

HIGH PERFORMANCE RESEARCH COMPUTING

Introduction to HPRC, Duo, VPN and Clusters

June 1, 2021



TEXAS A&M UNIVERSITY
Division of Research





<https://hprc.tamu.edu>

Quick Links

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

User Guides

- Ada
- Terra
- Grace
- Portal
- Galaxy

Cluster Status

Terra	
Nodes	307/313 (98%)
Cores	7195/9268 (78%)
Jobs	220R-65Q
Ada	

bacteriophage

sirtuin 2

peptide with nanomolar inhibition

unnatural amino acid

HPRC: TERRA cluster
MD: Desmond/Schrodinger
GPU, 150+ h

Synergism between Theory and Experiments

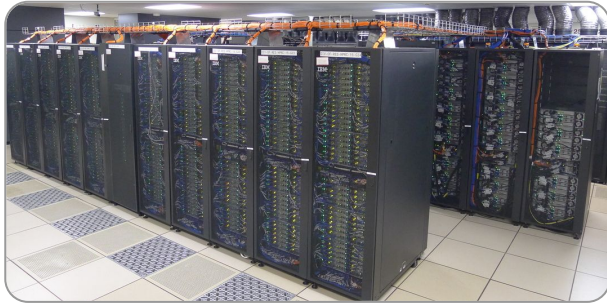
News

- APR 13** [New computational tool could help design futuristic turbines for jet engines](#)
- JAN 7** [XSEDE Welcomes New Service Providers](#)

Events

- May 24-26** [Texas A&M Research Computing Symposium](#)
- May 7** [Workshop: TensorDiffEq for Efficient and Scalable Physics-Informed Deep Learning](#)

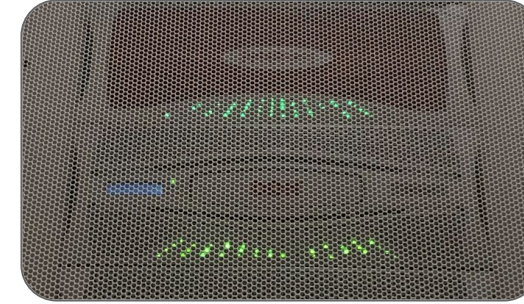
High Performance Research Computing Clusters



