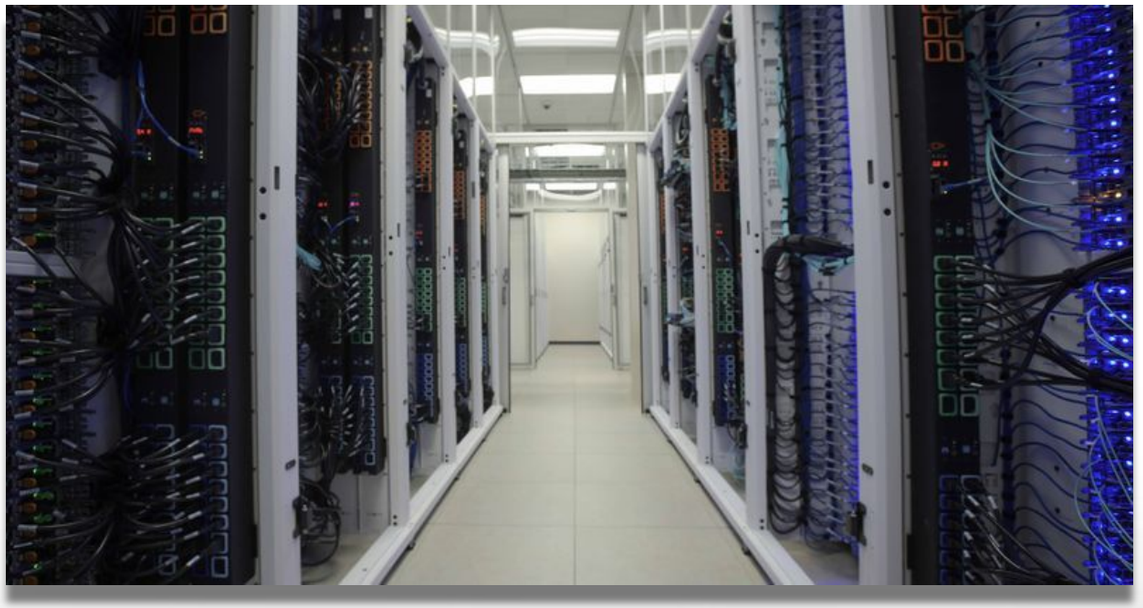
Things to Do While You are Waiting

- Open your web browser and visit hprc.tamu.edu
- Log into TAMU VPN (if you're off campus) and reconnect to Zoom
- If you don't have an HPRC account, please ask*
- If you don't know basic Linux commands, please ask*

*speak up in chat or email help@hprc.tamu.edu

Introduction to High Performance Research Computing



Slides by **Richard Lawrence**

Presented by **Xin Yang**

Spring 2022

Outline

- Usage Policies
- References
- Cluster Overview
- Break
- Accessing HPRC
- HPRC Computing Environment
- Break
- Cluster Computing Basics
- Break
- Cluster Computing Exercises
- Need Help?

Usage Policies
(Be a good compute citizen)

- It is illegal to share computer passwords and accounts by state law and university regulation
- It is prohibited to use HPRC clusters in any manner that violates the United States export control laws and regulations, EAR & ITAR
- Abide by the expressed or implied restrictions in using commercial software

hprc.tamu.edu/policies

Education Resources

- Knowledge Foundation:
  - Basic knowledge of LINUX commands
  - Slides from our LINUX short course are at:

    hprc.tamu.edu/training/intro_linux.html
  - Watch the relevant Introduction and Primer videos on our Youtube Channel

    youtube.com channel "Texas A&M HPRC"
  - Answers to frequently asked questions can be found on *our Wiki*

    https://hprc.tamu.edu/wiki/Main_Page

Follow Along

Simple exercises:

- Terra: hprc.tamu.edu/wiki/Terra:Exercises

Cluster computing exercises:

- Terra: Example files located in `/scratch/training/Intro-to-terra` directory

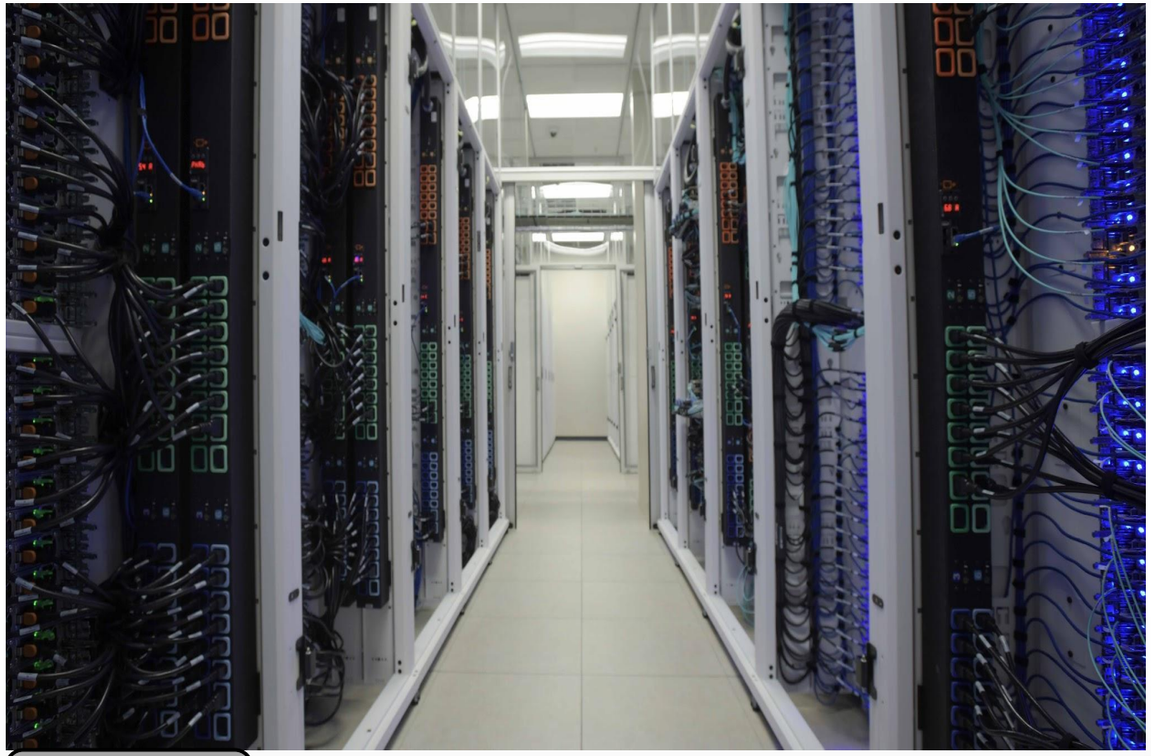
Interface for hands-on exercises:

