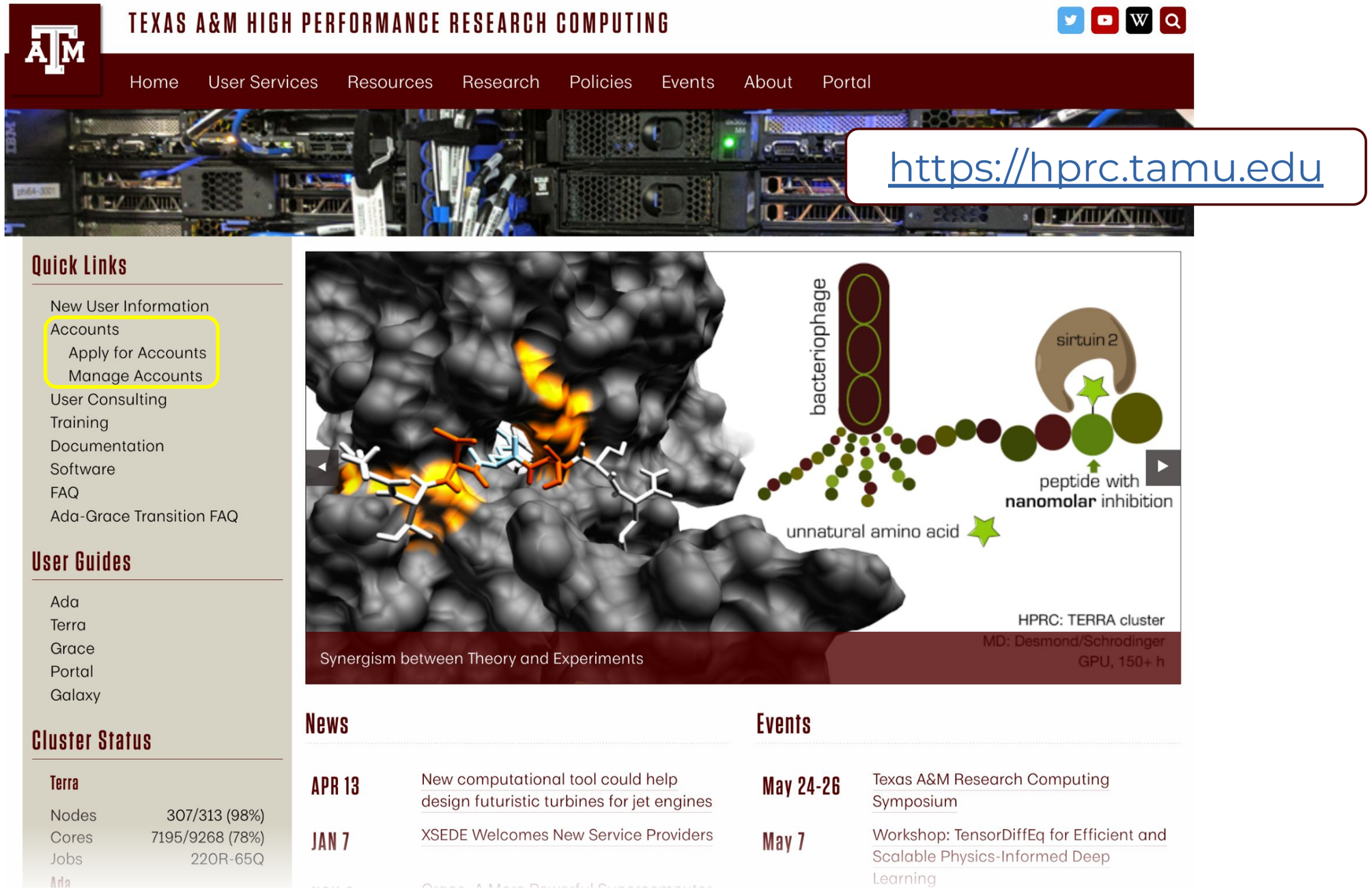
HIGH PERFORMANCE RESEARCH COMPUTING

Introduction to HPRC, Duo, VPN and Clusters

June 1, 2021

TEXAS A&M UNIVERSITY

Division of Research


TEXAS A&M HIGH PERFORMANCE RESEARCH COMPUTING
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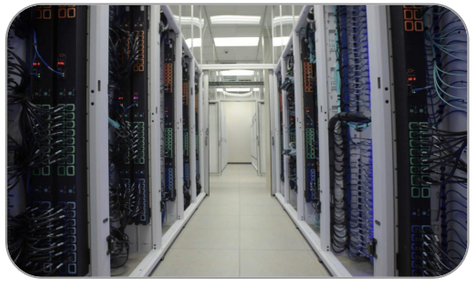
Cluster Status
Terra
Nodes 307/313 (98%)
Cores 7195/9268 (78%)
Jobs 220R-65Q
bacteriophage
sirtuin 2
peptide with
nanomolar inhibition
unnatural amino acid
HPRC: TERRA cluster
MD: Desmond/Schrodinger
GPU, 150+ h
Synergism between Theory and Experiments
News
APR 13
New computational tool could help design 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

*Retiring on June 30 2021

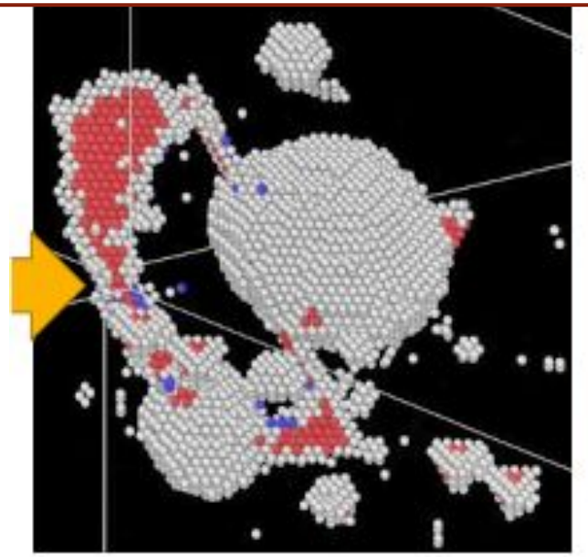
https://hprc.tamu.edu/resources

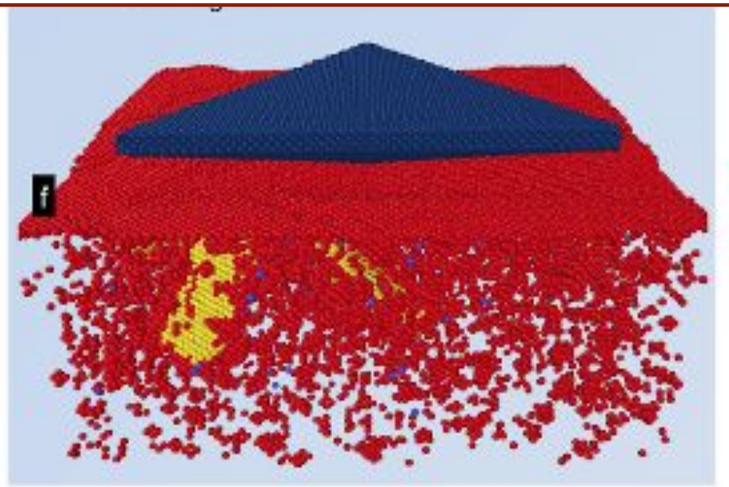
†Testing and early user onboarding

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)

