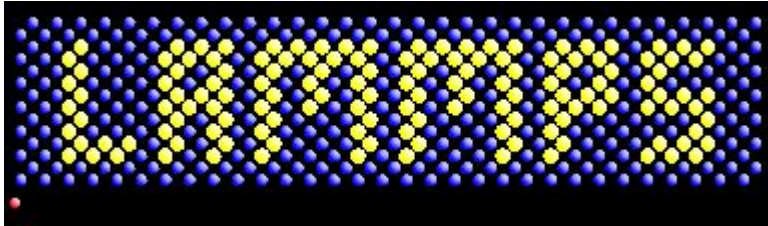
Activity:

- From the login node: (all on one line) **Following along live? add**
`srunk --mem=4G --time=60` **--reservation=workshop_pvc**
`--gres=gpu:1 --partition=pvc` `--pty bash -i`
- On the compute node (if necessary):
`cd /scratch/training/singularity` or `cd $TRAINING`
- From the compute node: (all on one line)
`singularity exec pytorch_2.1.20-xpu-idp-jupyter.sif python3`
`-c "import torch; import intel_extension_for_pytorch as ipex;`
`print(torch.xpu.device_count())"`



LAMMPS Molecular Dynamics on GPUs


- LAMMPS is a classical MD code
- <https://www.lammps.org/> has a cool animated logo.
- NVIDIA provides GPU-ready container images for lammps.
<https://catalog.ngc.nvidia.com/orgs/hpc/containers/lammps>



LAMMPS on H100 GPUs

- *This specific build works with H100 GPUs*

The screenshot shows the NVIDIA NGC Catalog interface for the LAMMPS container. The browser address bar displays `catalog.ngc.nvidia.com/orgs/hpc/containers/lammps/tags`. The page header includes the NVIDIA NGC | CATALOG logo and a 'Welcome Guest' message. The left sidebar shows the navigation path: Catalog > Containers > LAMMPS. The main content area has tabs for Overview, Tags (selected), Layers, Security Scanning, and Related Collections. A search bar for tags is present. A table lists the available tags, with the 'patch_15Jun2023' tag highlighted by a yellow border. The table columns include a tag icon, the tag name, the creation timestamp, size, and architecture count. The 'patch_15Jun2023' tag is associated with the image `nvcr.io/hpc/lammps:patch_15Jun2023`.

Tag	Created	Size	Architectures	Image
 patch_15Jun2023	08/09/2023 11:34 AM	561.38 MB	2 Architectures	nvcr.io/hpc/lammps:patch_15Jun2023

LAMMPS on NVIDIA GPUs

- Image file: `lammps-nv-patch_15Jun2023.sif`
from: `docker://nvcr.io/hpc/lammps:patch_15Jun2023`
Located at: `/scratch/training/singularity/`

Activity (step 1):

- From the login node: (all on one line) **Following along live? add**
`srunch --mem=4G --time=60` **--reservation=workshop_h100**
`--gres=gpu:1 --partition=gpu --pty bash -i`
- From the compute node:
`cd /scratch/training/singularity or cd $TRAINING`

LAMMPS on NVIDIA GPUs

- Image file: `lammps-nv-patch_15Jun2023.sif`
from: `docker://nvcr.io/hpc/lammps:patch_15Jun2023`
Located at: `/scratch/training/singularity/`

Activity (step 2):

- From the compute node: (all on one line)
`singularity run --nv lammps-nv-patch_15Jun2023.sif mpirun
lmp -k on g 1 -sf kk -pk kokkos cuda/aware on neigh full
comm device binsize 2.8 -var x 4 -var y 4 -var z 4 -in
in.lj.txt -log $TMPDIR/log.lammps`

Learn More About Containers



CCEP Community
Grant Awarded



I ACES: Fundamentals of Containers

Prerequisites: Current ACCESS ID, basic Linux/Unix skills

This course introduces concepts of containers and covers common containerization tasks using the Charliecloud and Singularity container engines on the ACES cluster.



I ACES: Containers for Scientific Workflows (Singularity / Apptainer)

Prerequisites: Current ACCESS ID, basic Linux/Unix skills

This course introduces the use of containers for scientific workflows using the Singularity container engine. Exercises will be performed using the ACES cluster, a composable accelerator testbed at Texas A&M University.



I ACES: Containers for Scientific Workflows (Charliecloud)

Prerequisites: Current ACCESS ID, basic Linux/Unix skills

This course introduces the use of Containers using the Charliecloud software suite. Exercises will be performed using the ACES cluster, a composable accelerator testbed at Texas A&M University.



Texas A&M at PEARC24

Talk/Event	Date/Time	Room
Tutorial: Hands-on exercises on the Intel Data Center GPU Max 1100 (PVC-GPU) for AI/ML and Molecular	Mon, July 22, 2024 9:00 AM-12:30 PM ET	Room 553B
Seventh Workshop on Strategies for Enhancing HPC Education and Training (SEHET24)	Mon, July 22, 2024 9:00 AM-12:30 PM ET	Room 557
Workshop: Providing cutting-edge computing testbeds to the science and engineering community	Mon, July 22, 2024 1:30 PM-5:00 PM ET	Room 554A
Workshop: Engaging Secondary Students in Computing: K12 Outreach	Mon, July 22, 2024 1:30 PM-5:00 PM ET	Room 553A
Cultivating Cyberinfrastructure Careers through Student Engagement at Texas A&M University High Performance Research Computing	Tue, July 23, 2024 11:00 AM-11:25 AM ET	Junior Ballroom
Insight Gained from Migrating a Machine Learning Model to Intelligence Processing Units	Tue, July 23, 2024 11:00 AM-11:25 AM ET	Room 551 A&B
BOF 4: What's in it for me? How can we truly democratize the research computing and data community?	Tue, July 23, 2024 1:30 PM-2:30 PM ET	Room 551 A&B



Texas A&M at PEARC24

Talk/Event	Date/Time	Room
BRICCs: Building Pathways to Research Cyberinfrastructure at Under Resourced Institutions	Tue, July 23, 2024 3:25 PM-3:50 PM ET	Junior Ballroom
Memory Bandwidth Performance across Accelerators	Tue, July 23, 2024 3:25 PM-3:50 PM ET	Ballroom B
Container Adoption in Campus High Performance Computing	Wed, July 24, 2024 11:00 AM-11:25 AM ET	Ballroom B
Engaging Secondary Students in Computing and Cybersecurity	Wed, July 24, 2024 3:15 PM-3:30 PM ET	Room 557
Exploring the Viability of Composable Architectures to Overcome Memory Limitations in High Performance Computing Workflows	Wed, July 24, 2024 3:45 PM-4:00 PM ET	Room 553 A&B
Performance of Molecular Dynamics Acceleration Strategies on Composable Cyberinfrastructure	Wed, July 24, 2024 4:15 PM-4:30 PM ET	Room 551 A&B
BOF 17: Fantastic ACCESS Cyberinfrastructure Resources and Where to Find Them	Wed, July 24, 2024 4:45 PM-5:45 PM ET	Room 553 A&B
BOF 18: Recipes to build successful cross-institutional collaborative computing	Wed, July 24, 2024 4:45 PM-5:45 PM ET	Junior Ballroom





High Performance
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Thank you

- Please visit our talks and BoFs at PEARC23
- Please join the [ACES affinity group](https://support.access-ci.org/affinity-groups/aces) support.access-ci.org/affinity-groups/aces
- Questions? help@hprc.tamu.edu
- We gratefully acknowledge support from National Science Foundation awards #2112356 (ACES), #2019129 (FASTER) and #19257614 (SWEETER)