- Terra: portal-terra.hprc.tamu.edu/
  or choose “Terra OnDemand” from portal.hprc.tamu.edu/

HPRC Clusters

Terra

320-node cluster,
deployed in 2017



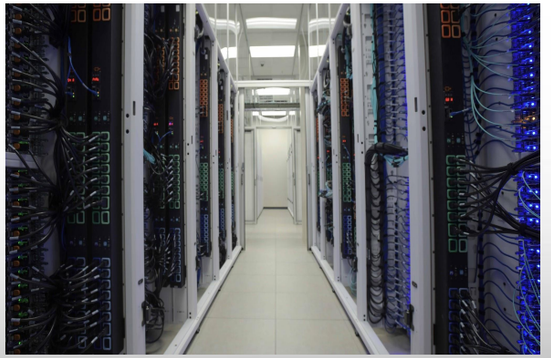
Grace

Flagship cluster,
deployed in 2021!

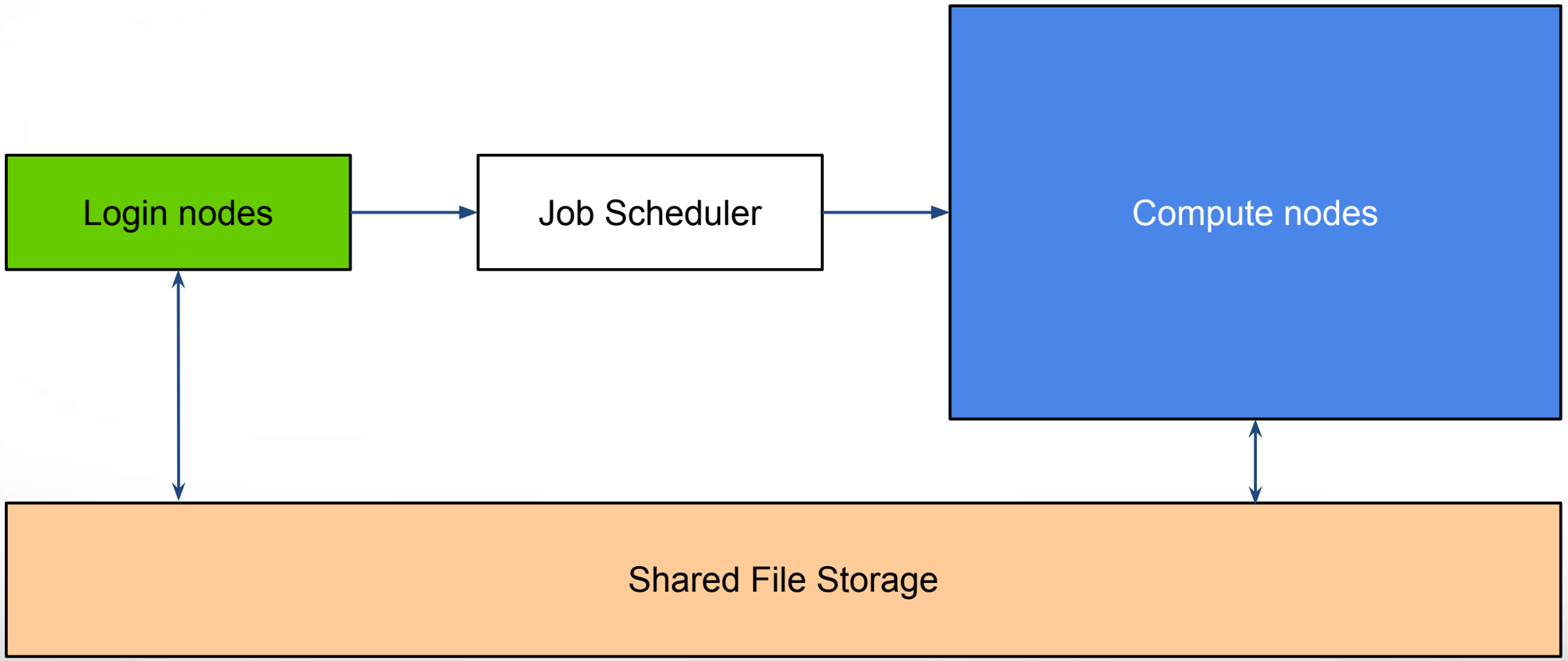
Clusters Are For You!

What kinds of problems are solved by cluster computing?

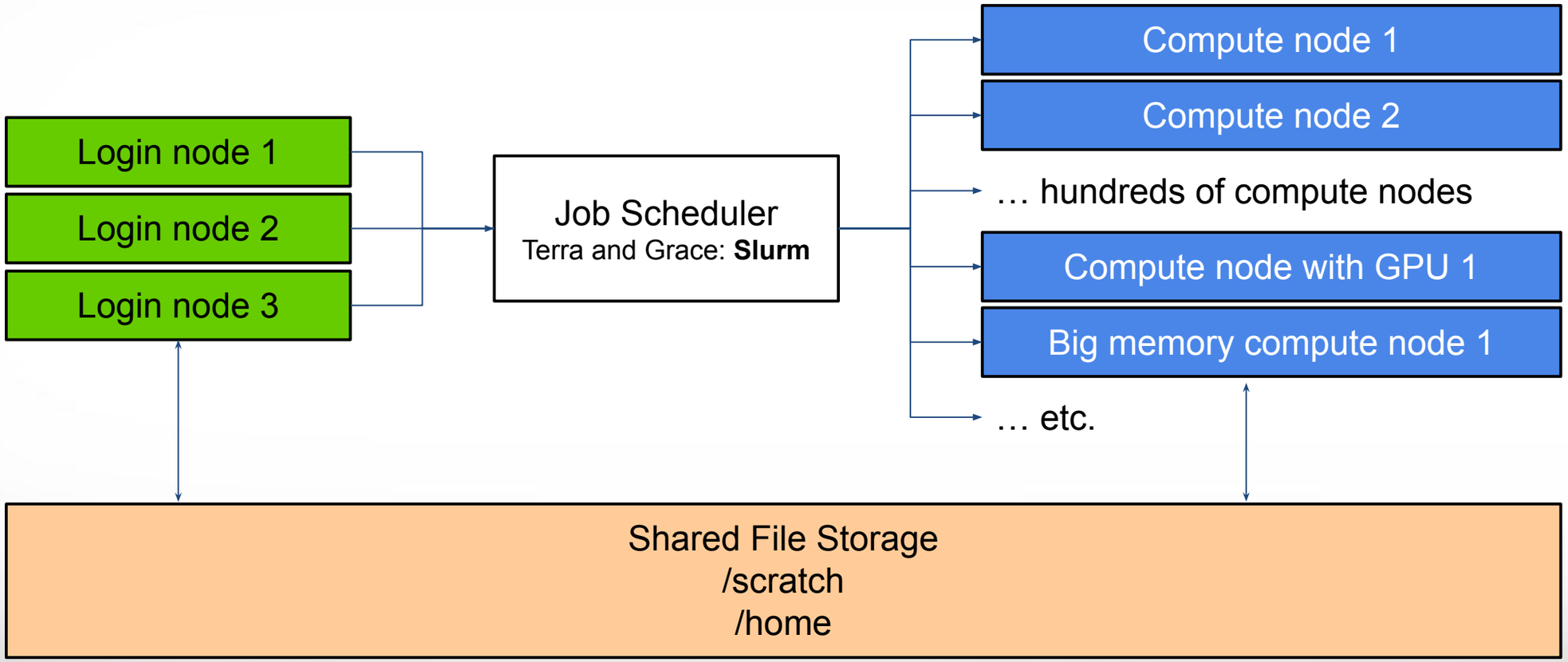
- Problems that are too big to fit in one laptop or workstation, due to limitation on memory, core count, or node count
- Problems that scale well with more CPU cores or memory
- Single-threaded problems with millions of permutations
- Problems that require large high speed storage and/or interconnect



