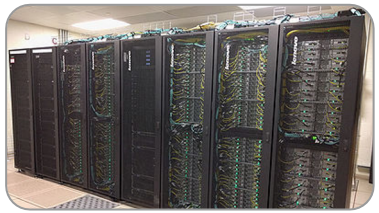
HPRC PI Meeting : Ada-Grace Transition

April 30, 2021

High Performance
Research Computing
DIVISION OF RESEARCH

High Performance Research Computing Clusters

Ada*



Terra

ViDaL

Grace†

	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

Ada Retiring and Disseminating

- Ada refresh planning started in early 2019
- RFP - Transitioning Racks of the Ada and Curie Supercomputers was issued in October, 2020
- 11 Ada Racks awarded to 7 research groups.
- 3 Ada Racks awarded to the Laboratory of Molecular Simulations (LMS) under HPRC

PI	Dept	Awards
Debjyoti Banerjee	MEEN/PETE	3 standard racks
Charlie Johnson	TxGen	1 large memory rack
Daniel Tabor	CHEM	1 large memory rack
Daniel Jimenez	CSE	1 standard rack
Ping Chang	iHESP	1 standard rack
Sherry Yennello	Cyclotron Institute	3 standard racks
Phanourios Tamamis	CHEN	1 standard rack

Ada Retirement Timeline

May 17

- Retire some of the compute racks

June 1

- All compute racks will be retired
- Login and data transfer nodes will be available to migrate data

June 30

- Ada cluster will be completely shutdown.
- Data retrieval and migration MUST be completed by this date

- Only migrate data from Ada to Grace that will be used for future work
- Please move remaining data from Ada to non-HPRC storage
- Quota increase requests over 10TB on Grace MUST be submitted by PIs with strong justification, and will be reviewed by the HPRC Director

Grace By The Numbers

- Total 925 compute nodes with aggregate computing capacity over 5 PFLOPS
- 917 compute nodes equipped with 2 Intel 24-core 3.0 GHz Cascade Lake processors and 384 GB memory
  - 100 GPU compute nodes have 2 NVIDIA A100 48 GB GPUs
  - 8 GPU compute nodes with 4 single precision T4 16GB GPUs
  - 9 GPU compute nodes with 2 RTX 6000 24GB GPUs
- 8 large memory compute nodes with 4 Intel 20-core 2.5GHz processors and 3.072 TB memory
- 6.7 PB Lustre storage (5.12 PB usable)
  - 1PB reserved for Prof. Elaine Oran's group.
- 2 connected GPFS storage systems- Profs. Ping Chang and Junjie Zhang's groups

