

HIGH PERFORMANCE RESEARCH COMPUTING

HPRC MATH OUTREACH EVENT

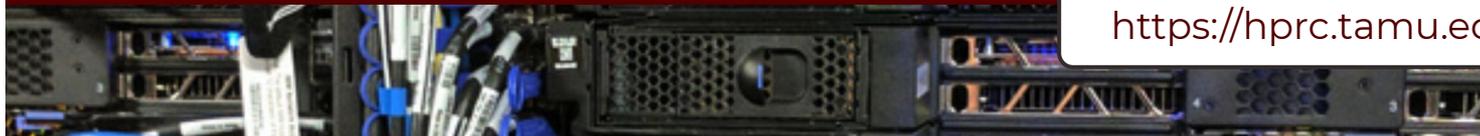
March 17, 2021



High Performance
Research Computing

DIVISION OF RESEARCH





https://hprc.tamu.edu

Quick Links

- New User Information
- Accounts
 - Apply for Accounts
 - Manage Accounts
- User Consulting
- Training
- Documentation
- Software
- FAQ

User Guides

- Ada
- Terra
- Grace
- Portal
- Galaxy

Cluster Status

Terra

Nodes	303/315 (96%)
Cores	7692/9324 (82%)
Jobs	509R-379Q

Ada

Nodes	763/775 (98%)
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TEXAS A&M UNIVERSITY TO ACQUIRE A NEXT-GENERATION COMPOSABLE HIGH PERFORMANCE COMPUTING PLATFORM

NSF Grant Supports Texas A&M's Acquisition Of High Performance Computing Platform

News

- JAN 7** [XSEDE Welcomes New Service Providers](#)
- NOV 9** [Grace, A More Powerful Supercomputer For Texas A&M Research Is Coming Soon](#)

Events

- FEB 12** [Short Course: Introduction to HPRC](#)
- FEB 12** [Short Course: SLURM Job Scheduling](#)

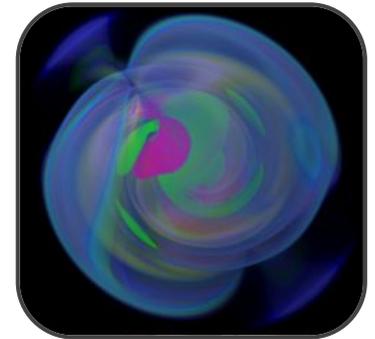


High Performance Research Computing

An interdisciplinary research environment that advances computational and data-enabled sciences, engineering, and scholarship

Our Mission:

- Enable research and discoveries that advance science and technology.
- Enable computational and data-enabled research activities of students, faculty, and staff at Texas A&M University.
- Provide consulting, technical documentation, and training to support users of these resources.



HPRC Services

- **Free of charge** to all faculty, research staff, students and external collaborators
- Computing cycles and networking for researchers
- **Application is required for access**
- Staff consists of 15 professionals and 8 student workers
- User Services
 - Helpdesk: New user start-up assistance and general support
 - Training: Short Courses, Workshops, & YouTube videos
 - Advanced Support: Software installation and consulting
 - Expertise in many science and engineering research domains
- Access to state and national advanced computing resources

High Performance Research Computing Clusters



Ada*



Terra



ViDaL



Grace†

Total Nodes (Cores)	864 (17,596)	307 (8,512)	24 (1,120)	925 (44,656)
General Nodes	20 cores 64GB	28 cores 64GB	40 cores 192 GB	48 cores 384GB
Features	GPUs (K20) Phi Large Memory Nodes	GPUs (K80, V100) KNL	Compliant Computing GPUs (V100) Large Memory Nodes	GPUs (A100, RTX 6000, T4) Large Memory Nodes
Interconnect	FDR10 InfiniBand	Omni-Path	40Gb Ethernet	HDR100 InfiniBand
Global Disk (raw)	5.6 PB	7.4 PB	2 PB	8.9 PB

*Retiring in Spring 2021

<https://hprc.tamu.edu/resources>

†Testing and early user onboarding

HPRC Training Short Courses

<https://hprc.tamu.edu/training>

Primers:

Linux
HPRC Clusters
Data Management
SLURM
Jupyter Notebook

Technology Lab:

Using AI Frameworks
in Jupyter Notebook

Short Courses:

Python
Scientific Python
PyTorch
TensorFlow
MATLAB
Scientific ML
Julia
CUDA
Drug Docking
Quantum Chemistry
and more...