Cluster Diagram

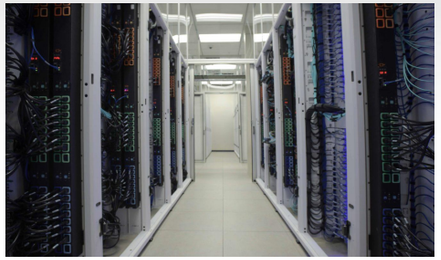


Cluster Diagram



HPRC Clusters

Terra



Grace

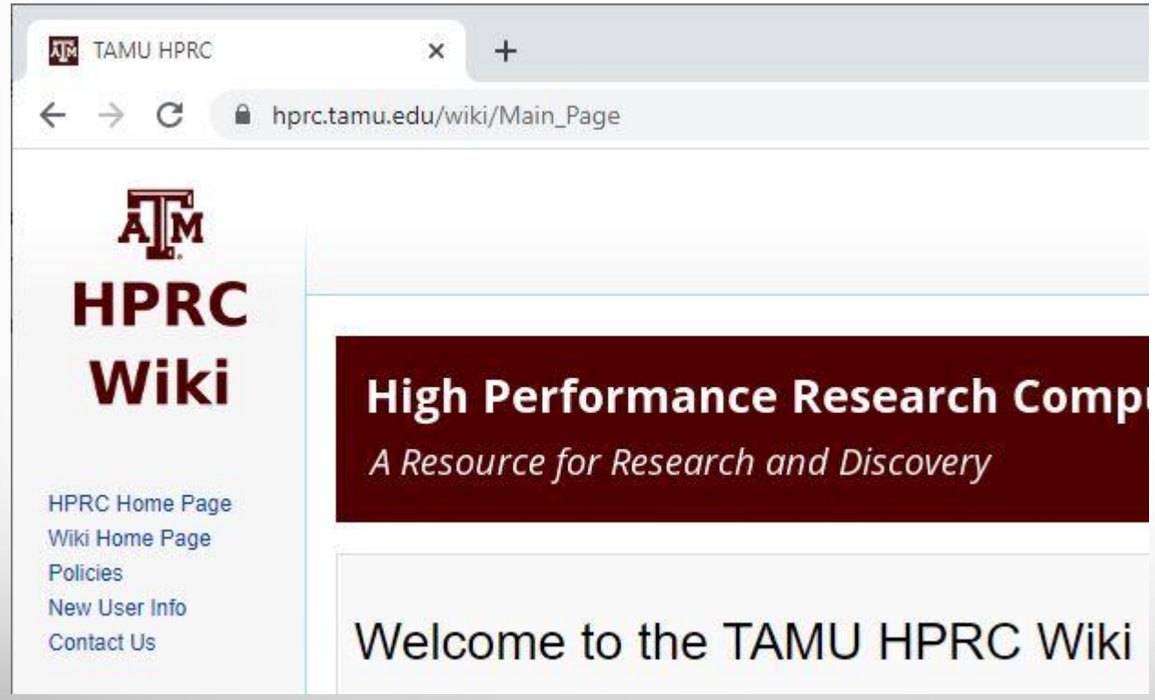
Total Nodes (Cores)	307 (8,512)	925 (44,656)
General Nodes	28 cores 64GB	48 cores 384GB
Features	GPUs Many-core nodes	GPUs - multiprecision Big Memory Nodes
Job Scheduler	Slurm	Slurm
Online Since	2017	2021