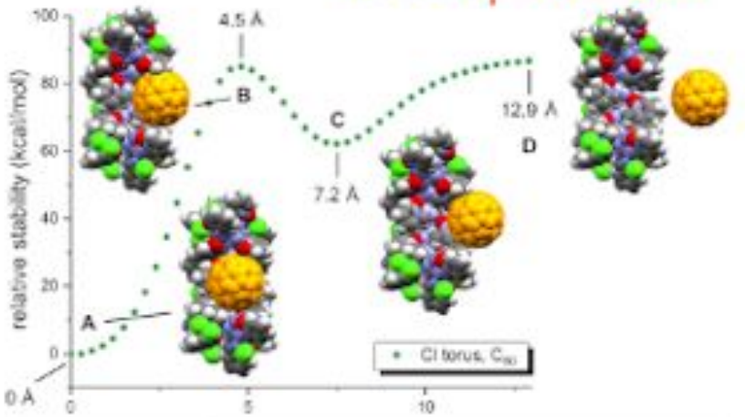
https://hprc.tamu.edu/events/conferences/sc20/

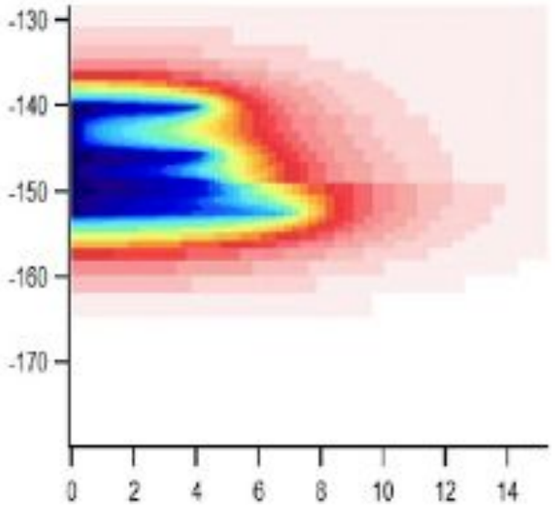


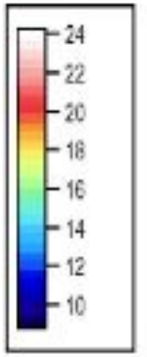


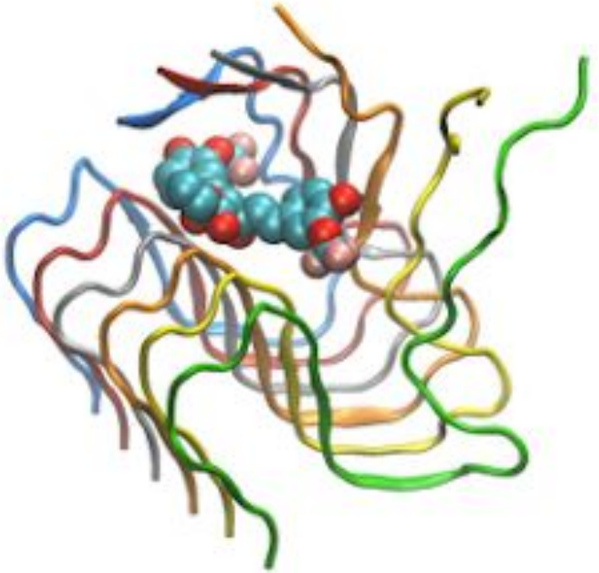
SC20

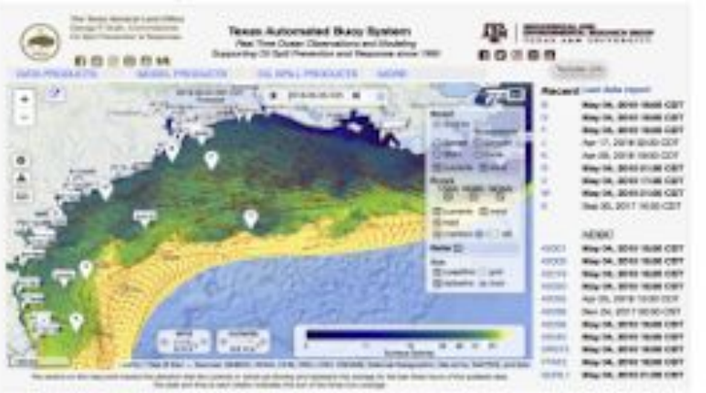
Everywhere we are | more than hpc.