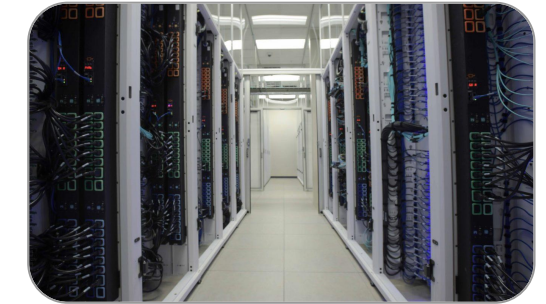
Ada*



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

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

*Retiring on June 30 2021

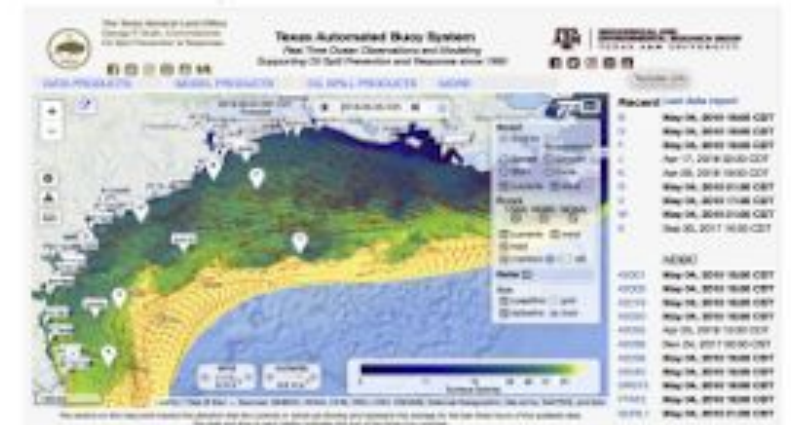
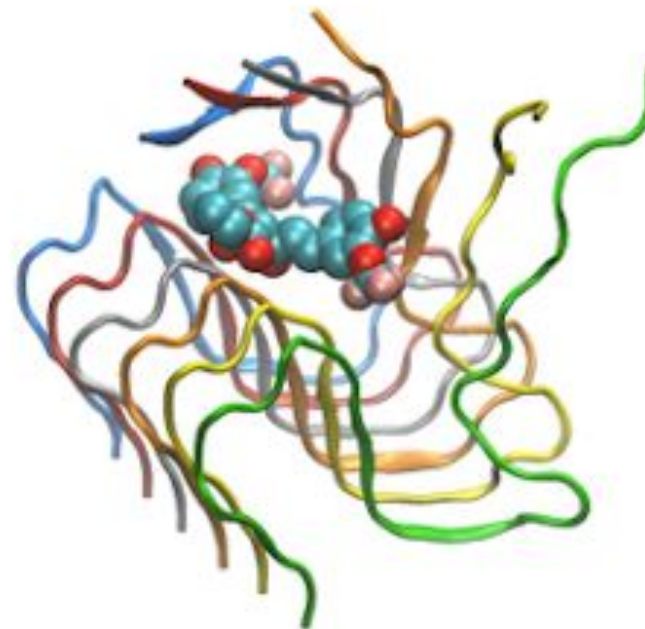
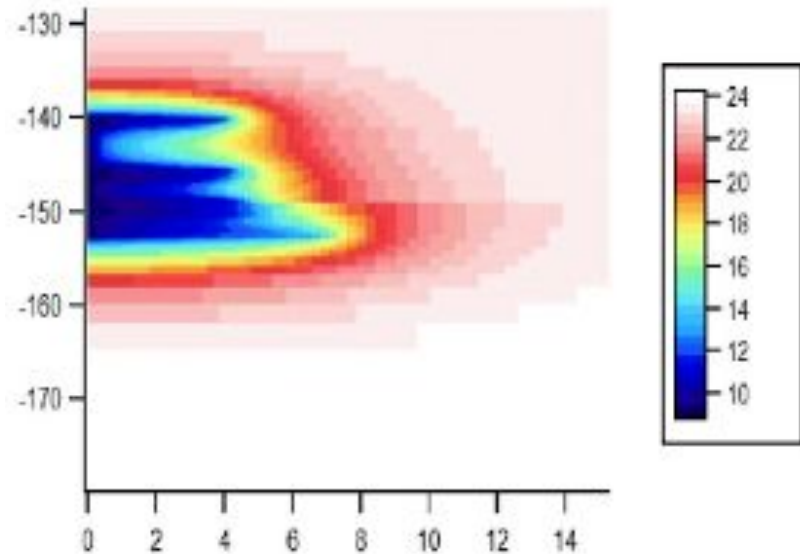
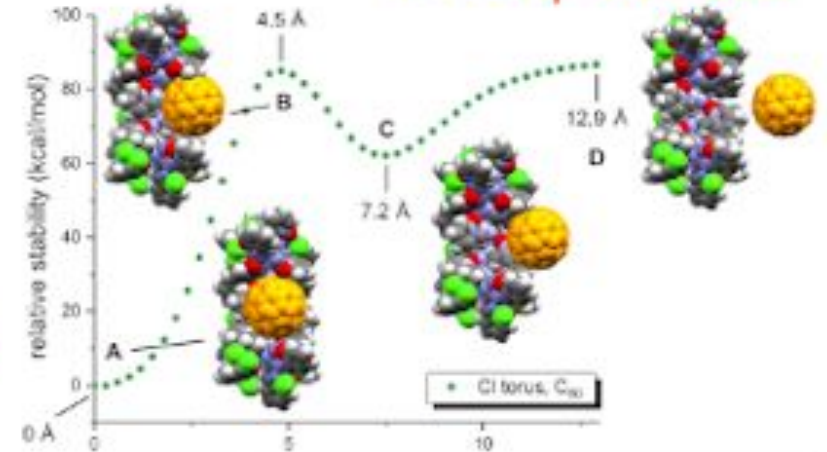
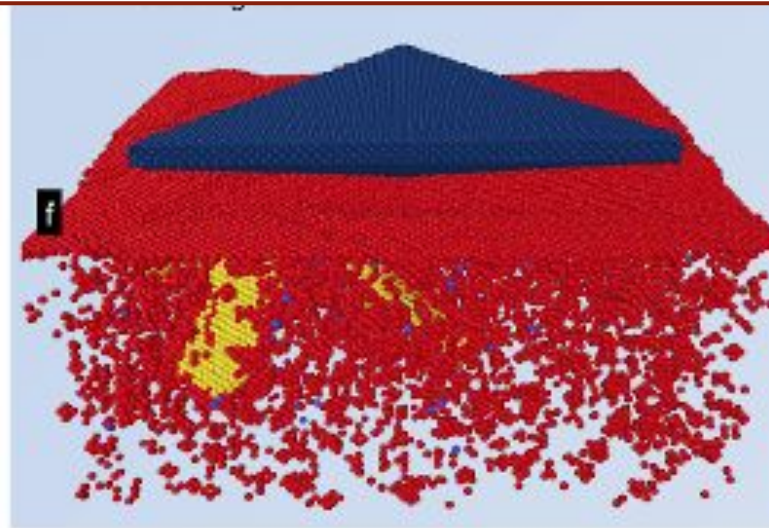
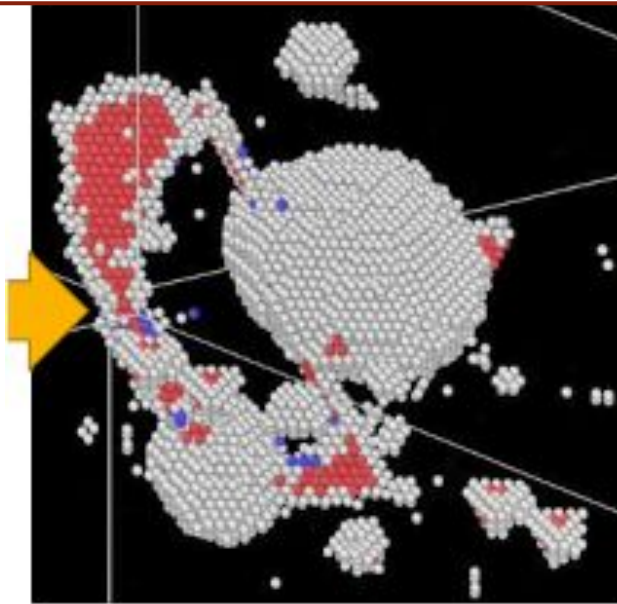
†Testing and early user onboarding