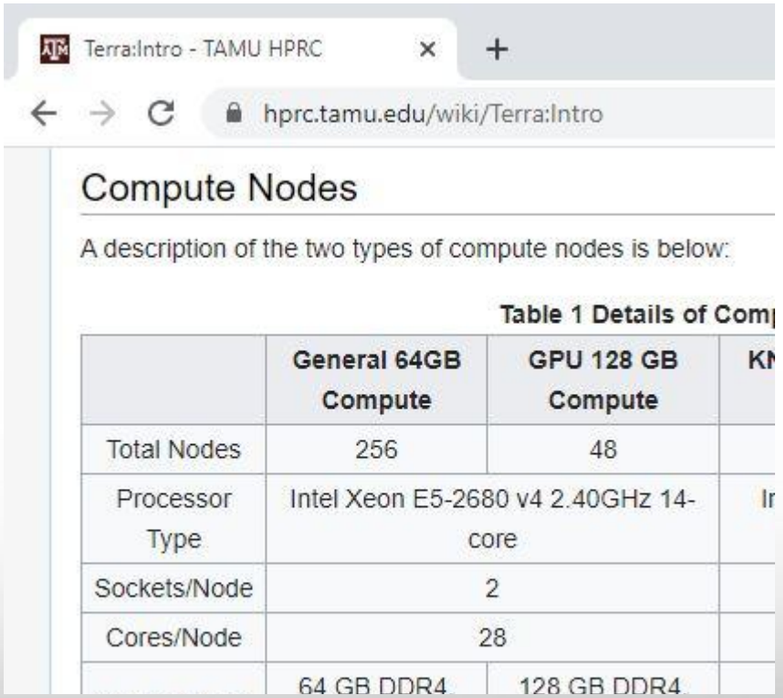
hprc.tamu.edu/resources

HPRC Wiki - Hardware

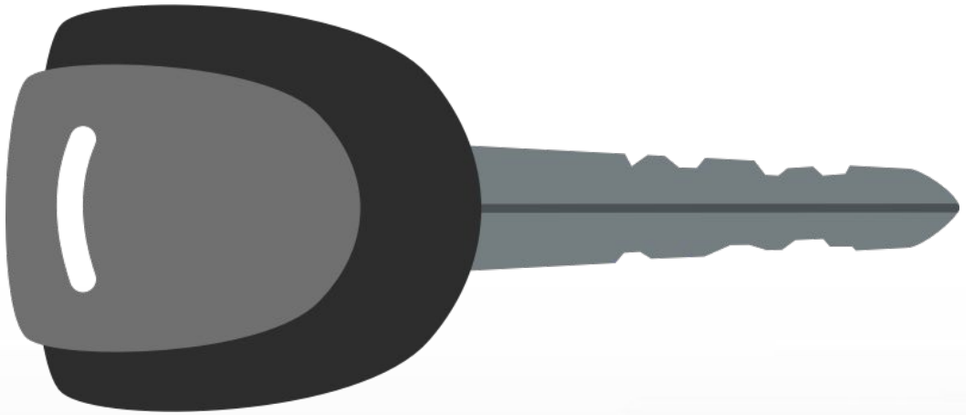
Visit our wiki https://hprc.tamu.edu/wiki/Main_Page to learn more about our clusters.

For example, information about Terra hardware is on page https://hprc.tamu.edu/wiki/Terra:Intro.





Getting Started



Authentication and Access

Three steps to access HPRC resources.

1. Get a HPRC account
2. VPN to TAMU campus
3. Web login (**Portal**, Globus) through CAS
   or
   SSH/SFTP to HPRC clusters

- Duo NetID two-factor authentication used to enhance security (it.tamu.edu/duo/)
- (Faculty and staff) Use Duo Keys - u.tamu.edu/get_duo_keys
- Instructions in two-factor wiki page (hprc.tamu.edu/wiki/Two_Factor)

Example: SSH login with Duo

```
$ ssh terra.tamu.edu
**************************************************************
…. warning message (snipped) …….
**************************************************************

Password:
Duo two-factor login for UserNetID

Enter a passcode or select one of the following options:

 1. Duo Push to XXX-XXX-1234
 2. Phone call to XXX-XXX-1234
 3. SMS passcodes to XXX-XXX-1234 (next code starts with: 9)

Passcode or option (1-3): 1
Success. Logging you in...
```

File Systems and User Directories

Directory	Environment Variable	Space Limit	File Limit	Intended Use
/home/$USER	$HOME	10 GB	10,000	Small amounts of processing.
/scratch/user/$USER	$SCRATCH	1 TB	250,000	Temporary storage of actively used large files. Not a long-term storage area.

File Systems and User Directories

Directory	Environment Variable	Space Limit	File Limit
/home/$USER	$HOME	10 GB	10,000
/scratch/user/$USER	$SCRATCH	1 TB	50,000

- **`$HOME`** and **`$SCRATCH`** are not shared between clusters.
- View usage and quota limits using the command:
- Quota and file limit increases can be requested
- Group directory for sharing files upon request.
- Do not share your home or scratch directories.

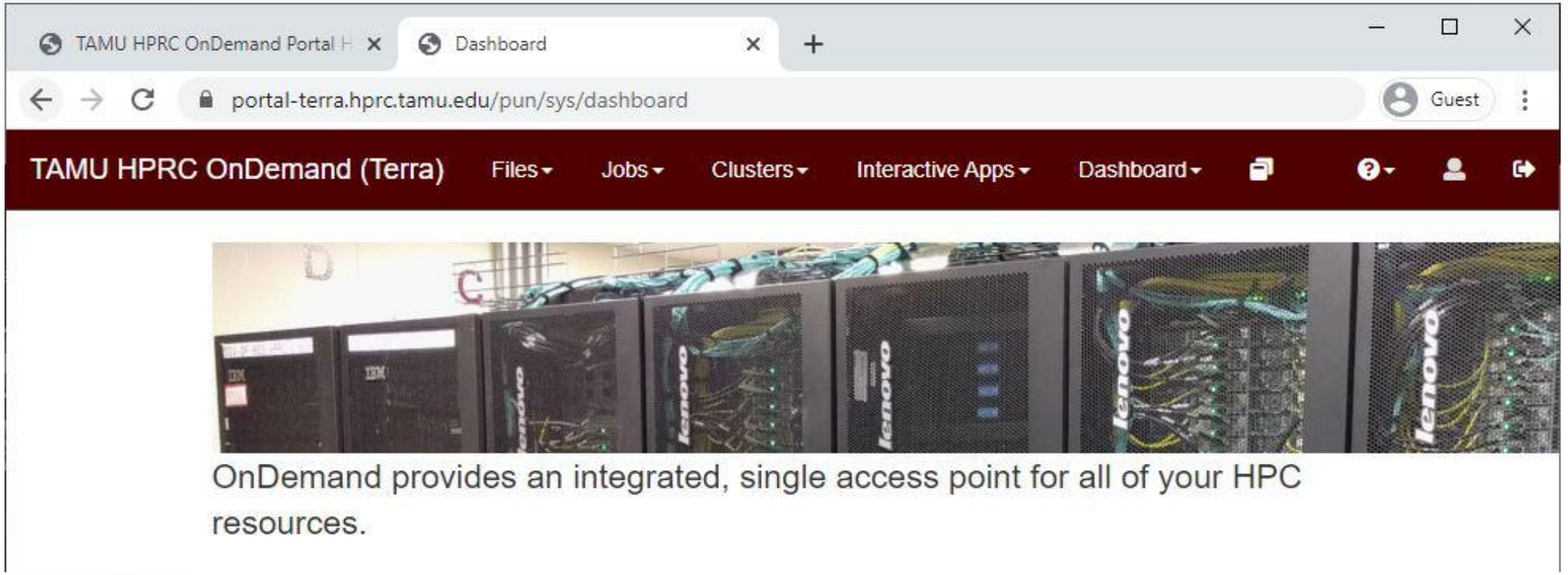
`showquota`

hprc.tamu.edu/wiki/Terra:Filesystems_and_Files
hprc.tamu.edu/wiki/Grace:Filesystems_and_Files