Short Courses:

NGS Analysis
NGS Metagenomics
NGS RADSeq/GBS
NGS Assembly
HPRC Galaxy
Linux
R
Perl
Fortran
OpenMP
MPI



High Performance
Research Computing
DIVISION OF RESEARCH

YouTube training videos



Texas A&M HPRC

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HPRC Intro #12: Transferring Files on TAMU HPRC

15 views • 3 days ago

CC



HPRC Short Course: Post-Processing CESM Model...

36 views • 3 months ago

CC



HPRC Short Course: Introduction to Python

77 views • 3 months ago

CC



HPRC Intro #11: Submitting a Job Using LSF

142 views • 4 months ago

CC



HPRC Primers: Introduction to Linux

80 views • 5 months ago

CC



HPRC Intro #8: Submitting a Job Using SLURM

245 views • 5 months ago

CC



HPRC Intro: #6 The Modules System

122 views • 5 months ago

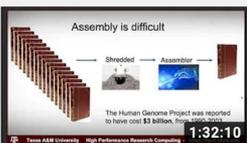
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HPRC Intro #3: Accessing Clusters from a Windows...

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NGS Assembly

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NGS RNA Sequencing

98 views • 7 months ago

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NGS Genotyping with Sequencing

59 views • 7 months ago

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HPRC Short Course: Introduction to Quantum...

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Texas A&M University High Performance Research Computing <https://hprc.tamu.edu>

Advanced Support Program

HPRC offers collaborations in research projects with a large computational component. Under the **ASP**, one or more HPRC analysts will contribute expertise and experience in several areas of high performance computing in a sustained and focused way.

- Porting applications to our clusters
- Optimizing and analyzing serial code performance
- Developing parallel code from serial versions and analyzing performance
- Optimizing serial and parallel I/O code performance
- Assisting in the optimal use of mathematical libraries
- Assisting with code development and design
- Assisting with the improvement of workflow automation in scientific processes

If you are interested in a collaboration through our **ASP** program, please send us an e-mail at help@hprc.tamu.edu.

ASP is supported in part by NSF award #1925764, CC* Team: SWEETER -- SouthWest Expertise in Expanding, Training, Education and Research.



Welcome to the TAMU HPRC Wiki

- [Ada Guide](#)
- [Terra Guide](#)
- [Software](#)
- [Usage Policies](#)
- [Contact Us](#)

Announcements

- **Grace Cluster Status:** Cluster deployed, currently in testing and early user access mode.
- **New GPU nodes in the Terra cluster:** Two new GPU nodes are now available in the Terra Cluster. Each GPU node has two Intel Skylake Xeon Gold 5118 20-core processors, 192 GB of memory and two NVIDIA 32GB V100 GPUs. To use these new GPU nodes, please submit jobs to the `gpu` queue on Terra by including the following job directive in your job scripts:

```
#SBATCH --gres=gpu:v100:1      #Request 1 GPU per node can be 1 or 2
#SBATCH --partition=gpu        #Request the GPU partition/queue
```

Getting an Account

- **Understanding HPRC:** For a brief overview of what services HPRC offers, see [this video](#) in our getting started series on YouTube.
- **New to HPRC's resources?** [This page](#) explains the HPRC resources available to the TAMU community. Also see the [Policies Page](#) to better understand the rules and etiquette of cluster usage..
- **Accessing the clusters:** All computer systems managed by the HPRC are available for use to TAMU faculty, staff, and students who require large-scale computing capabilities. The HPRC hosts the [Ada](#), [Terra](#), and [Grace](#) clusters at TAMU. To apply for or renew an HPRC account, please visit the [Account Applications](#) page. For information on how to obtain an allocation to run jobs on one of our clusters, please visit the [Allocations Policy](#) page. *All accounts expire and must be renewed in September of each year.*