Terra: A Lenovo x86 Cluster

- A 8,512-core hybrid system with NVIDIA K80 & V100 GPUs
- 304 28-core compute nodes equipped with the INTEL 14-core 2.4GHz Broadwell processor
- 48 nodes have 1 K80 GPU with 128GB memory each
- 4 nodes with 2 V100 GPUs with 32GB memory each
- Interconnect fabric is Intel OmniPath Architecture (OPA)

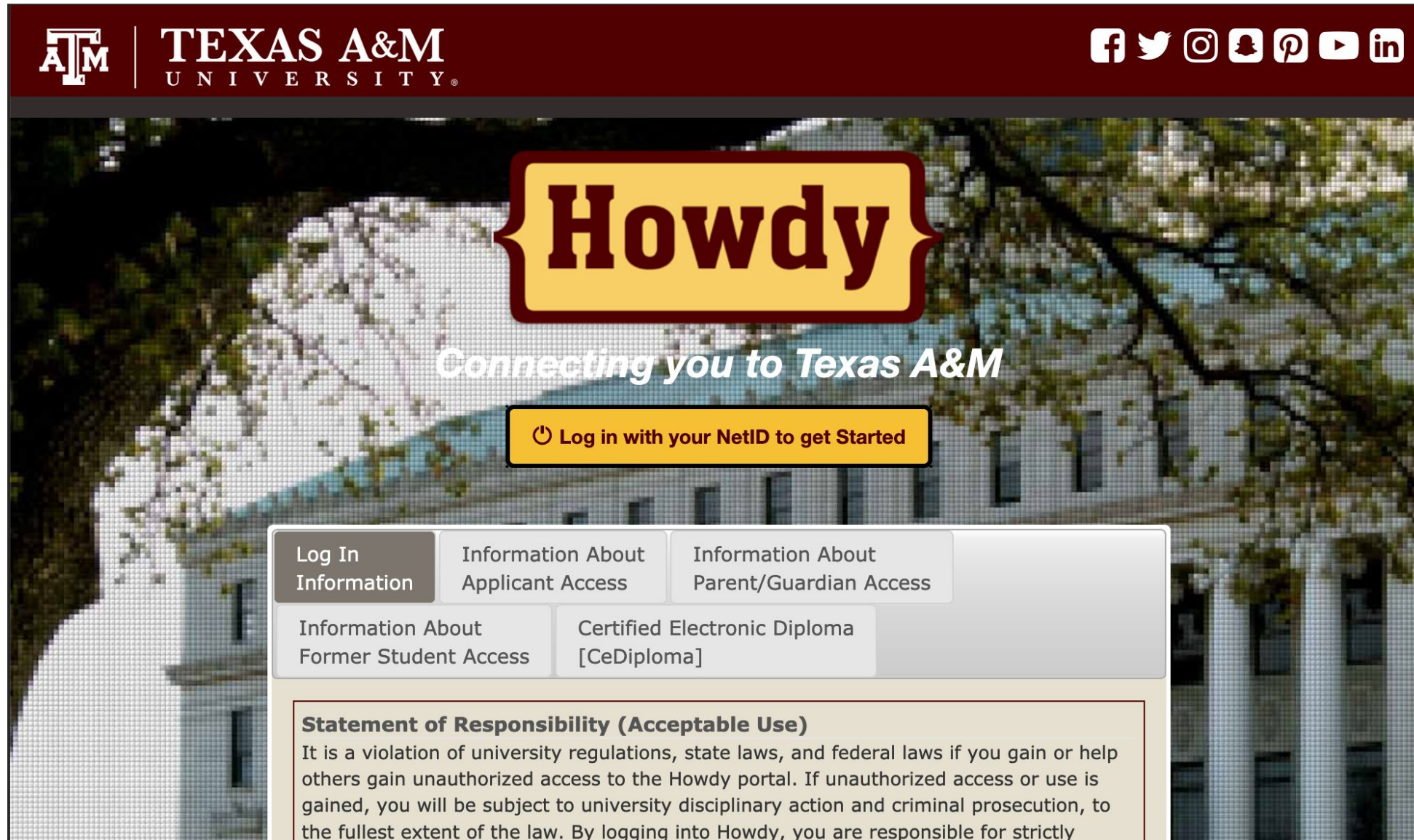


<https://hprc.tamu.edu/events/conferences/sc20/>



NETID - username you use to login to various systems and services
(<https://howdy.tamu.edu>)

For help with your netid: <https://it.tamu.edu/help/>



VPN (Virtual Private Network) <https://connect.tamu.edu>
Required to access the university's network from off campus.
For help with VPN: <https://it.tamu.edu/help/>



Texas A&M SSL VPN Service

DIVISION OF INFORMATION TECHNOLOGY

VPN users are required to use Duo NetID Two-Factor Authentication. If you use the Duo phone call feature, additional steps are required.

Once VPN is downloaded, type **connect.tamu.edu** in the empty box. Click Connect.