Hands-on exercises:

Activate TAMU VPN
Go to:
portal.hprc.tamu.edu

portal.hprc.tamu.edu



- Files > copy and edit files on the cluster's filesystems
- Jobs > submit and monitor cluster jobs
- Clusters > open a shell terminal (command line) on a login node
- Interactive Apps > start graphical software on a compute node and connect to it
- Dashboard > view file quotas and computing account allocations

Hands-on exercise:

Upload a File to Terra in Portal

Menu > Files > /scratch/user/<netid>

use the '↥ Upload' button near the top-right,
pick something small from your desktop

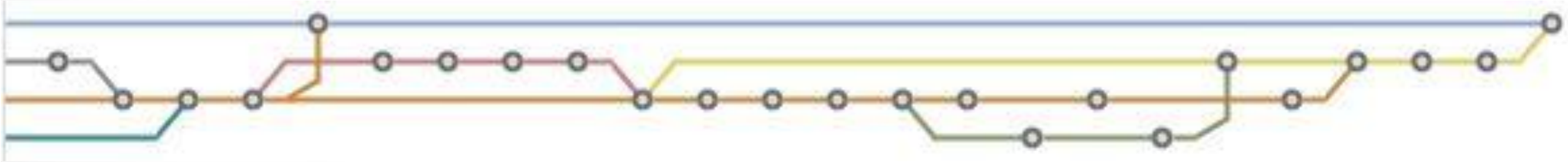
Hands-on exercise:

Check your file Quota on Terra in Portal

Menu > Dashboard > Terra Dashboard

Locate your /scratch disk usage stats

Software Infrastructure



Software

HPRC provides both pre-installed Software and installation assistance

- Software wiki page includes instructions and examples
  - hprc.tamu.edu/wiki/SW
- License-restricted software
  - Contact license owner for approval
- Contact us for software installation help/request
  - User can install software in their home/scratch dir
  - Do not run the "*sudo*" command when installing software

Computing Environment

- **Path:** the location on disk where an executable or library may be found.
- Paths are saved as **environment variables**, so you can choose which libraries and executables will be used by modifying the variables.
- There is a lot of software, many versions, and many paths to manage

..... How do you manage all these software versions?

hprc.tamu.edu/wiki/Terra:Computing_Environment#Modules

Computing Environment

Managing software versions using lmod

- Uses the command: **`module`**
- Each version of a software, application, library, etc. is available as a module.
  - Module names have the format:

software-name / version toolchain [dependency-version]

`TopHat/2.1.1-intel-2017A-Python-2.7.12`

- **`module`** sets the correct environment variables for you.

hprc.tamu.edu/wiki/Terra:Computing_Environment#Modules

Module Usage Basics: Terra

```
module avail or mla          # list all available modules (sometimes it is very slow)
                             # space bar down, page up/down, q to quit
                             # / for case sensitive search (similar to a Unix man page)

module spider <word>         # case insensitive search for modules with 'word' in name

module load <module>         # add <module> paths to the current environment variables
```

- Information about specific modules can also be found on our software page: https://hprc.tamu.edu/software/terra/#
- Learn more about `module` commands on our wiki: https://hprc.tamu.edu/wiki/SW:Modules

Module Usage Basics: Grace

- Installed applications are made available with the module system
  Grace uses a *software* ***hierarchy*** inside the module system

- Example:

```
mla perl
```

```
# search for a specific piece of software by keyword
```

```
module spider Perl/5.32.0
```

```
# find how to load a particular module using the full module name based on the above results
```

```
module load  GCCcore/10.2.0 Perl/5.32.0
```

```
# Load the base dependency module(s) first then the full module name
```

Hands-on exercises:

Open a terminal on Terra in Portal

Menu > Clusters > _terra Shell Access

use your Netid password and your two-factor Authentication method.

Module Loading Exercise

1. `ml list` # list all loaded modules
2. `mla blast+` # see which versions of BLAST+ and FastQC are available
3. `ml BLAST+/2.8.1-intel-2018b` # load a specific module version
4. `ml list` # list all loaded modules
5. `ml FastQC/0.11.8-Java-11` # load a compatible module version (intel + Java)
6. `ml Java/1.7.0` # change version of a loaded module (Java/11 to Java/1.7.0)
   # notice the message about reloaded modules
7. `ml list` # list all loaded modules
8. `ml purge` # remove all loaded modules

Development Environment - Toolchains

- Toolchains are combinations of compilers, MPI libraries, and highly optimized math libraries.
- Toolchain components are primarily either Intel or Open Source.

Example toolchains for `C++` development:

Components	**Open Source**	**Intel Source**	**Mixed Source**
Compiler only	`GCCcore`	`iccifort`	-
Compiler + MPI	`gompi`	`iimpi`	`iompi`
Compiler + MPI + MKL, BLAS, FFTW, LAPACK	`foss`	`intel`	`iomkl`
Compiler + all of the above + CUDA Compiler	`fosscuda`	`intelcuda`	`iomklc`

Example usage: `module load foss/2019b`

As usual, see our Wiki for more information. hprc.tamu.edu/wiki/SW:Toolchains

Module Usage Practices

- Applications installed as modules are available to all users
  - (except for restricted modules)
- It's a good habit to unload unused modules before loading new modules.
- It is recommended to load a specific software version instead of the defaults
- **Avoid loading modules in your `~/.bashrc`**
- Avoid mixing toolchains when loading multiple modules at the same time. This usually leads to one of them not working.

hprc.tamu.edu/wiki/Terra:Computing_Environment#Modules

Software Install Example: Virtual Env

Python is a language which supports many external libraries in the form of extensions. (called Python Packages).