Using the Clusters

- **QuickStart Guides:** For just the "need-to-know" information on getting started with our clusters, visit our QuickStart pages. Topics discussed include cluster access, file management, the batch system, setting up a software environment using modules, creating your own job files, and project account management. [Ada QuickStart Guide](#), [Terra Quickstart Guide](#), [Grace Quickstart Guide](#)
- **Batch Jobs:** As a shared resource between many users, each cluster must employ a batch system to schedule a time for each user's job to run. Without such a system, one user could use a disproportionate amount of resources, and cause other users' work to stall. Ada's batch system is called LSF, and Terra's batch system is called SLURM. While similar in function, they differ in their finer details, such as job file syntax. Information relevant to each system can be found below.

[Ada / LSF Batch Pages](#)
[Complete Ada Batch Page](#)
[Job Submission \(bsub\)](#)
[Ada Queue Structure](#)

[Terra and Grace / SLURM Batch Pages](#)
[Complete Terra Batch Page](#)
[Job Submission \(sbatch\)](#)
[Terra Queue Structure](#)

Available Software Modules



TEXAS A&M HIGH PERFORMANCE RESEARCH COMPUTING



Home User Services Resources Research Policies Events About Portal

<https://hprc.tamu.edu/software/terra>

SOFTWARE MODULES ON THE TERRA CLUSTER

Last Updated: Mon Nov 23 00:00:01 CST

The available software for the Terra cluster is listed in the table. Click on any software package name to get more information such as the available additional documentation if available, etc.

Show 10 entries Search: mumps

Name	Description
MUMPS	A parallel sparse direct solver URL: https://graal.ens-lyon.fr/MUMPS/

Showing 1 to 1 of 1 entries (filtered from 1,702 total entries)

<https://hprc.tamu.edu/wiki/SW:Modules>

MUMPS

Home Page:
<https://graal.ens-lyon.fr/MUMPS/>

Description:
A parallel sparse direct solver URL: <https://graal.ens-lyon.fr/MUMPS/>

Notes:

Versions:
MUMPS/5.0.1-intel-2017b-parmetis
MUMPS/5.0.1-intel-2017b-metis
MUMPS/5.1.2-intel-2017b-parmetis
MUMPS/5.1.2-intel-2017b-metis
MUMPS/5.2.1-foss-2018b-metis
MUMPS/5.2.1-foss-2019a-metis-seq
MUMPS/5.2.1-foss-2019a-metis
MUMPS/5.2.1-foss-2019b-metis
MUMPS/5.2.1-foss-2020a-metis
MUMPS/5.2.1-intel-2019a-metis-seq
MUMPS/5.2.1-intel-2019a-metis
MUMPS/5.2.1-intel-2019b-metis
MUMPS/5.2.1-intel-2020a-metis