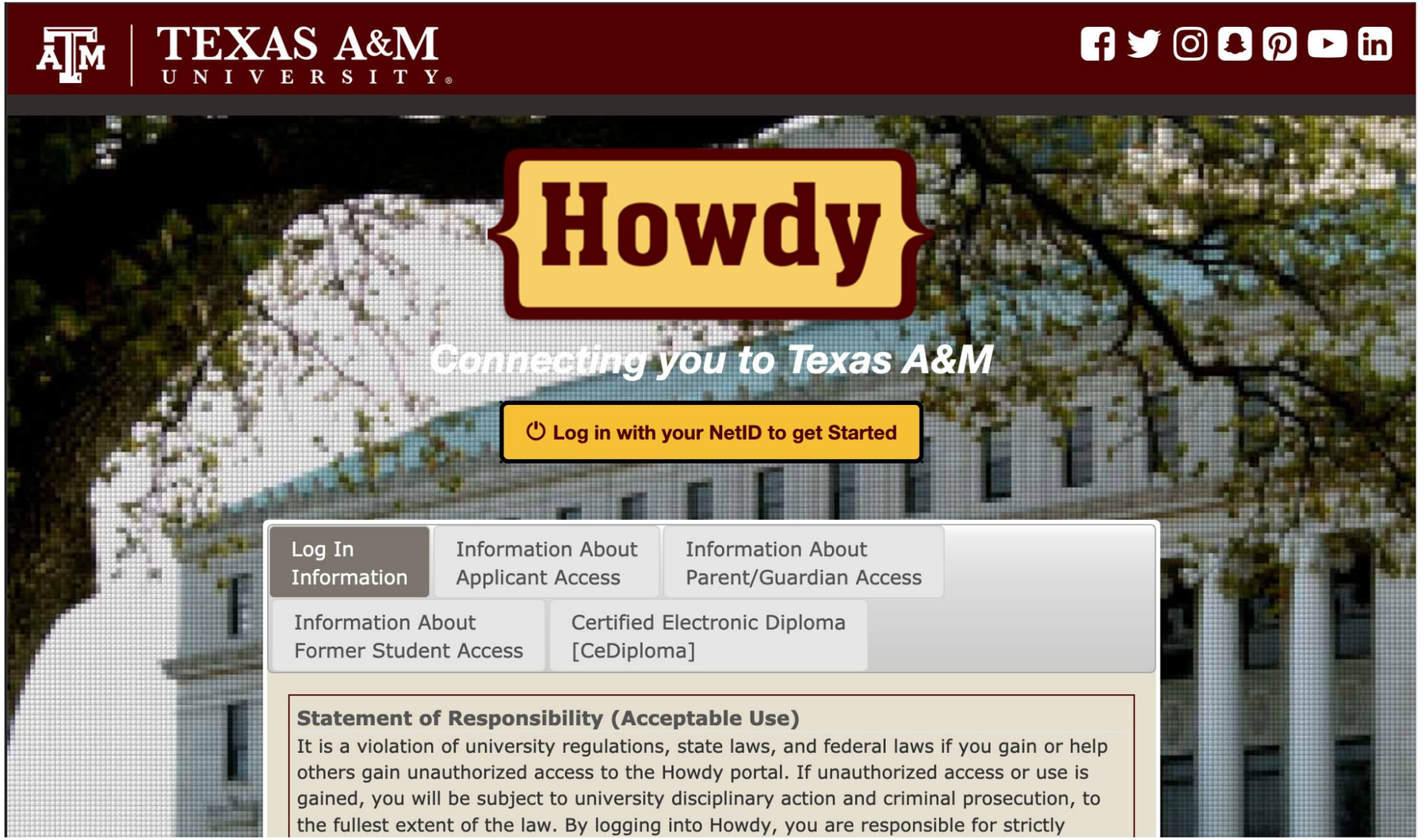






NETID - username you use to login to various systems and services (https://howdy.tamu.edu)

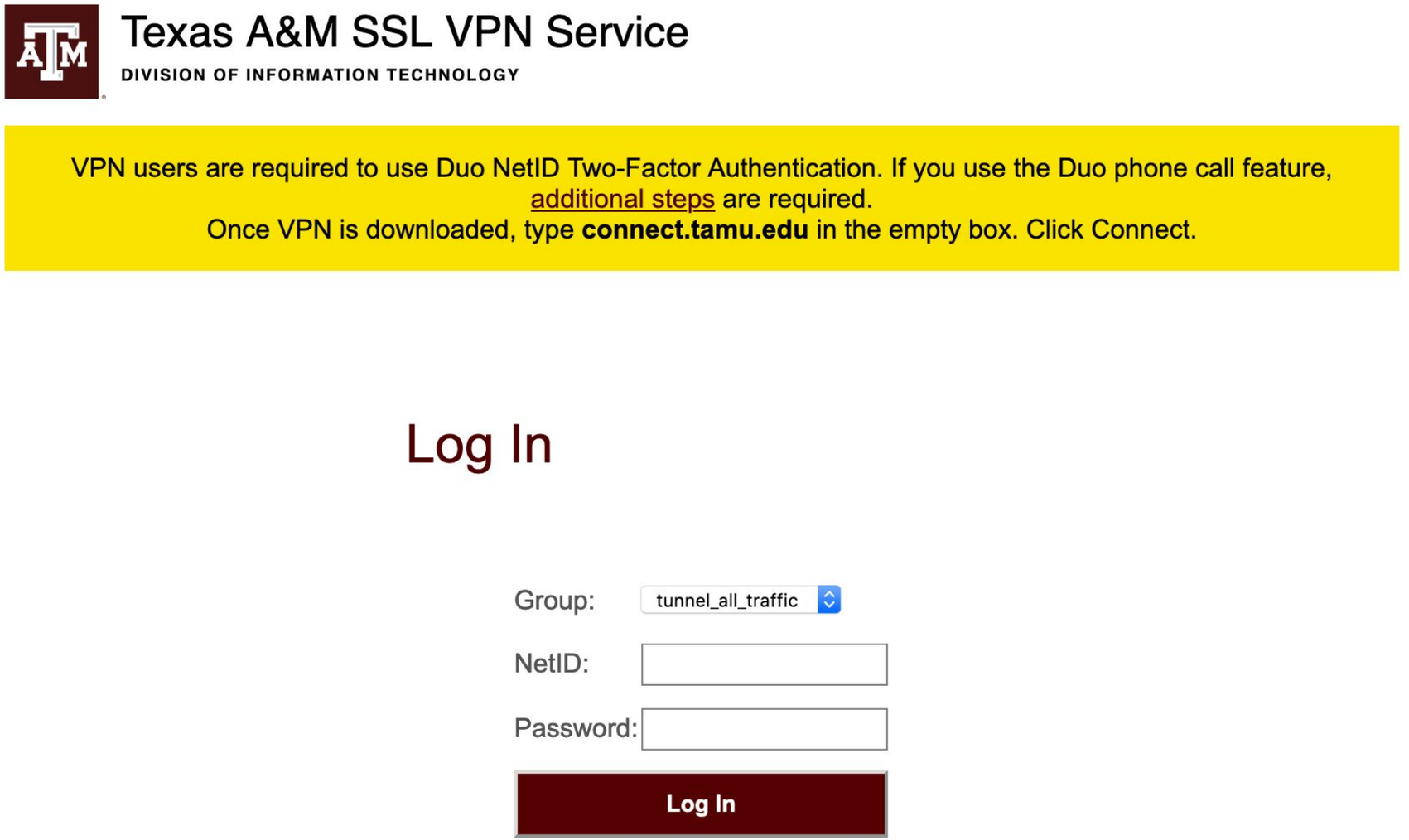
For help with your netid: https://it.tamu.edu/help/



VPN (Virtual Private Network) https://connect.tamu.edu

Required to access the university's network from off campus.