Some commonly used packages:

- SciPy & NumPy
- Jupyter notebook
- Scikit-learn

You can install these yourself using the Virtual Environment feature. Instructions are on the wiki:

https://hprc.tamu.edu/wiki/SW:Python#Create_a_virtual_environment

Software Install Exercise

1.
```
cd $SCRATCH
mkdir python_example
cd python_example
```
setup workspace

2.
```
module purge
module load Python/3.6.6-intel-2018b
```
setup Python module

3.
```
virtualenv my_example_venv
source my_example_venv/bin/activate
```
setup your virtual environment

4.
```
python -c "import pytime"
```
check if python-time is installed (it's not)

5.
```
pip install python-time
```
install a cute little python package

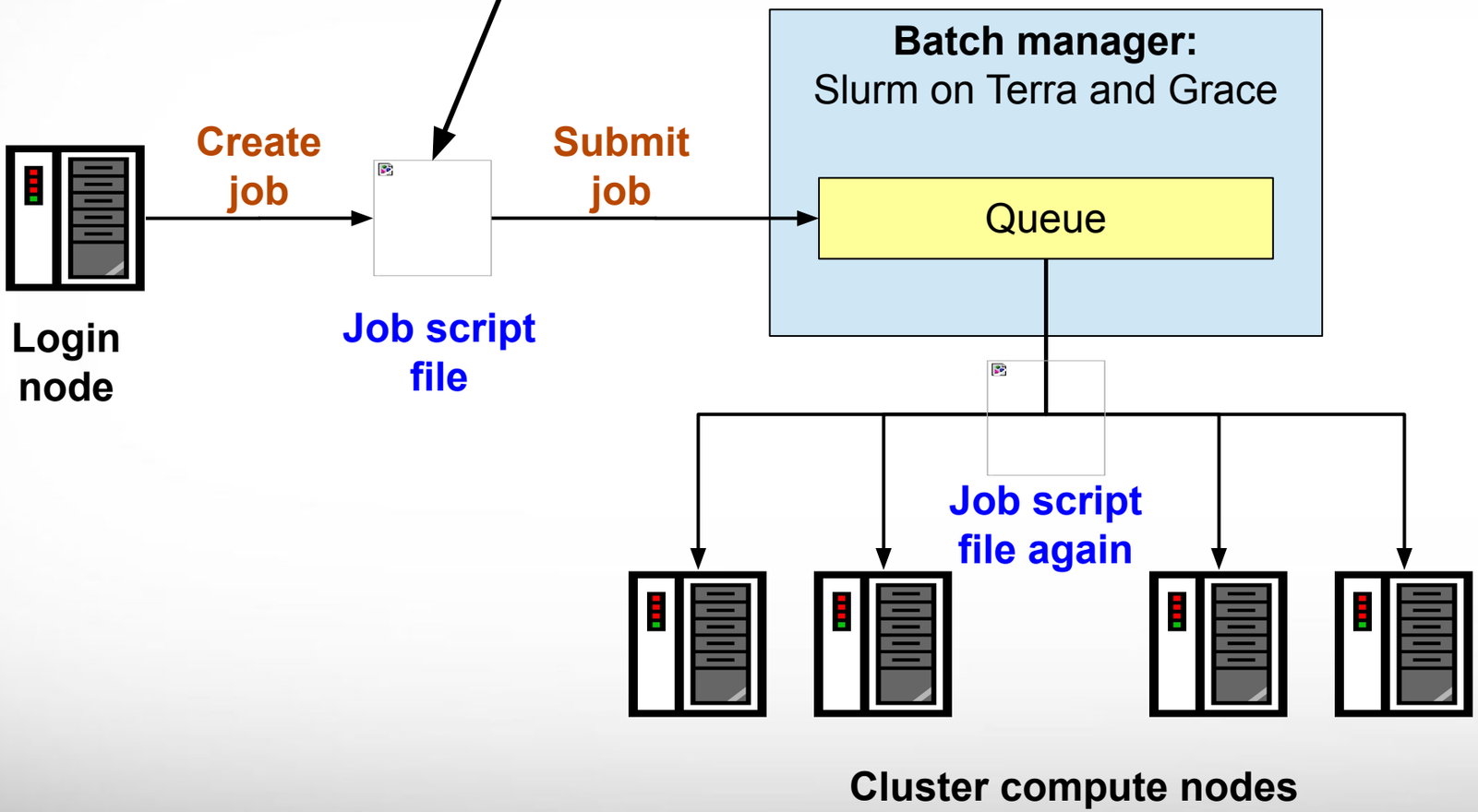
6.
```
python -c "import pytime"
```
check if python-time is installed (it is)

7.
```
deactivate
```
all done

Cluster Computing

Batch Computing on HPRC Clusters

A batch job script is a text file that contains both Unix commands and Batch manager job parameters



Consumable Computing Resources

- Resources specified in a job file:
  - Processor cores
  - Memory
  - Wall time
  - GPU
- Service Unit (SU) - Billing Account
  - Use "**`myproject`**" to query
    hprc.tamu.edu/wiki/HPRC:AMS:Service_Unit

`myproject`

```
================================================================================================
              List of YourNetID's Project Accounts
------------------------------------------------------------------------------------------------
|   Account    |   FY   | Default | Allocation |Used & Pending SUs|   Balance   |    PI      |
------------------------------------------------------------------------------------------------
|1228000223136|  2019  |       N|    10000.00|              0.00|    10000.00|Doe, John   |
------------------------------------------------------------------------------------------------
|1428000243716|  2019  |       Y|     5000.00|            -71.06|     4928.94|Doe, Jane   |
------------------------------------------------------------------------------------------------
```

Consumable Computing Resources

- Software license/token:
  - Use "**`license_status`**" to query
  - hprc.tamu.edu/wiki/SW:License_Checker

Find available license for "ansys":

```
license_status -s ansys
```

```
License status for ANSYS:
-------------------------------------------------------------
|License Name                |  # Issued|  # In Use|# Available|
-------------------------------------------------------------
|aa_mcad                     |        50|         0|         50|
|aa_r                        |        50|        32|         18|
|aim_mp1                     |        50|         0|         50|
|   ......                                                    |
-------------------------------------------------------------
```

Find detail options:

```
license_status -h
```

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

A Service Unit (SU) on **Grace** and **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

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

Batch Queues

- Job submissions are auto-assigned to batch queues based on the resources requested (number of cores/nodes and walltime limit)
- Some jobs can be directly submitted to a queue:
  - For example, if gpu nodes are needed, use the **gpu** partition/queue.
- Batch queue policies are used to manage the workload and may be adjusted periodically.