Log In

Group:

NetID:

Password:

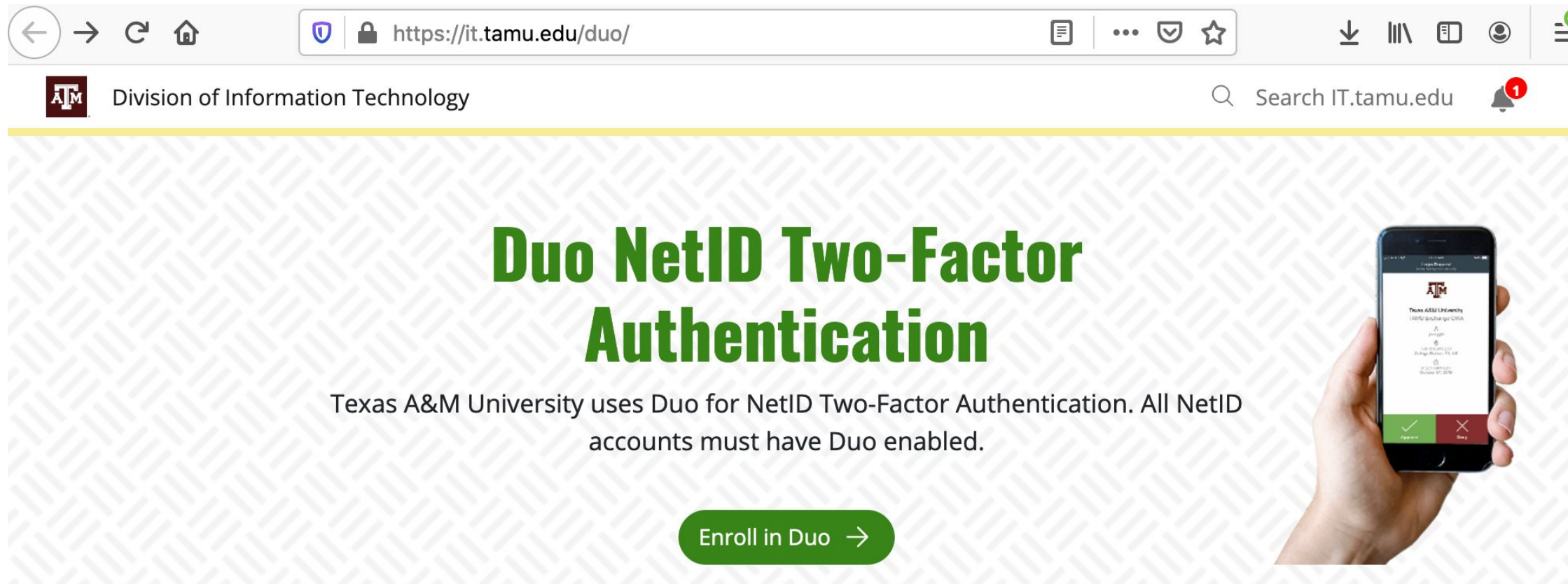
Log In



Two-Factor Authentication (DUO)

For help with enabling DUO: <https://it.tamu.edu/help/>

- Duo NetID two-factor authentication to enhance security (<https://it.tamu.edu/duo/>)
 - All web login (howdy, portal.hprc.tamu.edu, Globus) through CAS
 - VPN to TAMU campus (<https://connect.tamu.edu>)
 - SSH/SFTP to HPRC clusters (https://hprc.tamu.edu/wiki/Two_Factor)





<https://hprc.tamu.edu>

Quick Links

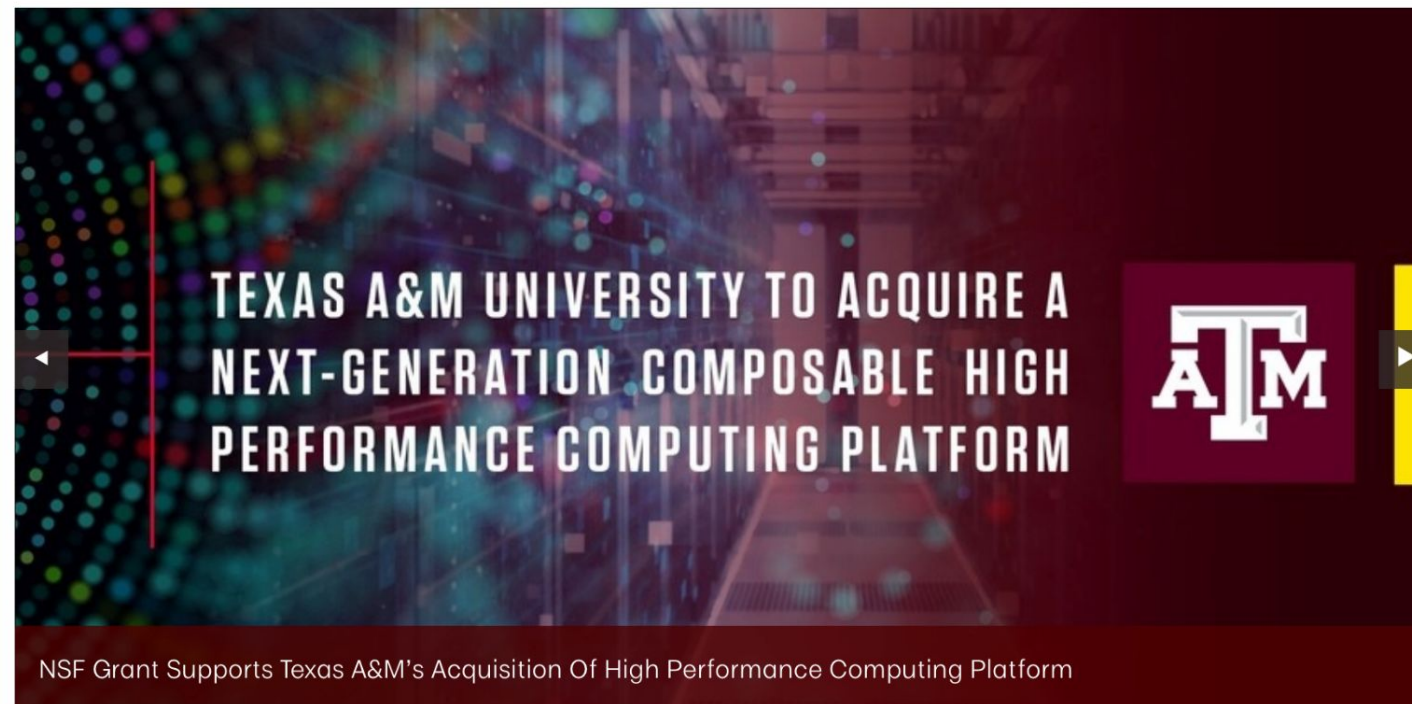
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High Performance
Research Computing
DIVISION OF RESEARCH