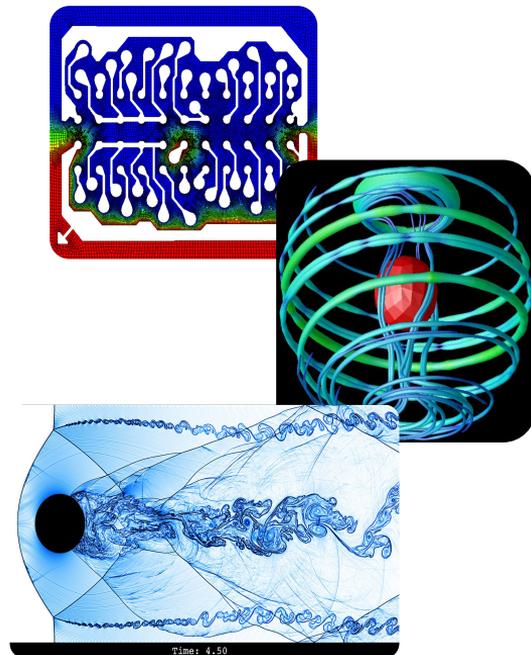
Available Software Modules

<https://hprc.tamu.edu/wiki/SW:Modules>

mla command to quickly search for installed software:

```
[mouse@terra3 ~]$ mla mumps
Using /home/mouse/module.avail.terra
MUMPS/
MUMPS/5.0.1-intel-2017b-parmetis
MUMPS/5.0.1-intel-2017b-metis
MUMPS/5.1.2-intel-2017b-parmetis
MUMPS/5.1.2-intel-2017b-metis
MUMPS/5.2.1-foss-2018b-metis
MUMPS/5.2.1-foss-2019a-metis-seq
MUMPS/5.2.1-foss-2019a-metis
MUMPS/5.2.1-foss-2019b-metis
MUMPS/5.2.1-foss-2020a-metis
MUMPS/5.2.1-intel-2019a-metis-seq
MUMPS/5.2.1-intel-2019a-metis
MUMPS/5.2.1-intel-2019b-metis
MUMPS/5.2.1-intel-2020a-metis
```

Compilers: C++, Fortran,
intel, gnu, ...
openmpi, intelmpi
Python
Matlab
Paraview
Visit
Deal.II
FFTW
ScaLAPACK
Gmsh
MUMPS
METIS
p4est
PETSc
SLEPc
Trilinos
...



Images: <https://www.dealii.org/code-gallery.html>



OnDemand provides an integrated, single access point to HPRC resources.

Message of the Day

IMPORTANT POLICY INFORMATION

- Unauthorized use of HPRC resources is prohibited and subject to disciplinary action.
- Use of HPRC resources in violation of United States export control regulations is prohibited. Current HPRC accounts will be DISABLED if they are found to be in violation.
- Sharing HPRC account and password information is in violation of HPRC policies.
- Authorized users must also adhere to ALL policies at: <https://hprc.tamu.edu/policies>

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

Terra Cluster Maintenance, March 23

The Terra cluster will be unavailable from 9am to 6pm on Tuesday, March 23rd. Maintenance will be performed if they will overlap with this maintenance window.

Open OnDemand (OOD) Portal enables advanced web and graphical interface for HPC users.



- BIO
- Beauti
- DIYABC
- FigTree
- IGV
- JBrowse
- Krait
- Mauve
- Structure
- Tracer
- GUI
- ANSYS Workbench
- Abaqus/CAE
- LS-PREPOST
- LS-PREPOST (workshop)
- MATLAB
- ParaView
- VNC
- Imaging
- Chimera
- Coot
- Diffusion Toolkit & TrackVis
- FSL
- Fiji
- ICY
- ImageJ
- Vaa3D
- cisTEM
- Servers
- Jupyter Notebook
- JupyterLab
- RStudio
- Spark-Jupyter Notebook



HPC resources.