hprc.tamu.edu/wiki/Terra:Batch#Queues

sinfo : Current Queues

File Edit View Search Terminal Help

```
[  netid @terra2 ~]$ sinfo
PARTITION        AVAIL  TIMELIMIT    JOB_SIZE    NODES(A/I/O/T)   CPUS(A/I/O/T)
short*           up     2:00:00      1-16        156/145/3/304    3667/4761/84/8512
medium           up     1-00:00:00   1-64        156/145/3/304    3667/4761/84/8512
long             up     7-00:00:00   1-32        156/145/3/304    3667/4761/84/8512
gpu              up     2-00:00:00   1-48        48/0/0/48        797/547/0/1344
vnc              up     12:00:00     1           48/0/0/48        797/547/0/1344
xlong            up     21-00:00:00  1-32        108/145/3/256    2870/4214/84/7168
staff            up     infinite     1-infinite  156/145/3/304    3667/4761/84/8512
low_priority     up     1-00:00:00   1-infinite  156/145/3/304    3667/4761/84/8512
special          up     7-00:00:00   1-infinite  156/145/3/304    3667/4761/84/8512
knl              up     7-00:00:00   1-8         0/14/2/16        0/980/140/1120
```

For the NODES and CPUS columns:
A = Active (in use by running jobs)
I = Idle (available for jobs)
O = Offline (unavailable for jobs)
T = Total

Batch Job Scripts

Sample Job Script Structure (Slurm)

```
#!/bin/bash

##NECESSARY JOB SPECIFICATIONS
#SBATCH --job-name=JobExample1
#SBATCH --time=01:30:00
#SBATCH --ntasks=1
#SBATCH --mem=2G
#SBATCH --output=stdout.%j

##OPTIONAL JOB SPECIFICATIONS
#SBATCH --account=123456
#SBATCH --mail-type=ALL
#SBATCH --mail-user=email_address

# load required module(s)
module purge
module load Python/3.7.0-intel-2018b

./my_program.py
```

See also `example01.job`

These parameters describe your job to the job scheduler

This is single line comment and not run as part of the script

Load the required module(s) first

This is a command that is executed by the job

Important Batch Job Parameters (**Slurm**)

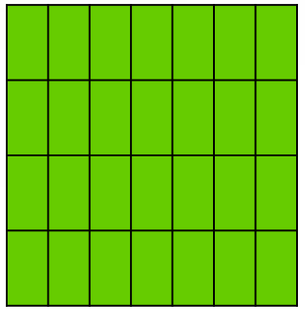
Slurm parameter	Comment
`#SBATCH --time=HH:MM:SS`	Specifies the time limit for the job. Must specify seconds SS on Terra
`#SBATCH --ntasks=NNN`	Total number of tasks (cores) for the job.
`#SBATCH --ntasks-per-node=XX`	Specifies the maximum number of tasks (cores) to allocate per node

`#SBATCH --mem=nnnnM`
`or`
`#SBATCH --mem=nG`
 	
`(memory per NODE)`
	Sets the maximum amount of memory (MB).
	
	G for GB is supported on Terra

hprc.tamu.edu/wiki/HPRC:Batch_Translation

Mapping Jobs to Cores per Node on Terra

A.

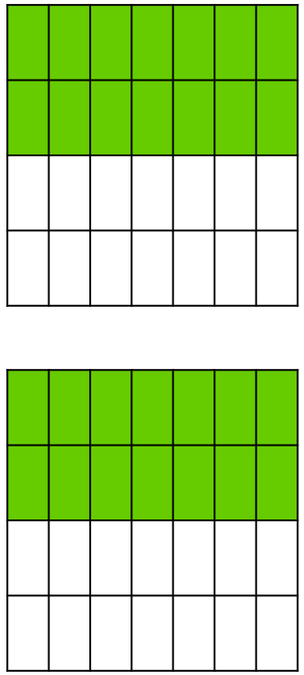


28 cores on
1 compute node

#SBATCH --ntasks 28
#SBATCH --tasks-per-node=28

Preferred Mapping
(if applicable)

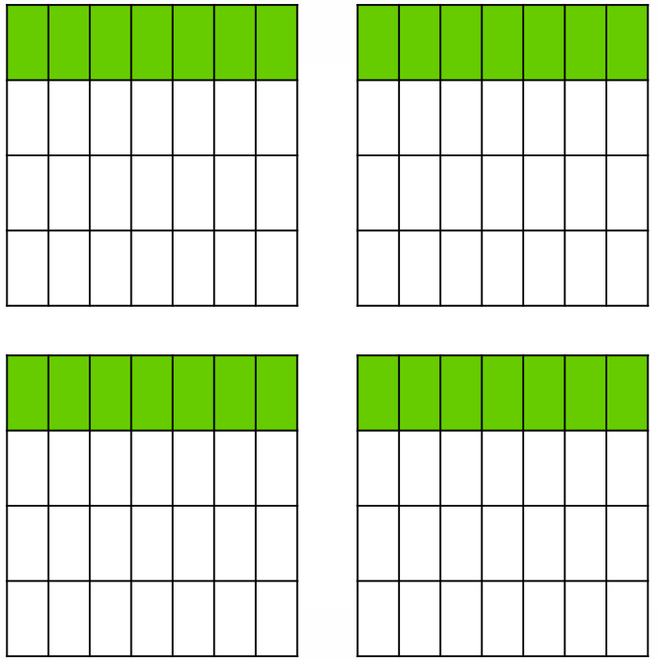
B.



28 cores on
2 compute nodes

#SBATCH --ntasks 28
#SBATCH --tasks-per-node=14

C.



28 cores on
4 compute nodes

#SBATCH --ntasks 28
#SBATCH --tasks-per-node=7

Job Memory Requests on Terra

- Specify memory request based on memory per node:

  #SBATCH --mem=xxxxM # memory per node in MB

  or

  #SBATCH --mem=xG # memory per node in GB

- On 64GB nodes, usable memory is at most 56 GB. The per-process memory limit should not exceed 2000 MB for a 28-core job.
- On 128GB nodes, usable memory is at most 112 GB. The per-process memory limit should not exceed 4000 MB for a 28-core job.

Job Memory Requests on **Grace**

- Specify memory request based on memory per node:

  #SBATCH --mem=xxxxM # memory per node in MB

  or

  #SBATCH --mem=xG # memory per node in GB

- On 384GB nodes, usable memory is at most 360 GB.

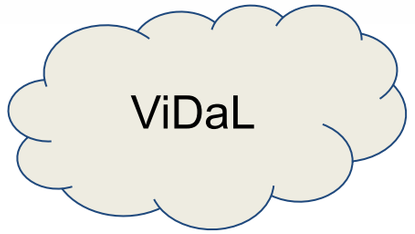
  The per-process memory limit should not exceed ~7500 MB for a 48-core job.