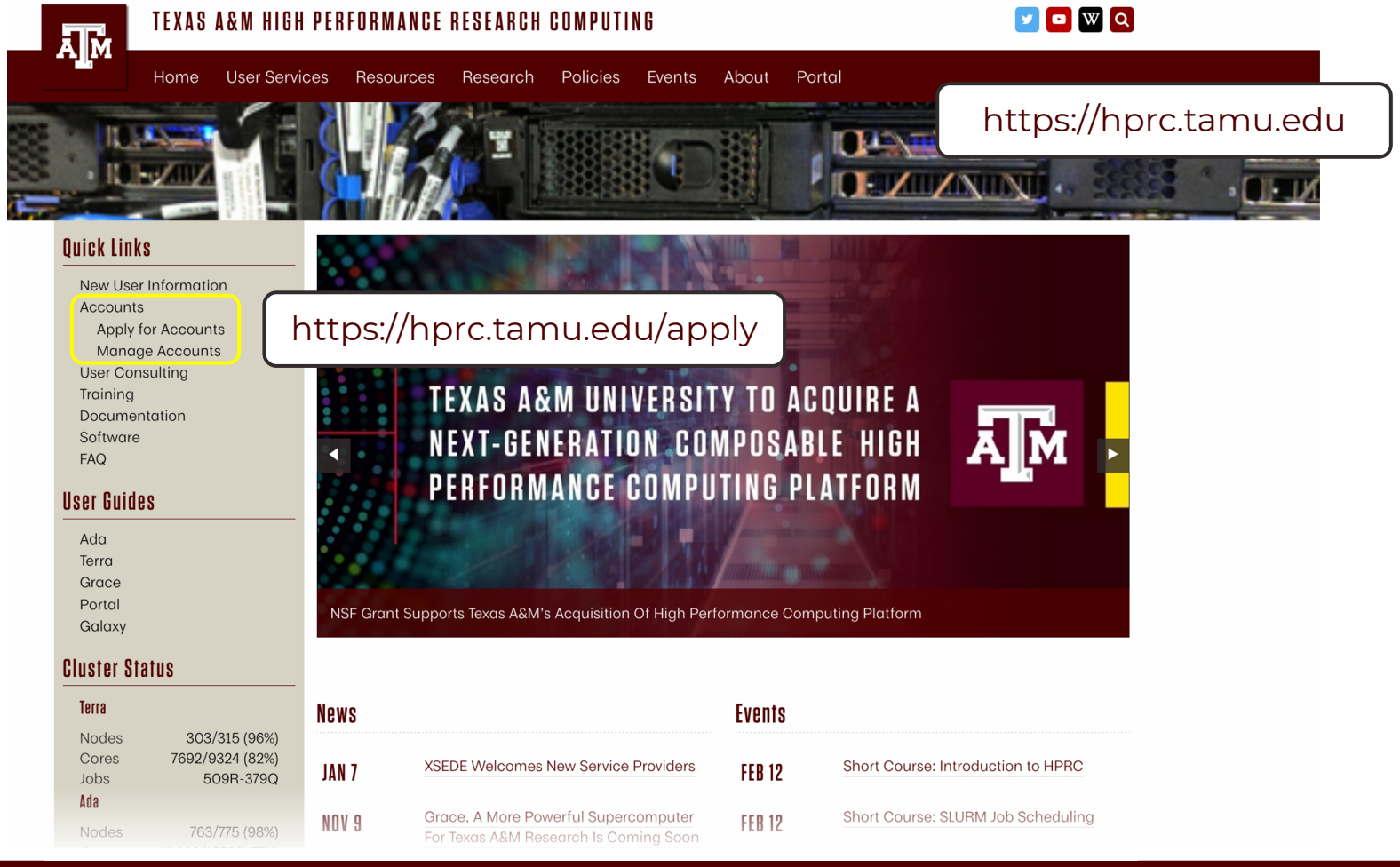
Special Allocations on Grace

- Request soliciting Condo Partners for the Supercomputer ADA Refresh was issued in March 2019.
- The rates ($0.004/SU and $130/TB) are calculated based on solely on hardware costs.
- HPRC has subsidized all other costs.
- PIs who made commitments before October 2019 were offered 1:1 matching by VPR

PI	Dept.	Contribution ($)	Allocations (SU or TB)
Elaine Oran	Aerospace Eng.	$100K	**10M SUs/year**
Elaine Oran	Aerospace Eng.	$130K	1 PB Storage
Thomas Overbye	ECE	$60K	**6M SUs/year**
Akram Abu-Odeh	TTI	$50K	**5M SUs/year**
Ping Chang	Oceanography	VPR Cost Share for iHESP	20M SUs/year
Phanourios Tamamis	Chemical Eng.	$25K	1.25M SUs/year
Goong Chen	Mathematics	$8000	**800K SUs/year**