prohibited. Current HPRC accounts will be DISABLED

maintenance will be performed

HPRC Portal

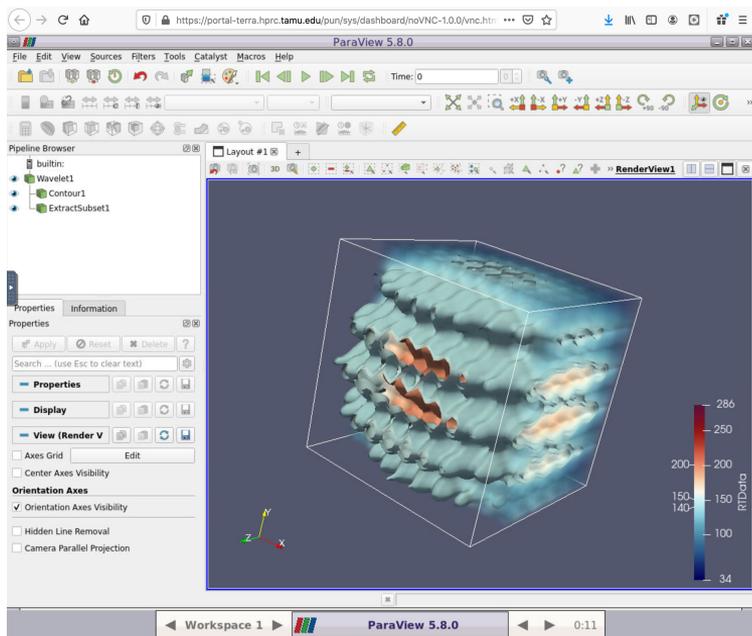
<https://portal.hprc.tamu.edu>

HPRC Portal YouTube tutorials



HPRC Open OnDemand Portal

<https://portal.hprc.tamu.edu>



The image shows the HPRC Terra Toolbox dashboard. The header includes the HPRC logo and the text 'High Performance Research Computing DIVISION OF RESEARCH'. The main content is divided into several sections:

- CLUSTER STATISTICS**: Contains two pie charts. The first is 'Node Utilization' with categories: Allocated (red), Mixed (blue), and Idle (green). The second is 'Core Utilization' with categories: Used (red) and Free (green).
- Jobs**: A table showing the number of running and pending jobs.
- SUMMARY**: A table showing account information.
- Disk Quotas**: A table showing disk usage and limits for various directories.
- Your Jobs**: A table showing the status of individual jobs.

Account	Default	Allocation	Used	Balance
122853910111	Set Default	20000	0	20000
122853910233	Set Default	200000	198148.06	1851.94
122853913205	default	5000	-3735.43	1264.57
122853915531	Set Default	200000	50000	150000

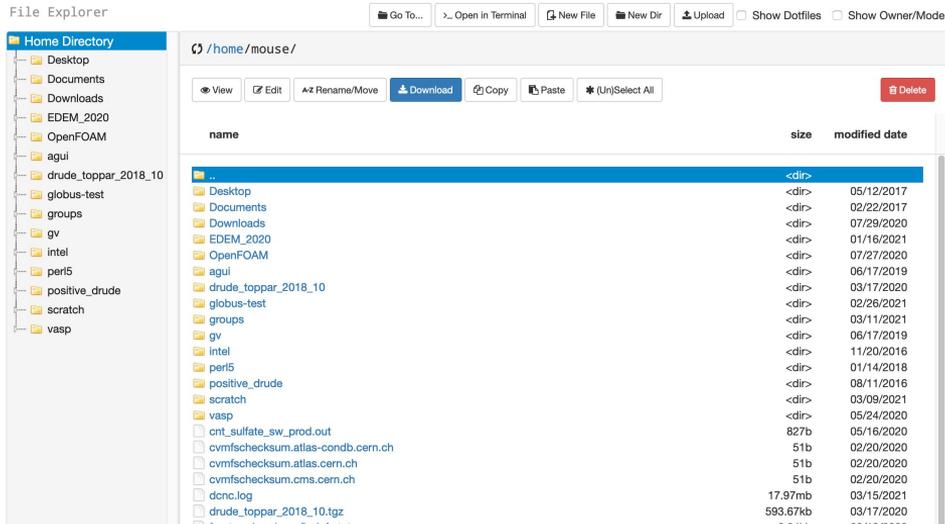
Disk	Disk Usage	Limit	File Usage	Limit
/home	2.76 GB (27.59 %)	10 GB	8882 (88.82 %)	10000
/scratch	282.87 GB (27.62 %)	1 TB	100574 (50.29 %)	200000

Job ID	Name	State	Partition
7522977	...rd/sys/vnc	RUNNING	gpu

Run GUI based software. You can start an interactive job, close your browser, log out of your computer and login later on the same or different computer to continue working on your interactive job.



Advantages of Using the HPRC Portal



Create, delete, copy, edit, rename upload and download files and directories on the HPRC clusters using a web browser. Transfer files between your local computer and the HPRC clusters.