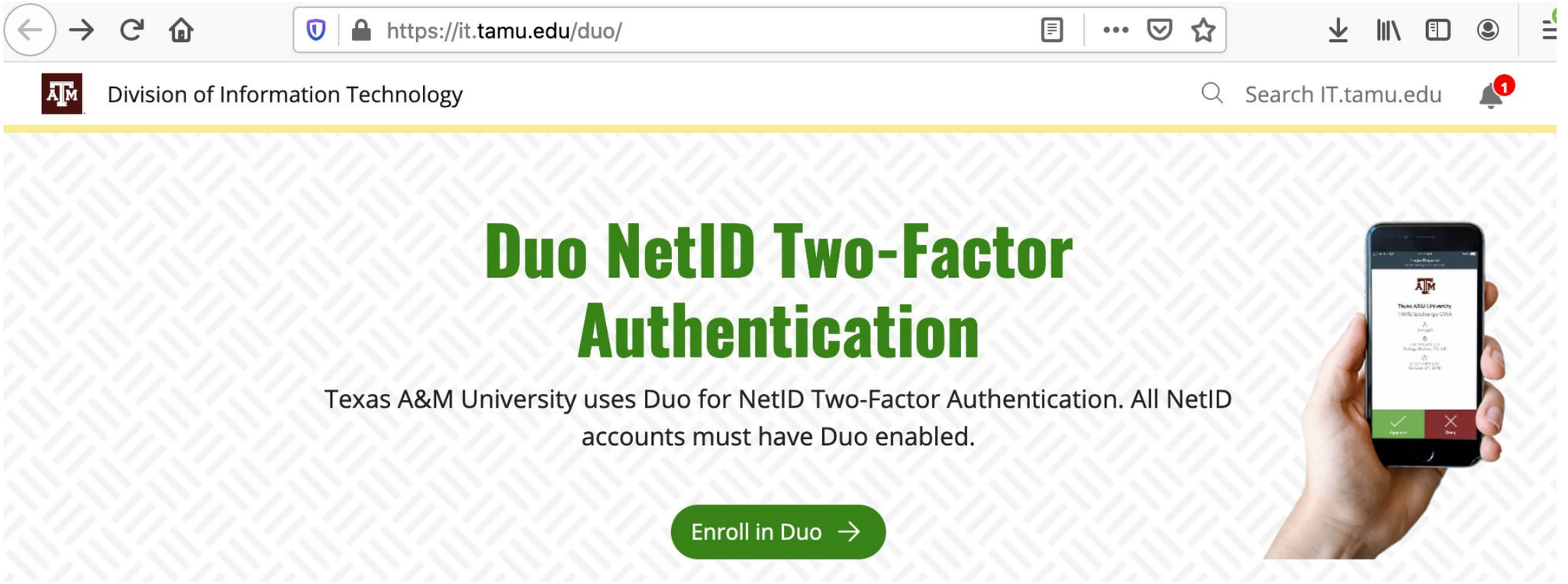
For help with VPN: https://it.tamu.edu/help/

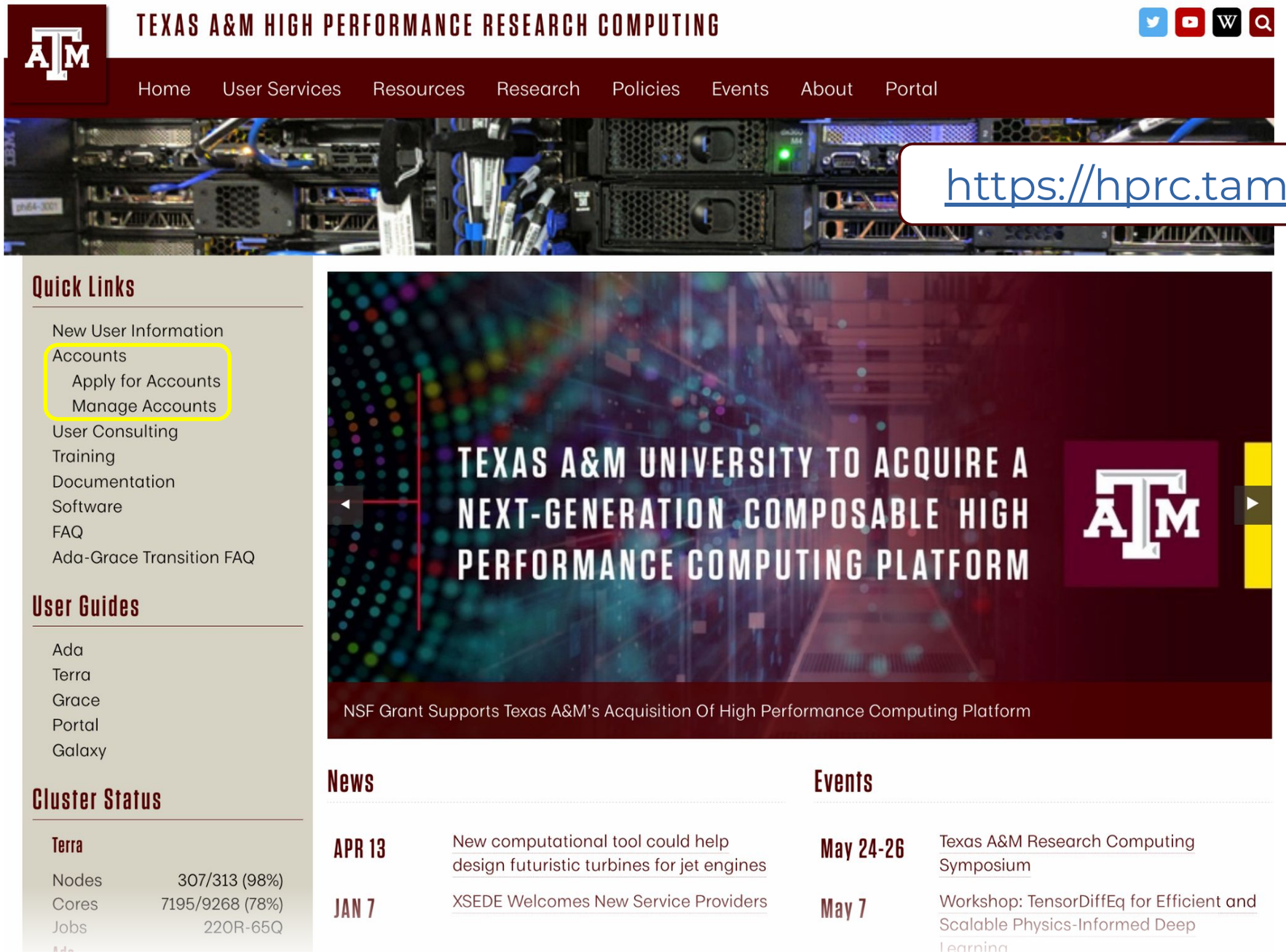


Two-Factor Authentication (DUO)

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)

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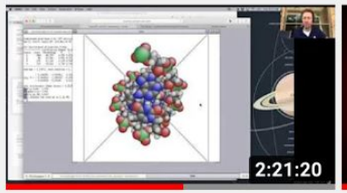

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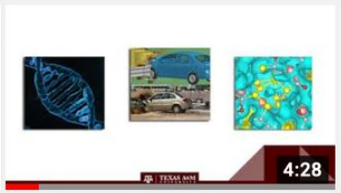

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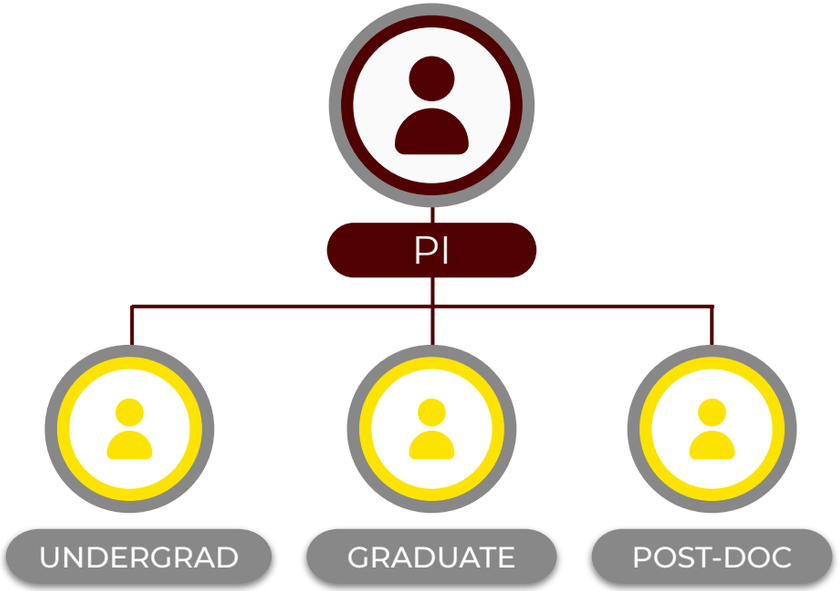
HPRC Account Allocations

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 HPRC-RAC	No	HPRC-RAC
Research (Terra)	Faculty, Research Scientists, Qualified Staff	300,000	5,000,000	5,000,000	Determined by HPRC-RAC	No	HPRC-RAC

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.