[YouTube training videos](#)



Texas A&M HPRC

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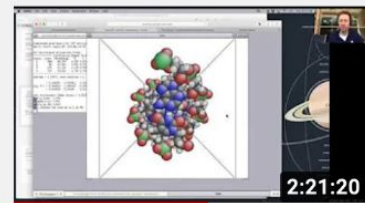
ABOUT



41 videos

Uploads PLAY ALL

SORT BY



OREU: Introduction to
LAMMPS Part 1

874 views • 11 months ago

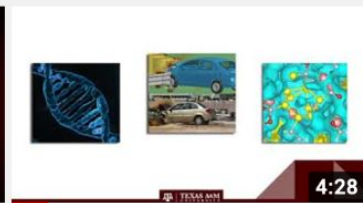
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HPRC Intro #8: Submitting a
Job Using SLURM

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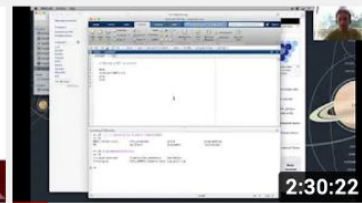
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HPRC intro: #0 What is
HPRC?

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OREU: Introduction to
LAMMPS Part 2

364 views • 11 months ago

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HPRC Primers: Ada

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HPRC Intro #11: Submitting
a Job Using LSF

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HPRC Intro: #7 Submitting a
Job File on Ada/Curie

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HPRC Intro: #2 Cluster
Access Using SSH

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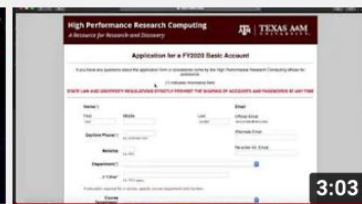
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HPRC Intro: #5 Managing
Allocations

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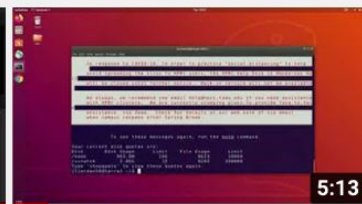
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HPRC Intro: #1 Applying for
Accounts

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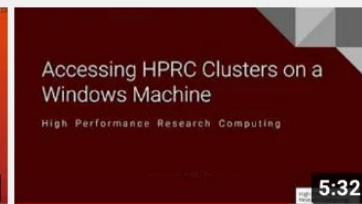
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HPRC Intro: #4 File
Management on the...

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

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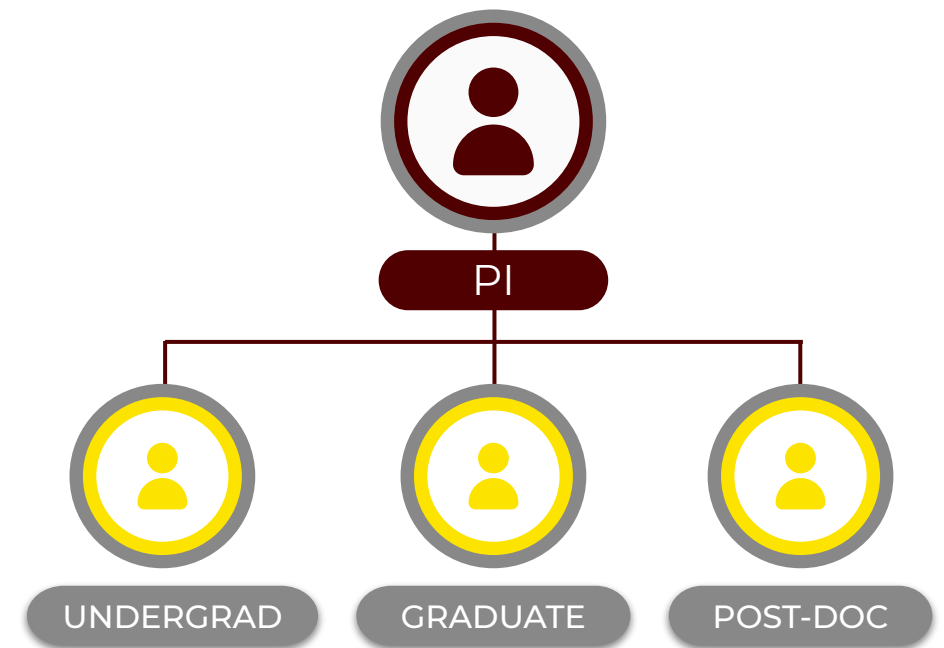
<https://hprc.tamu.edu>

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>



Undergraduate, Graduate & Postdoctoral researchers can apply for a Basic allocation.