Allocations on Grace

- Grace has been in friendly user mode since December 2020.
- Grace will be open to all active HPRC users by May 17. Early user requests are being accepted.
- No allocations and pre-charging for Grace until FY22 starting September 1.
- Current Ada allocations will not be transferred to Grace.
- FY22 allocation requests for Grace will be accepted starting July 1, 2021. Please begin planning.
- All special allocations/commitments on Ada will be expired when Ada is retired.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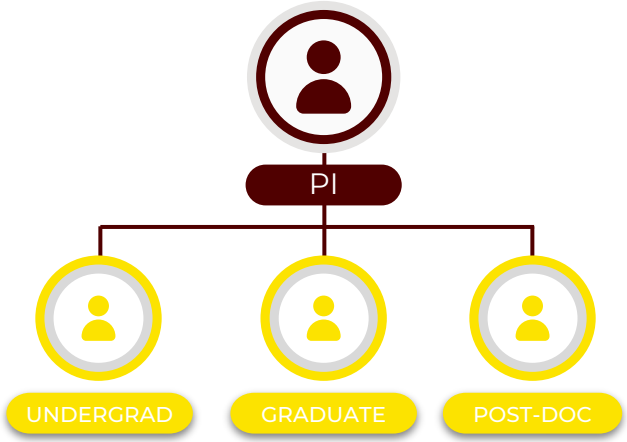
NSF Grant Supports Texas A&M's Acquisition Of High Performance Computing Platform
User Guides
Ada
Terra
Grace
Portal
Galaxy
Cluster Status
Terra
Nodes 303/315 (96%)
Cores 7692/9324 (82%)
Jobs 509R-379Q
Ada
Nodes 763/775 (98%)
News
JAN 7 XSEDE Welcomes New Service Providers
NOV 9 Grace, A More Powerful Supercomputer For Texas A&M Research Is Coming Soon
Events
FEB 12 Short Course: Introduction to HPRC
FEB 12 Short Course: SLURM Job Scheduling

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?	Review and approv 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 Direct
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
Research (Grace)	Faculty, Research Scientists, Qualified Staff	300,000	10,000,000	10,000,000	Determined by HPRC-RAC	No	HPRC RAC

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

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

A Service Unit (SU) on Grace is equivalent to one core or **7.5** GB memory usage for one hour.

Number of Cores	GB of memory per core	Total Memory (GB)	Hours	SUs charged
1	7.5	7.5	1	1
1	10	10	1	2
1	360	360	1	48
48	7.5	360	1	48

- **GPU jobs are charged 3 * 48 SUs per hour**
- Unused SUs expire at the end of each fiscal year (Aug 31) and won't be renewed

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

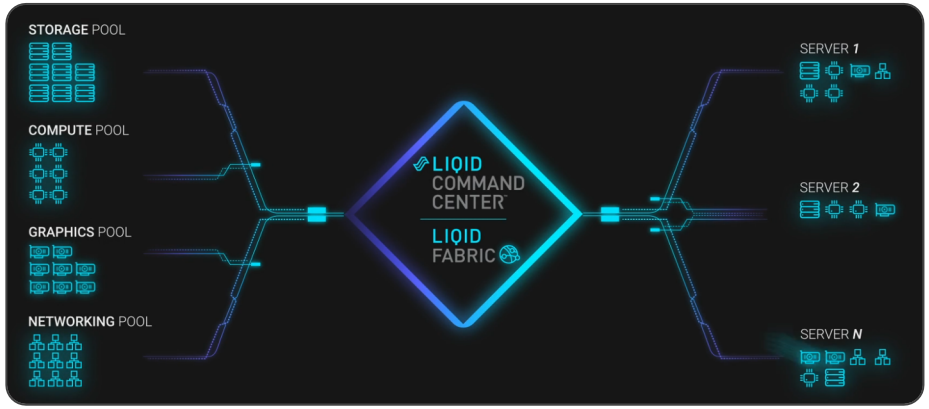
Special Requests

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 resources are reserved for special case assignments
  - Examples of special case assignments
    - working with HPRC on new capabilities of general value to research communities across campus
    - new faculty startup
    - grant in-kind match
    - other operations that go beyond normal research projects
  - Granted by the Director or the VPR.
- Committed Allocations
  - PIs who made “condo” contributions to the HPRC infrastructure will have committed allocations related to their contributions in addition to the common pool.