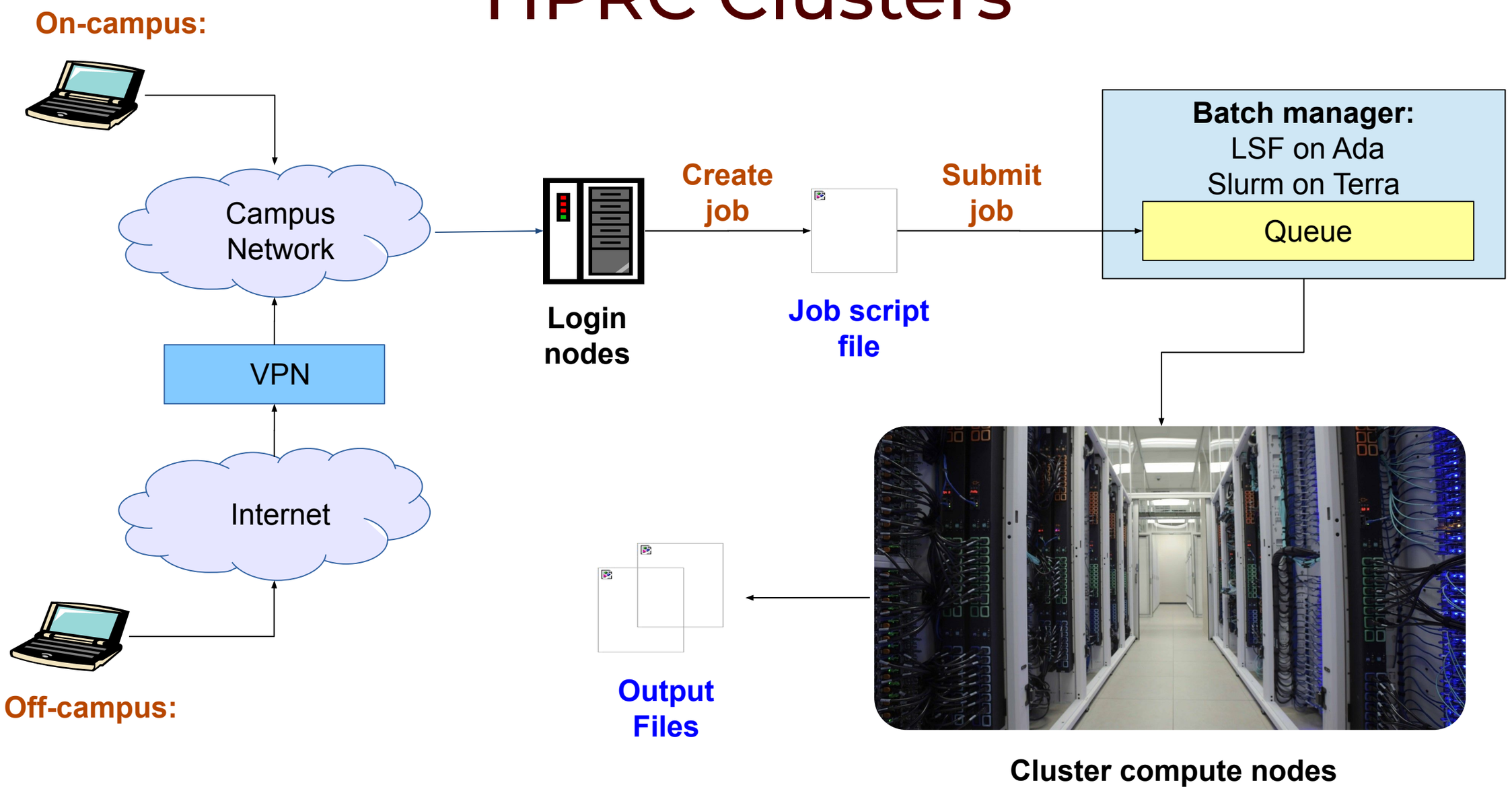
Examples of SUs charged based on Job Cores, Time and Memory Requested

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

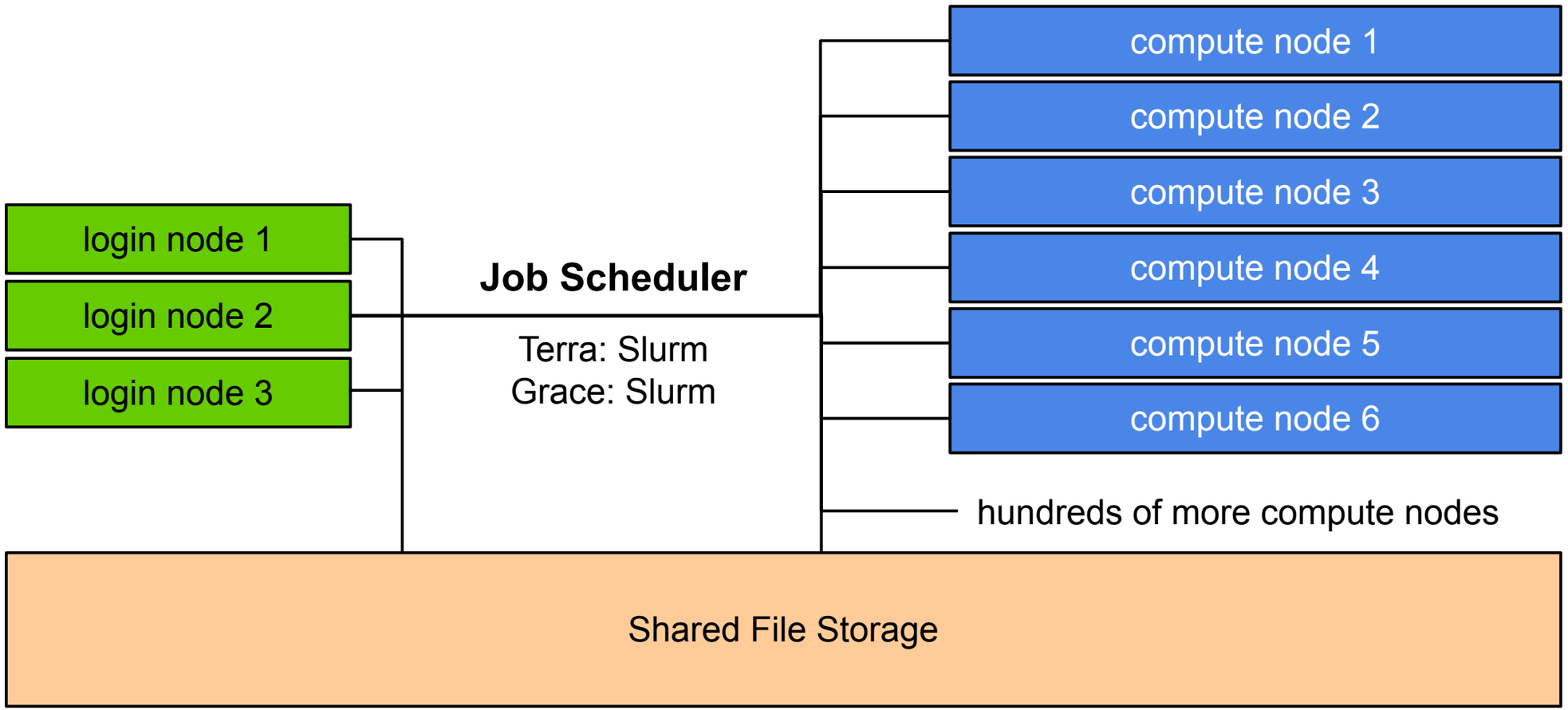
Number of Cores	GB of memory per core	Total Memory (GB)	Hours	SUs charged
1	2	2	1	1
1	3	3	1	2
1	56	56	1	28
28	2	56	1	28