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

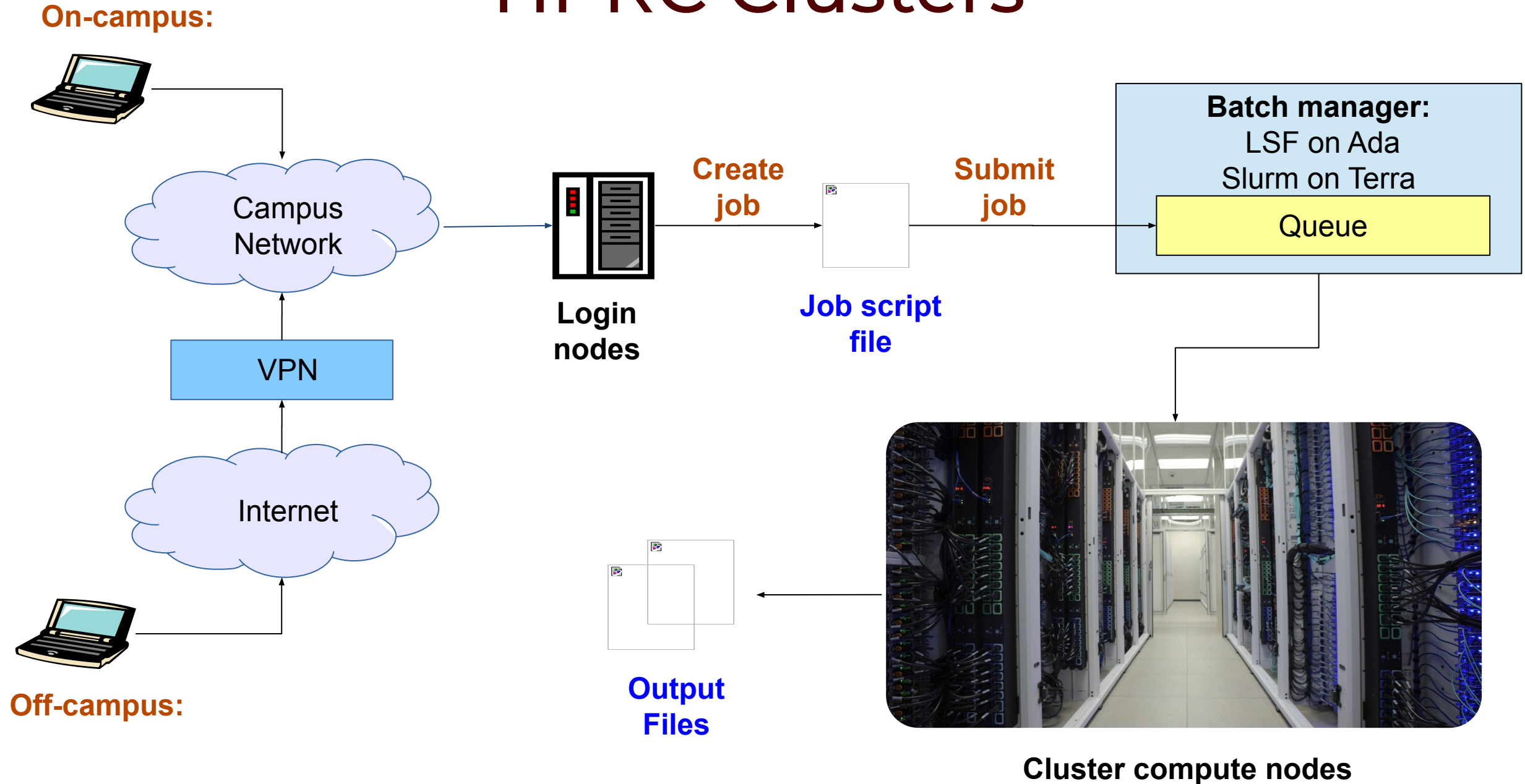
Examples of **SUs** charged based on Job Cores, Time and Memory Requested