Upcoming System: FASTER

Fostering Accelerated Scientific Transformations, Education, and Research



Available in Summer 2021

- Adopts the innovative LIQID **composable** software-hardware approach combined with cutting-edge technologies.
- Equipped with Intel 32-core **Ice Lake processors**, **NVIDIA A100 (40)**, **T4 (200), and A40/A10 (TBD)** GPUs for AI/DL/ML workloads.
- 180 compute nodes. Each node can access 16+ GPUs.
- 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.

HIGH PERFORMANCE RESEARCH COMPUTING
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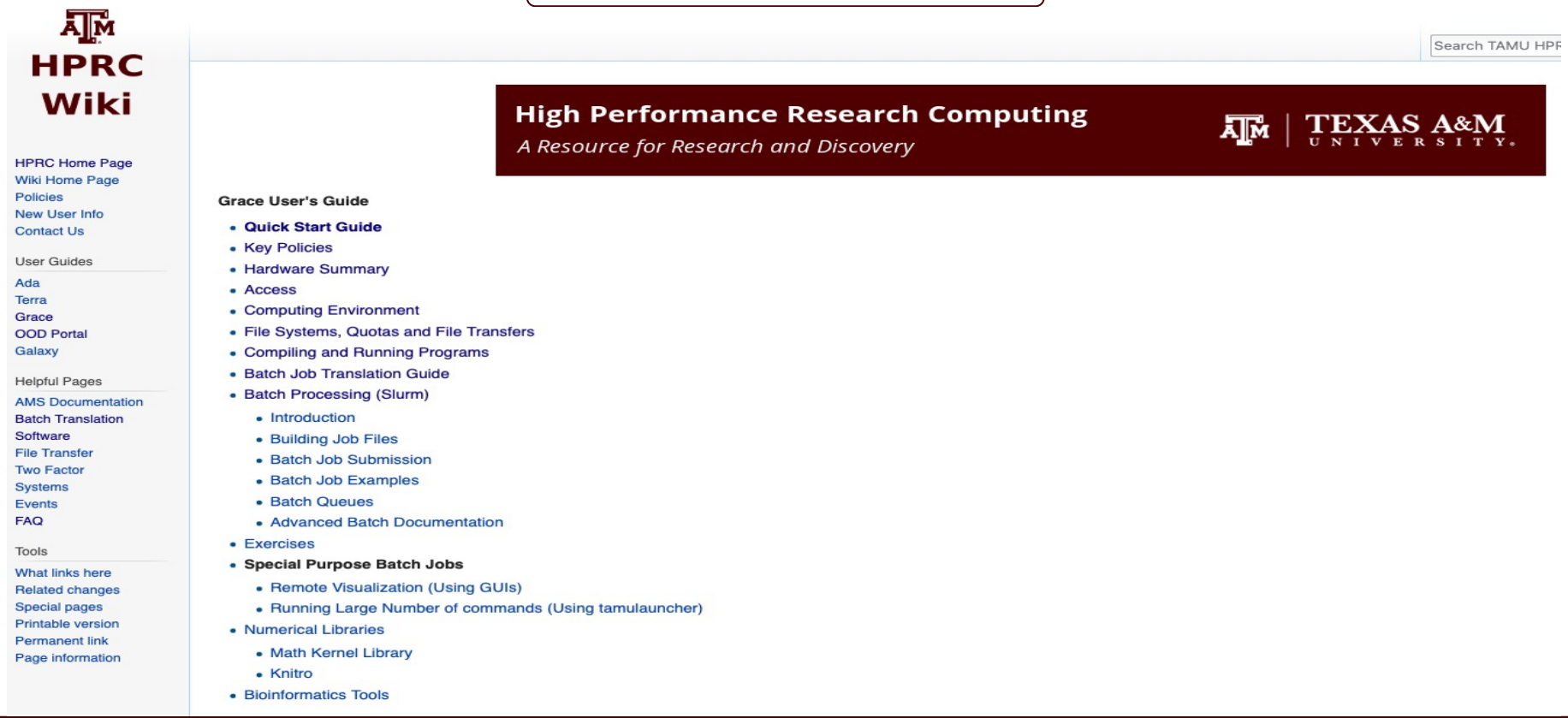
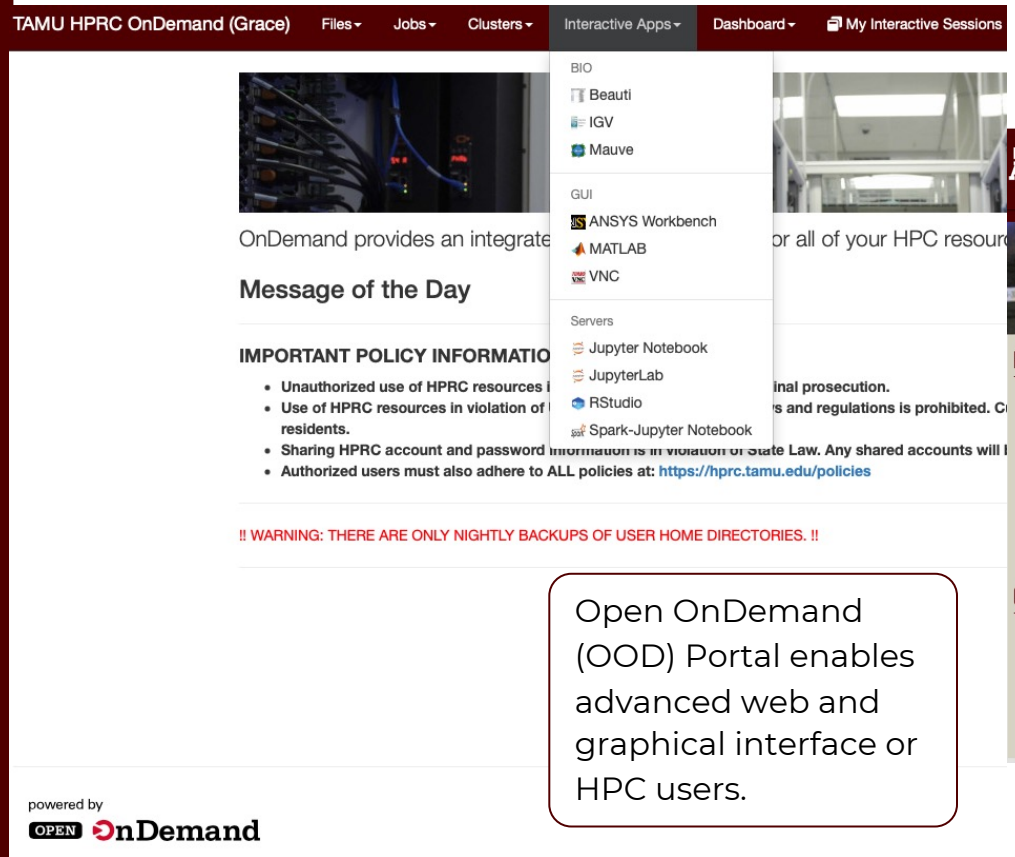
Thank you!