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

HPRC Clusters

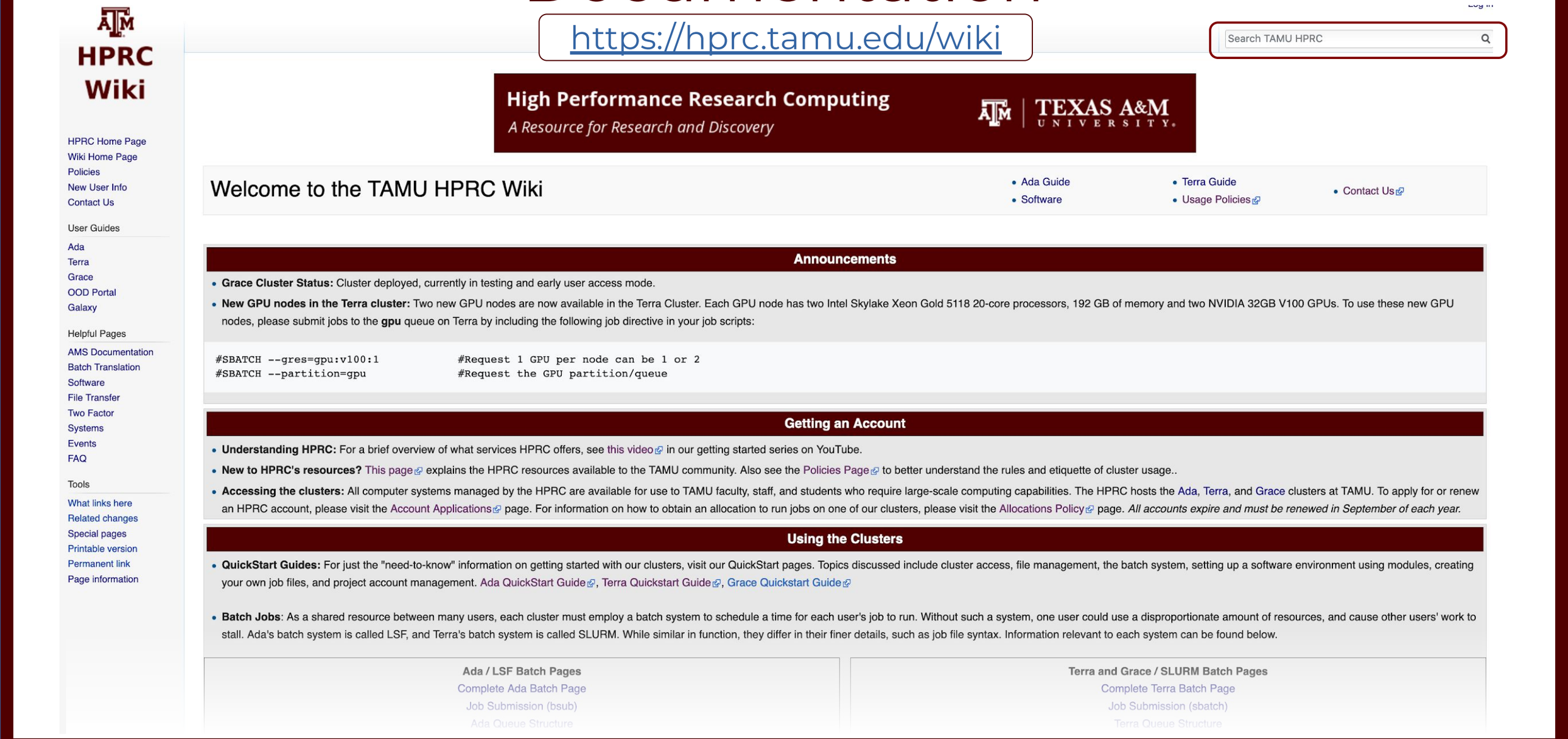


HPC Diagram


compute node 1
compute node 2
compute node 3
compute node 4
compute node 5
compute node 6
login node 1
login node 2
login node 3
Job Scheduler
Terra: Slurm
Grace: Slurm
hundreds of more compute nodes
Shared File Storage

Documentation

https://hprc.tamu.edu/wiki



Available Software Modules

SOFTWARE MODULES ON THE TERRA CLUSTER

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

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) Previous 1 Next

```
[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

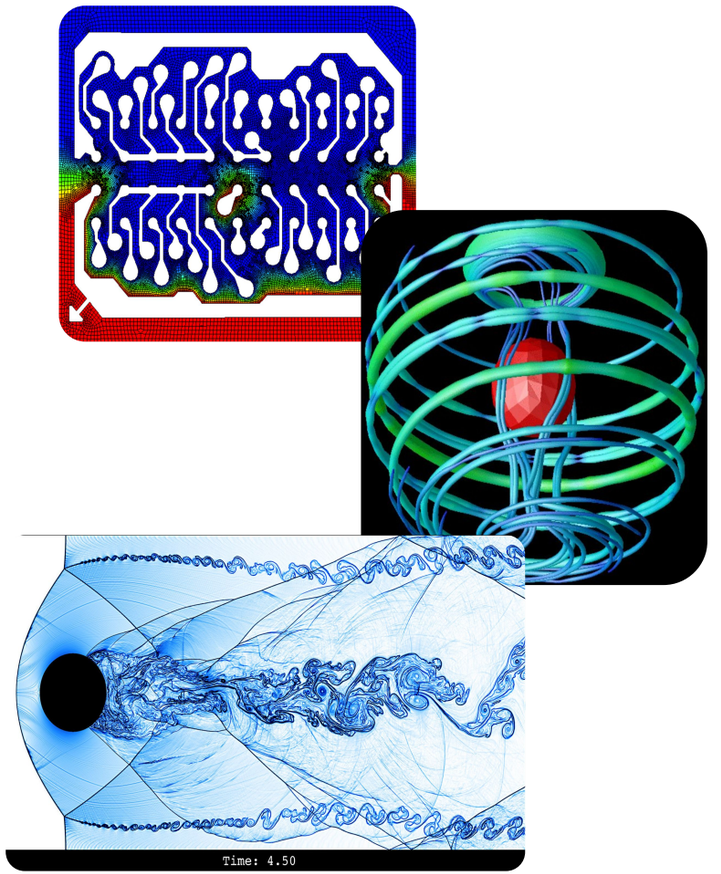
Available Software Modules

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
```