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

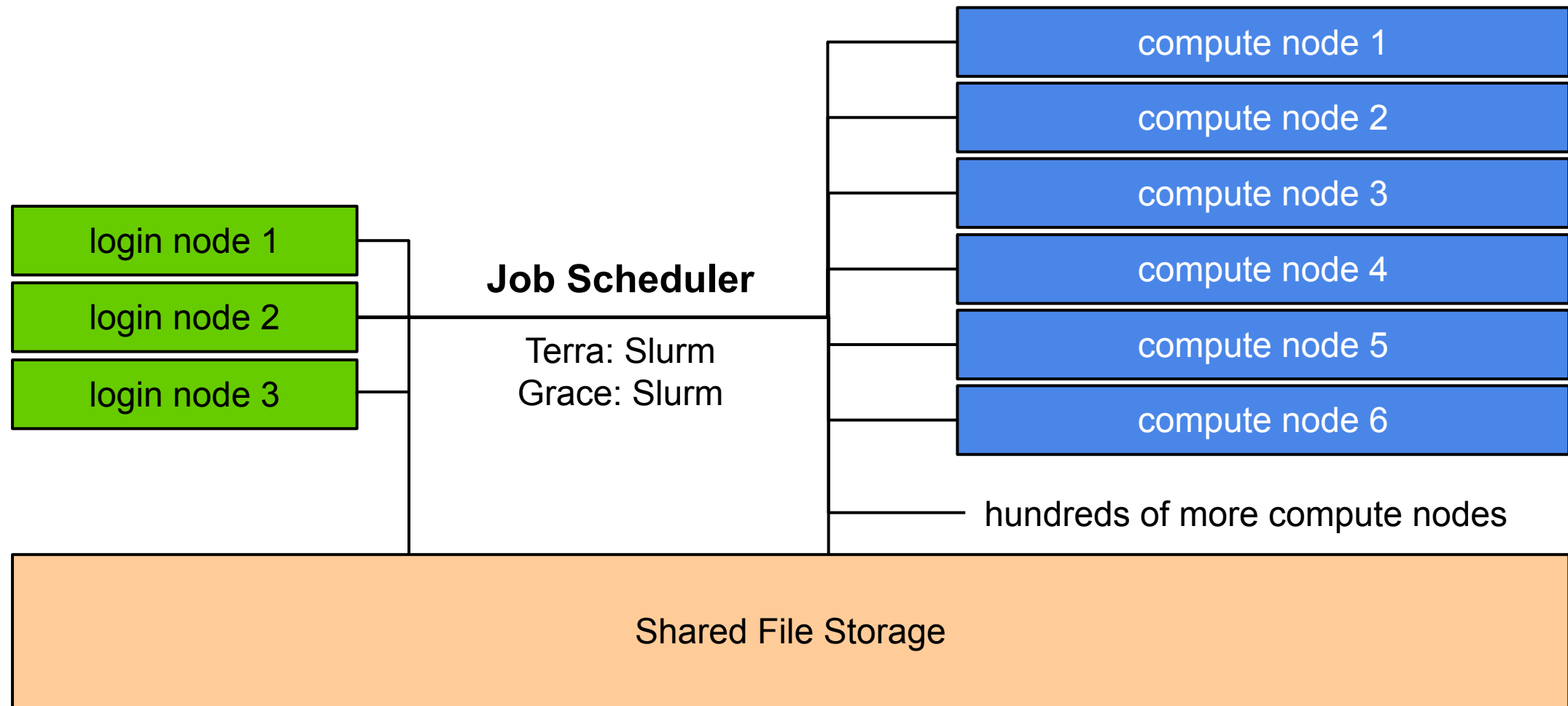
Number of Cores	GB of memory per core	Total Memory (GB)	Hours	SUs charged
1	2	2	1	1
1	3	3	1	2
1	56	56	1	28
28	2	56	1	28

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

HPRC Clusters



HPC Diagram





HPRC Home Page
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New User Info
Contact Us

User Guides

Ada
Terra
Grace
OOD Portal
Galaxy

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Two Factor
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Documentation

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

Search TAMU HPRC

High Performance Research Computing

A Resource for Research and Discovery



Welcome to the TAMU HPRC Wiki

• [Ada Guide](#)
• [Software](#)

• [Terra Guide](#)
• [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](#)



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High Performance Research Computing

<https://hprc.tamu.edu>

Available Software Modules

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 versions, additional documentation if available, etc.

Show 10 entries

Search: computer vision

Name	Description
OpenCV	OpenCV (Open Source Computer Vision Library) is an open source computer vision and machine learning software library. OpenCV was built to provide a common infrastructure for computer vision applications and to accelerate the use of machine perception in the commercial products. URL: https://opencv.org/
opencv_contrib	OpenCV (Open Source Computer Vision Library) is an open source computer vision and machine learning software library. OpenCV was built to provide a common infrastructure for computer vision applications and to accelerate the use of machine perception in the commercial products.
plantcv	PlantCV: Plant phenotyping using computer vision. URL: https://pypi.org/project/plantcv/
POV-Ray	The Persistence of Vision Raytracer, or POV-Ray, is a ray tracing program which generates images from a text-based scene description, and is available for a variety of computer platforms. POV-Ray is a high-quality, Free Software tool for creating stunning three-dimensional graphics. The source code is available for those wanting to do their own ports.
torchvision	Datasets, Transforms and Models specific to Computer Vision URL: https://github.com/pytorch/vision
VXL	A multi-platform collection of C++ software libraries for Computer Vision and Image Understanding.
WebKitGTK+	WebKitGTK+ is a full-featured port of the WebKit rendering engine, suitable for projects requiring any kind of web integration, from hybrid HTML/CSS applications to full-fledged web browsers. It offers WebKit's full functionality and is useful in a wide range of systems from desktop computers to embedded systems like phones, tablets, and televisions. URL: https://webkitgtk.org/

Showing 1 to 7 of 7 entries (filtered from 1,702 total entries)