Documentation

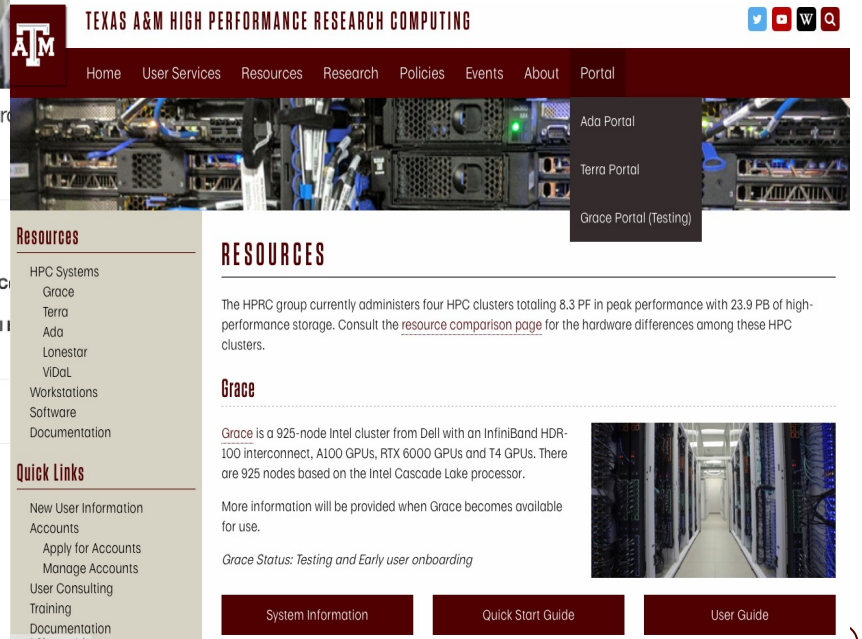
https://hprc.tamu.edu/wiki



HPRC Portal



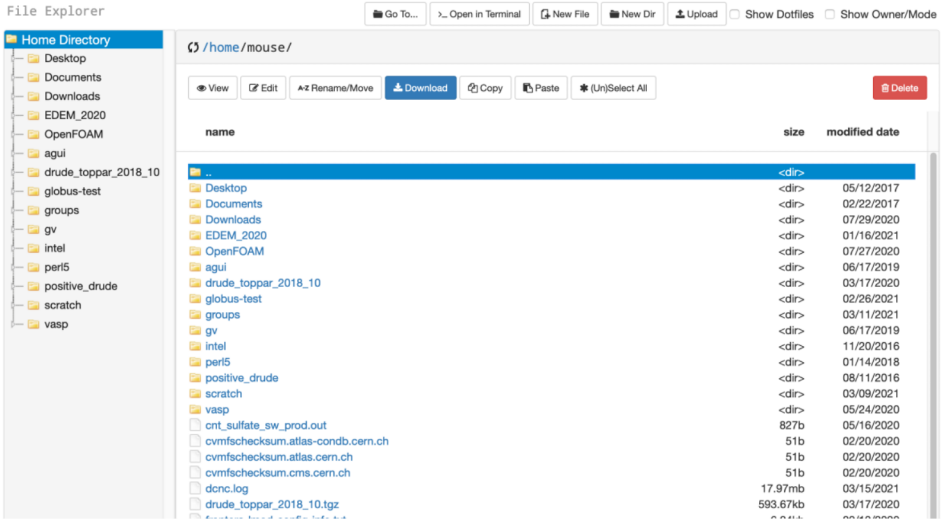
https://portal.hprc.tamu.edu



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

HPRC Portal YouTube tutorials

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

Available Software Modules

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

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 availa
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)

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

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

HPRC Training Short Courses
https://hprc.tamu.edu/training

Primers:

Linux
HPRC Clusters
Data Management
Schedulers
Jupyter Notebook

Technology Lab:

Using AI Frameworks in Jupyter Notebook

Short Courses:

Python
Scientific Python
Containers
PyTorch
TensorFlow
MATLAB
Scientific ML
Julia
CUDA
Drug Docking
Quantum Chemistry

Short Courses:

NGS Analysis
NGS Metagenomics
NGS RADSeq/GBS
Schedulers - SLURM
HPRC Galaxy
Linux
R
Perl
Fortran
OpenMP
and more...

YouTube training videos

Texas A&M HPRC
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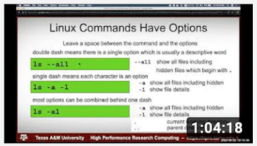

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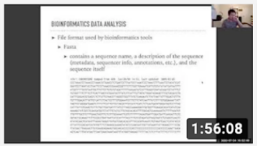

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