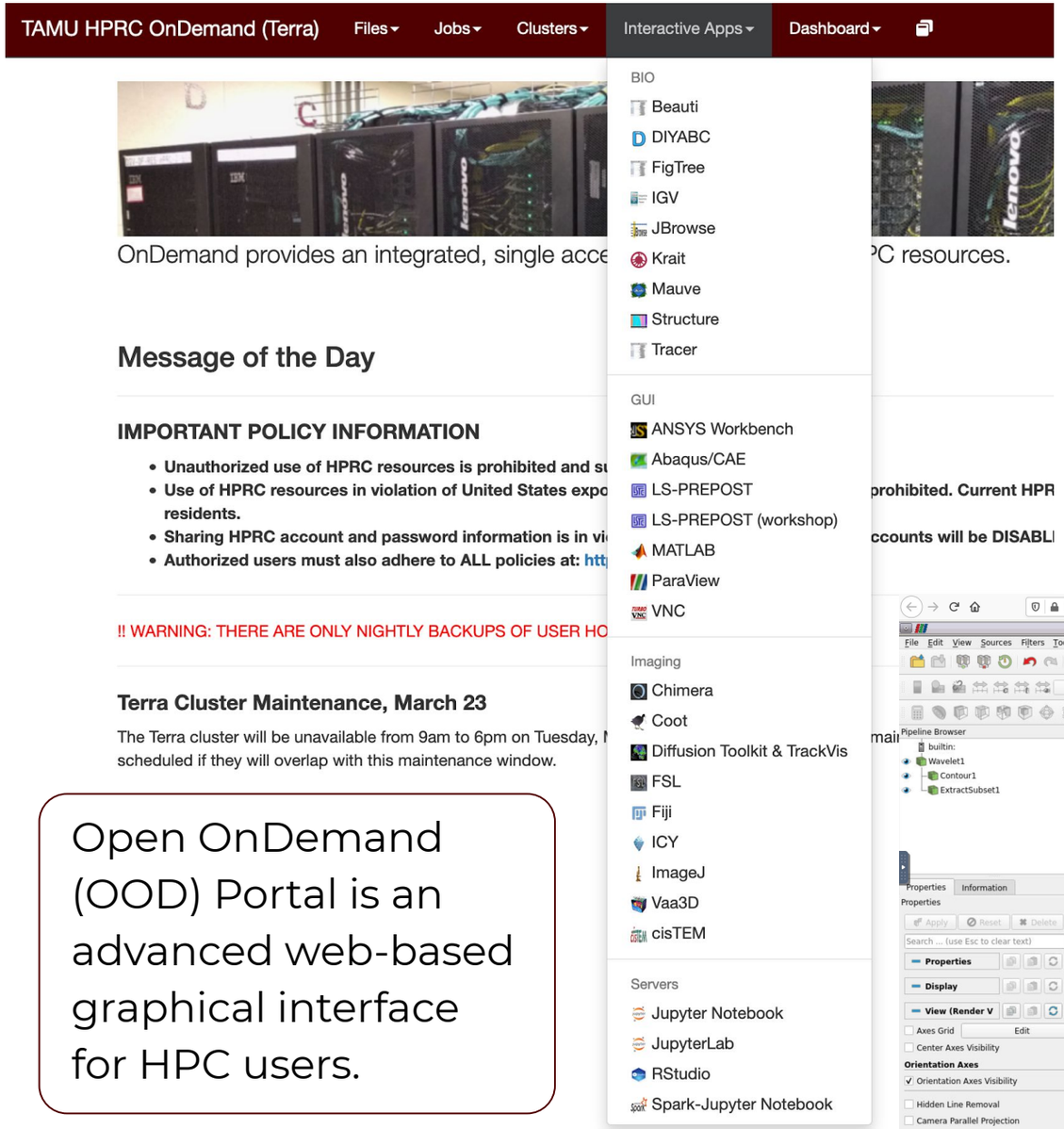
Compilers: C++, Fortran, intel, gnu, …
openmpi, intelmpi
Python
Matlab
Paraview
Visit
Deal.II
FFTW
ScaLAPACK
Gmsh
MUMPS
METIS
p4est
PETSc
SLEPc
Trilinos
…