Previous1Next

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

```
[mouse@terra3 ~]$ mla opencv
Using /home/mouse/module.avail.terra
OpenCV/
OpenCV/3.3.0-foss-2017b-Python-3.6.3
OpenCV/3.3.0-intel-2017A-Python-2.7.12
OpenCV/3.3.0-intel-2017b-Python-2.7.14
OpenCV/3.4.1-foss-2017b-Python-2.7.14-CUDA-9.0.176
OpenCV/3.4.1-foss-2017b-Python-2.7.14
OpenCV/3.4.1-foss-2018a-Python-2.7.14
OpenCV/3.4.1-foss-2018a-Python-3.6.4
OpenCV/3.4.1-intel-2018a-Python-3.6.4
OpenCV/3.4.5-foss-2018b-Python-2.7.15
OpenCV/3.4.5-fosscuda-2018b-Python-2.7.15
OpenCV/3.4.5-fosscuda-2018b-Python-3.6.6
OpenCV/3.4.7-foss-2019a-Python-2.7.15
OpenCV/3.4.7-foss-2019a-Python-3.7.2
OpenCV/3.4.7-fosscuda-2019a-Python-2.7.15
OpenCV/3.4.7-fosscuda-2019a-Python-3.7.2
OpenCV/4.0.1-foss-2018b-Python-2.7.15
OpenCV/4.0.1-foss-2018b-Python-3.6.6
OpenCV/4.2.0-foss-2019b-Python-3.7.4
OpenCV/4.2.0-foss-2020a-Python-3.8.2
OpenCV/4.2.0-fosscuda-2019b-Python-3.7.4
opencv_contrib/
opencv_contrib/3.4.1-foss-2018a-Python-3.6.4
```

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



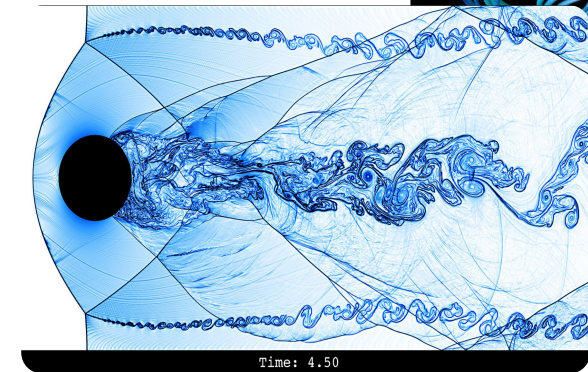
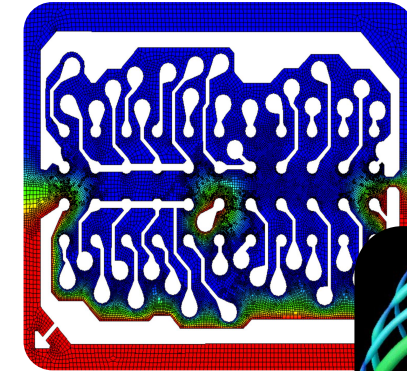
Available Software Modules

<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>

TAMU HPRC OnDemand (Terra)
Files
Jobs
Clusters
Interactive Apps
Dashboard

OnDemand provides an integrated, single access point to HPC 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 regulations is prohibited. Current HPRC accounts will be disabled if users are found in violation.
- Sharing HPRC account and password information is in violation of policy.
- Authorized users must also adhere to ALL policies at: [http://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 23, 2015. We will schedule maintenance windows if they will overlap with this maintenance window.

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

powered by

HPRC Portal

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

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Ada Portal
Terra Portal
Grace Portal (Testing)

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pDNA/peptide complex

Interaction with the negatively charged cell membrane and internalization

Methods to study, engineer and design

Events

International tool could help design more efficient wind turbines for jet engines

May 24-26 Texas A&M Research Computing Symposium

[HPRC Portal](#)

[YouTube tutorials](#)

Slack - Collaboration Software

<https://slack.com/resources/slack-101>

The screenshot displays a Slack workspace interface. On the left sidebar, the channel list includes #cesm2-discussion, #general, #gitter, #hpc_stuff (highlighted with a red arrow), #o-reu-fea-ansys, #o-reu-lammps, #random, #training, and #o-reu-texas-am-2021 (highlighted with a red arrow). The main chat area shows a message from Michael Demkowicz at 10:00 AM: "Interested in applying for a graduate fellowship? TAMUS LSAMP is collaborating with the TAMU Graduate and Professional School to sponsor a fellowship application writing boot camp. See attached pdf for detailed schedule (the events have also been added to the O-REU google calendar). Note that you have to register at the link provided to participate." Below the text is a PDF attachment titled "2021 Summer Fellowship Application Writing Boot Camp (AGENDA).pdf" (286 kB PDF). The PDF content includes: "Summer 2021 Fellowship Application Writing Boot Camp", "Presented by the Graduate and Professional School and Texas A&M University System - Louis Stokes Alliance for Minority Participation program (TAMUS LSAMP)", and a "Registration Link: https://gradconnect.tamu.edu/register/FellowshipBootCamp". Below the PDF, there is a reaction of 1 checkmark and a smiley face. The next message from Michael Demkowicz at 10:20 AM says: "Join Dr. Emily Pentzer here for an hour of round-robin virtual speed networking for women in the O-REU program. Monday, June 7, at 12pm (noon) CT. The event has been added to the O-REU calendar, as well. (edited)". The final message from Michael Demkowicz at 1:16 PM states: "Note to all those who will be taking the LAMMPS tutorial: last year, when I made the tutorial recordings, I used the Ada cluster at HPRC. That cluster has now been retired. Therefore, please use the Terra cluster instead: http://portal-terra.hprc.tamu.edu (You must be signed on to VPN for this link to work)".





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TEXAS A&M UNIVERSITY

Help with HPRC:

<https://hprc.tamu.edu>

help@hprc.tamu.edu

Help with TAMU IT (netid, VPN, enabling DUO):

<https://it.tamu.edu/help/>

helpdesk@tamu.edu