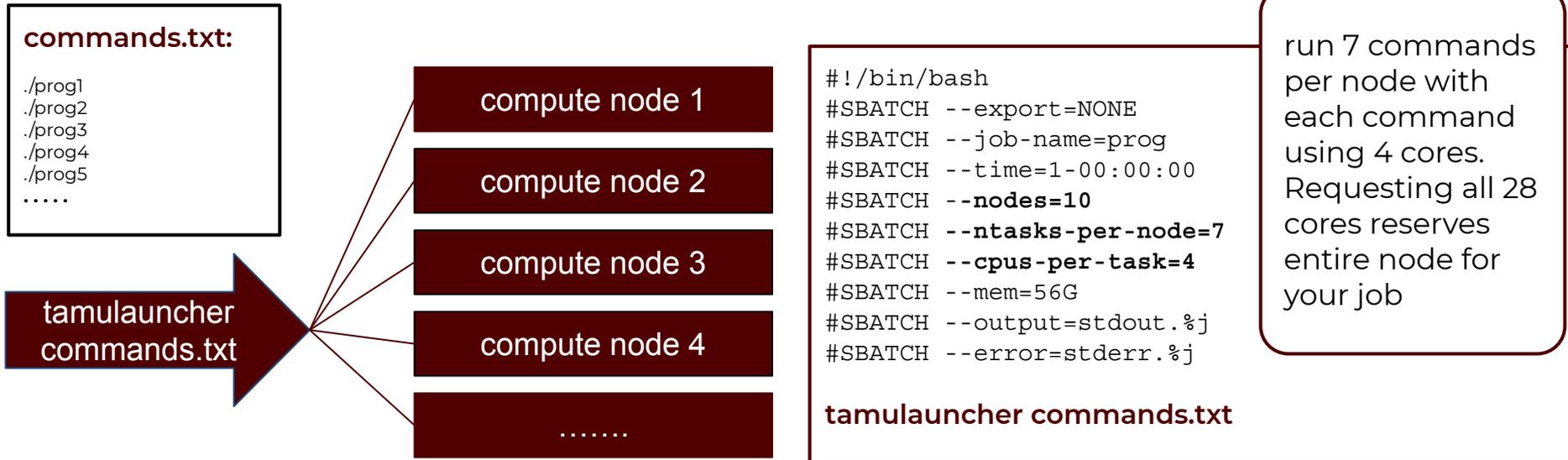
Access the command line

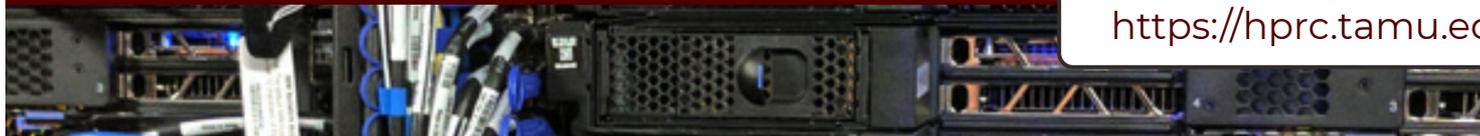


HPRC TAMULauncher

<https://hprc.tamu.edu/wiki/SW:tamulauncher>

tamulauncher provides a convenient way to run a large number of serial or multithreaded commands without the need to submit individual jobs or a Job array.





<https://hprc.tamu.edu>

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<https://hprc.tamu.edu/apply>

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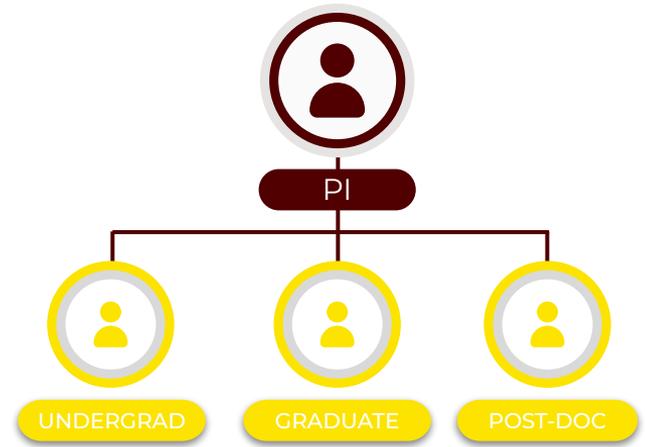