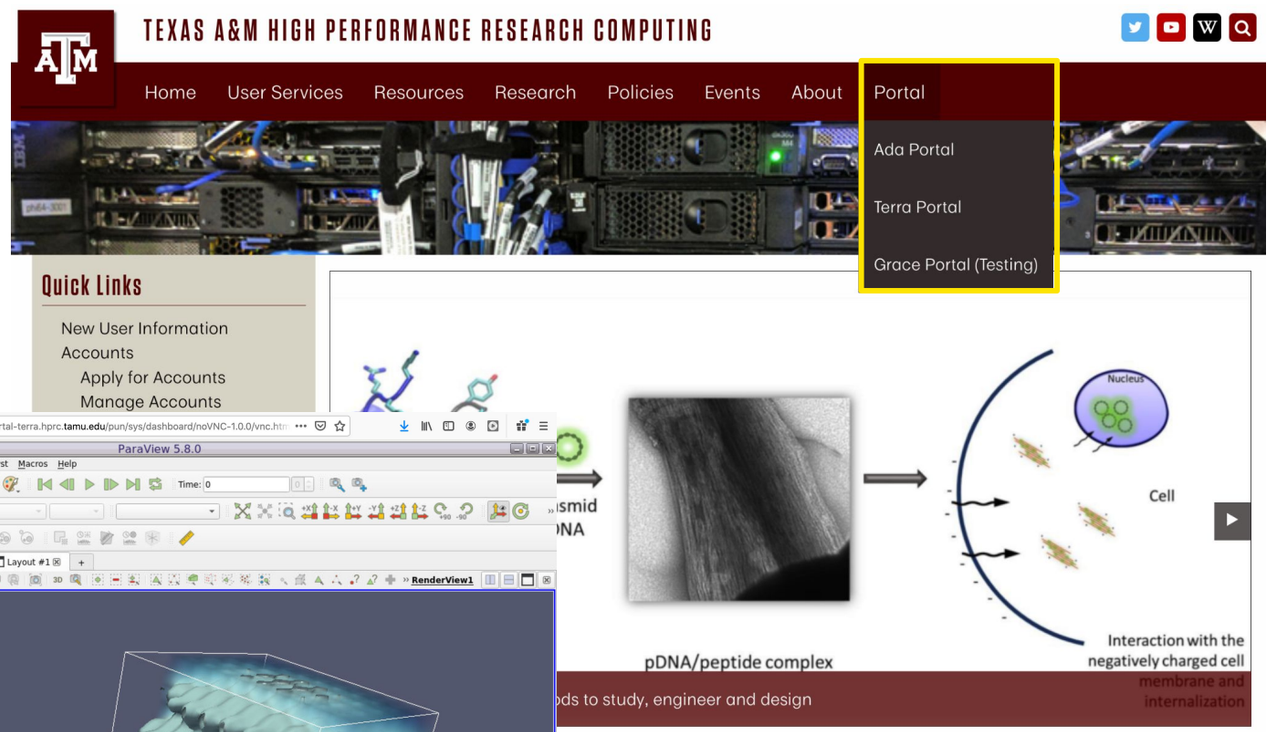


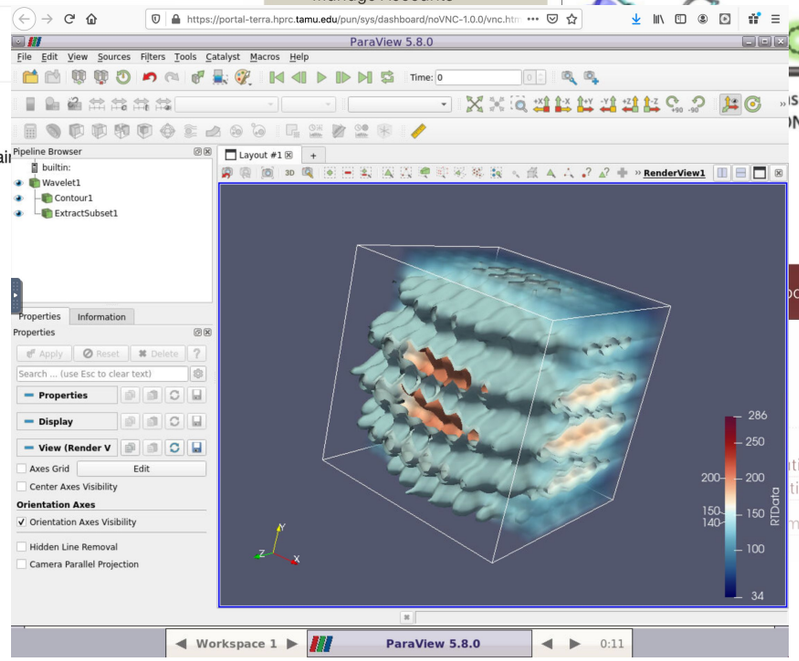
Images: https://www.dealii.org/code-gallery.html

HPRC Portal

https://portal.hprc.tamu.edu







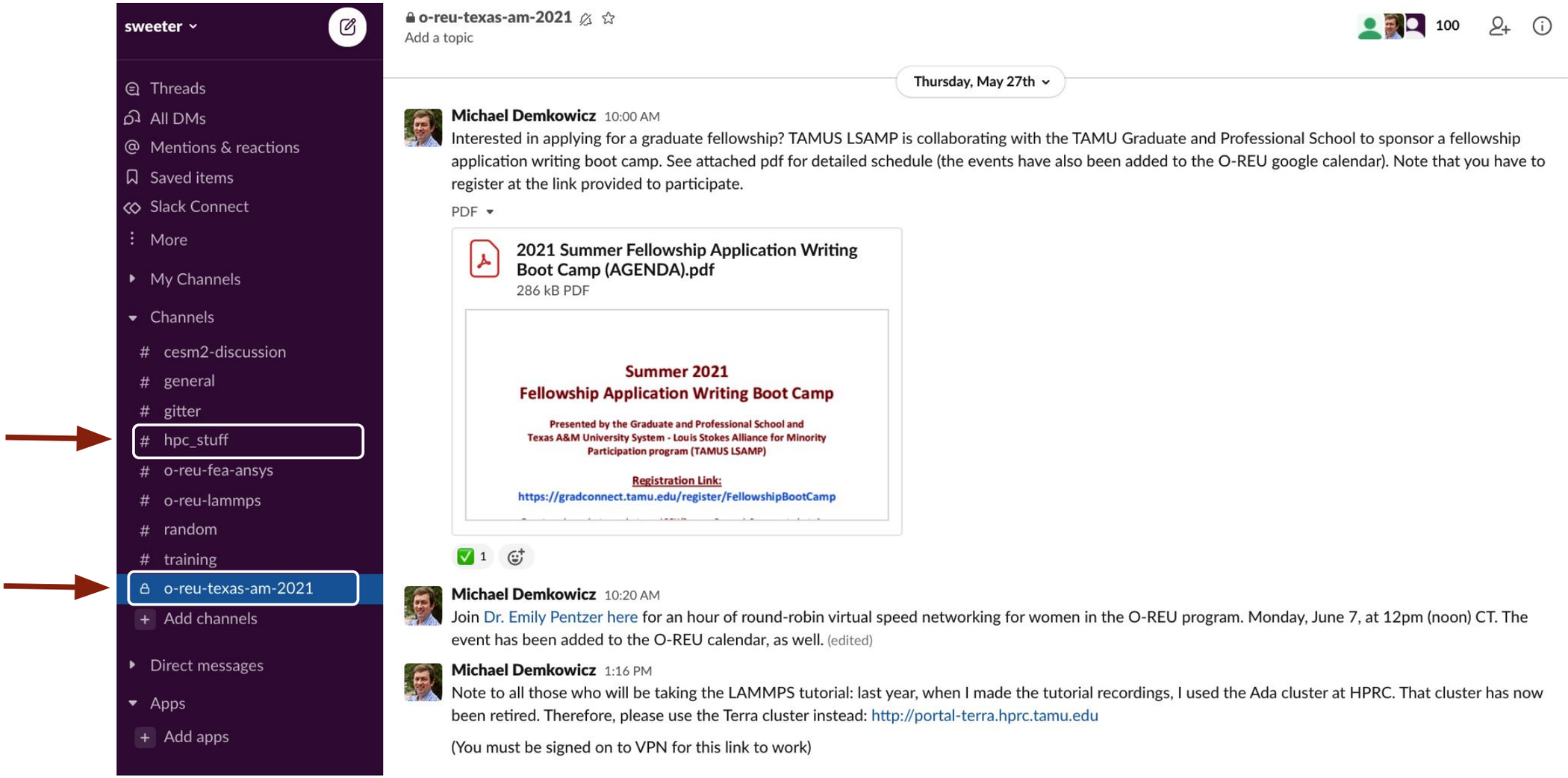
Open OnDemand (OOD) Portal is an advanced web-based graphical interface for HPC users.

powered by OPEN OnDemand

[HPRC Portal YouTube tutorials]

Slack - Collaboration Software

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



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Help with HPRC:

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help@hprc.tamu.edu

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

https://it.tamu.edu/help/
helpdesk@tamu.edu