HPRC Account Allocations

Allocation Type	Who can apply?	Minimum SUs per Allocation per Machine	Maximum SUs per Allocation per Machine	Maximum Total SUs per Machine	Maximum Number of Allocations per Machine	Allowed to spend more than allocation?	Reviewed and approved by
Basic	Faculty, Post-Docs*, Research Associates, Research Scientists, Qualified Staff, Students*, Visiting Scholars/Students*	5,000	5,000	5,000	1	No	HPRC Staff
Startup	Faculty, Research Associates, Research Scientists, Qualified Staff	5,000	200,000	400,000	2	No	HPRC Director
Research (Ada)	Faculty, Research Scientists, Qualified Staff	300,000	8,000,000	8,000,000	Determined by <u>HPRC-RAC</u>	No	<u>HPRC-RAC</u>
Research (Terra)	Faculty, Research Scientists, Qualified Staff	300,000	5,000,000	5,000,000	Determined by <u>HPRC-RAC</u>	No	<u>HPRC-RAC</u>

Note: '*' - requires a PI

<https://hprc.tamu.edu/policies/allocations.html>



Graduate Students & Postdoctoral researchers can apply for a Basic allocation.

PIs can apply for a Startup or Research allocation and sub-allocate SUs to their researchers.

HPRC Account: PI Eligibility

For the purpose of HPRC allocations, only **active faculty** members and **permanent research staff** (subject to HPRC-RAC Chair review and approval) of Texas A&M System Members headquartered in Brazos County can serve as a PI.

Adjunct and Visiting professors do not qualify themselves, but can use HPRC resources as part of a sponsoring PI's group.

Note that:

- A PI can have more than one allocation.
- A user can work on more than one project and with more than one PI

<https://hprc.tamu.edu/policies/allocations.html>



Special Requests

<https://hprc.tamu.edu/policies/allocations.html>

- **Dedicated Use**
 - Requests for dedicated cluster use require the approval of the Director.
 - To initiate the process, please send e-mail to the HPRC help desk at help@hprc.tamu.edu
- **Special case allocations**
 - 20% of common SUs are reserved for special case assignments
 - Example special case assignments
 - working with HPRC staff on new capabilities of general value to research communities across campus
 - new faculty startup
 - other operations that go beyond normal research projects
 - Granted by the Director or the VPR.
- **Committed Allocations**
 - PIs who have contributed to the HPRC infrastructure via the “condo” contributions will also have committed allocations related to their contributions which are outside the common pool.

Terra: Examples of SUs charged based on Job Cores, Time and Memory Requested

A Service Unit (SU) on Terra is equivalent to one core or **2** GB memory usage for one hour.

Number of Cores	GB of memory per core	Total Memory (GB)	Hours	SUs charged
1	2	2	1	1
1	3	3	1	2
1	56	56	1	28
28	2	56	1	28

GPU jobs are are charge 28 SUs per hour

Unused SUs expire at the end of each fiscal year (Aug 31) and must be renewed

hprc.tamu.edu/wiki/HPRC:AMS:Service_Unit

HPRC Cluster Queues

CLUSTER STATUS HISTORY

NOTE: Data for this graph is only updated every ten minutes.

Systems:

Ada

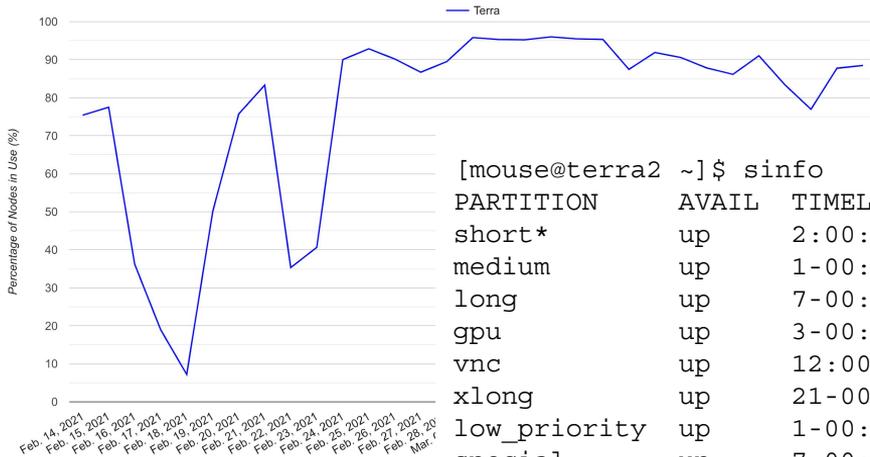
Terra

Number of days:

X-axis interval:

Statistic:

Update Graphs



```
[mouse@terra2 ~]$ sinfo
```

PARTITION	AVAIL	TIMELIMIT	JOB_SIZE	NODES (A/I/O/T)	CPUS (A/I/O/T)
short*	up	2:00:00	1-16	254/1/1/256	5428/1712/28/7168
medium	up	1-00:00:00	1-64	254/1/1/256	5428/1712/28/7168
long	up	7-00:00:00	1-32	254/1/1/256	5428/1712/28/7168
gpu	up	3-00:00:00	1-48	24/26/0/50	617/775/0/1392
vnc	up	12:00:00	1	22/26/0/48	569/775/0/1344
xlong	up	21-00:00:00	1-32	254/1/1/256	5428/1712/28/7168
low_priority	up	1-00:00:00	1-infinite	276/27/1/304	5997/2487/28/8512
special	up	7-00:00:00	1-infinite	276/27/1/304	5997/2487/28/8512
kn1	up	7-00:00:00	1-8	0/12/4/16	0/840/280/1120

Cluster Status

Terra

Nodes 277/315 (88%)
 Cores 6035/9324 (65%)
 Jobs 344R-9376Q

Ada

Nodes 762/775 (98%)
 Cores 10892/15768 (69%)
 Jobs 613R-1043Q

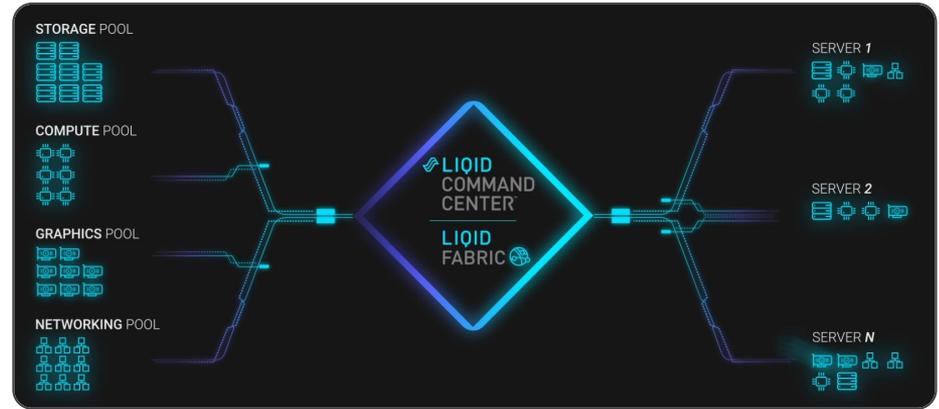
Historical Status

https://hprc.tamu.edu/wiki/Terra:Batch_Processing_SLURM
<https://hprc.tamu.edu/training/slurm.html>

FASTER

Fostering Accelerated Scientific Transformations, Education, and Research

Available summer 2021



- Equipped with **NVIDIA A100**, and **T4/T4-Next** GPUs for AI/DL/ML workloads. Each node can access 16+ GPUs.
- Adopts the innovative LIQID **composable** software-hardware approach combined with cutting-edge technologies.
- Funded by NSF MRI grant #2019129 (\$3.09M + \$1.32M TAMU match)



**HIGH PERFORMANCE
RESEARCH COMPUTING**
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 (Grace, Terra, Ada, ViDAL), NetID (UserID), Job information (Job id(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.