- On 3TB nodes, usable memory is at most 2900 GB.

  The per-process memory limit should not exceed 37120 MB for a 48-core job.

Pop Quiz

Pop Quiz



Which one of the following HPRC clusters is *not* in use?

A. Grace
B. Terra
C. FASTER
D. ViDaL

Slurm Pop Quiz

```
#SBATCH --job-name=stacks_S2
#SBATCH --ntasks 80
#SBATCH --ntasks-per-node=20
#SBATCH --mem=40G
#SBATCH --time=48:00:00
#SBATCH --output stdout.%J
#SBATCH --error stderr.%J
```

How many nodes is this job requesting?

A. 1600
B. 80
C. 20
D. 4

(end of Pop Quiz)

Job Submission and Tracking: Grace and Terra

Slurm commands	Description
`sbatch jobfile1`	Submit jobfile1 to batch system
`squeue [-u user_name] [-j job_id]`	List jobs
`scancel job_id`	Kill a job
`sacct -X -j job_id`	Show information for a job (can be when job is running or recently finished)
`sacct -X -S YYYY-HH-MM`	Show information for all of your jobs since YYYY-HH-MM
`lnu job_id`	Show resource usage for a job
`pestat -u $USER`	Show resource usage for a running job
`seff job_id`	Check CPU/memory efficiency for a job

hprc.tamu.edu/wiki/HPRC:Batch_Translation

Job Environment Variables

- **Terra**:
  - **$PATH** = list of directories where executables are found
  - **$LD_LIBRARY_PATH** = list of directories where libraries are found
  - **$SCRATCH** = short-hand for /scratch/user/<NetID>
- **Slurm**:
  - **$SLURM_JOBID** = job id, unique number for each job
  - **$SLURM_SUBMIT_DIR** = directory where job was submitted from
  - **$TMPDIR** = /work/job.$SLURM_JOBID
    - $TMPDIR is local to each assigned compute node for the job and is about 850GB
    - Use of $TMPDIR is recommended for jobs that use many small temporary files
    - Do not use $TMPDIR for software that has checkpoints to restart where it left off

hprc.tamu.edu/wiki/Ada:Batch_Processing_LSF#Environment_Variables
hprc.tamu.edu/wiki/Terra:Batch#Environment_Variables

Batch Job Exercises

Hands-on exercises:

Copy the example files into your scratch directory, if you haven't done so already.

```
cp -r /scratch/training/Intro-to-terra $SCRATCH
```

Inspect the contents.

```
cd $SCRATCH/Intro-to-terra
ls
ls *
```

Job Exercise: Check Output

Submit job

```
cd batch_examples
```

Terra:

```
sbatch example01.job
```

```
Submitted batch job <#####>
```

Check status

Terra:

```
squeue -u $USER
```

```
JOBID   NAME      USER      PARTITION  NODES  CPUS  STATE    TIME   TIME_LEFT  START_TIME          REASON      NODELIST
64039   somejob   someuser  medium     4      112   PENDING  0:00   20:00      2017-01-30T21:00:4  Resources
64038   somejob   someuser  medium     4      112   RUNNING  2:49   17:11      2017-01-30T20:40:4  None        tnxt-[0401-0404]
```

Check output

```
cat output.ex01.env_variables.<tab autocomplete>
```

This job output file was created by the parameter in your job script file

Terra: `#SBATCH -o output.ex01.env_variables.%j`

Job Exercise: Check Status

Submit job

```
cd batch_examples
```

Terra:

```
sbatch example02.job
```

```
Submitted batch job <#####>
```

Check status

Terra:

```
squeue -u $USER
```

```
JOBID   NAME      USER      PARTITION  NODES  CPUS  STATE    TIME   TIME_LEFT  START_TIME          REASON      NODELIST
64039   somejob   someuser  medium     4      112   PENDING  0:00   20:00      2017-01-30T21:00:4  Resources
64038   somejob   someuser  medium     4      112   RUNNING  2:49   17:11      2017-01-30T20:40:4  None        tnxt-[0401-0404]
```

Check output

```
cat output.ex02.echo_numbers.<tab autocomplete>
```

This job output file was created by the parameter in your job script file

Terra: `#SBATCH -o output.ex02.echo_numbers.%j`

Job Exercise: Debug job failures

Submit job

```
cd batch_examples
```

Terra:

```
sbatch example03.job
```

```
Submitted batch job <#####>
```

Check output

```
cat output.ex03.python_mem.<tab autocomplete>
```

This job output file was created by the parameter in your job script file

Terra: `#SBATCH -o output.ex03.python_mem.%j`

```
slurmstepd: error: Exceeded job memory limit at some point.
```

Make the necessary adjustments to memory parameters in your job script and resubmit the job

Job Exercise: Bad job script

Submit job

```
cd batch_examples
```

Terra:

```
sbatch example05.job
```

```
sbatch: error: CPU count per node can not be satisfied
sbatch: error: Batch job submission failed: Requested node configuration is not available
```

Quiz: what went wrong with this job script?

Check your Service Unit (SU) Balance

- List the SU Balance of your Account(s)

```
myproject
```

```
 ================================================================================
              List of YourNetID's Project Accounts
--------------------------------------------------------------------------------
|   Account    |    FY    | Default | Allocation |Used & Pending SUs|   Balance  |    PI    |
--------------------------------------------------------------------------------
|1228000223136|  2019    |       N|    10000.00|              0.00|    10000.00|Doe, John |
--------------------------------------------------------------------------------
|1428000243716|  2019    |       Y|     5000.00|            -71.06|     4928.94|Doe, Jane |
--------------------------------------------------------------------------------
|1258000247058|  2019    |       N|     5000.00|             -0.91|     4999.09|Doe, Jane |
--------------------------------------------------------------------------------
```

- To specify a project ID to charge in the job file
  - Grace & Terra: **`#SBATCH -A Account#`**
- Run "**`myproject -d Account#`**" to change default project account
- Run "**`myproject -h`**" to see more options

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

Job submission issue: insufficient SUs

Bonus Assignment: modify a job file so that the requested SU's are too much for your account. I.e.: make an error message (like the following) appear.

Grace & Terra:

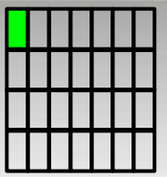
```
$ sbatch myjob
sbatch: error: (from job_submit) your account's balance is not sufficient to submit your job
               Project Account: 123940134739
               Account Balance: 382.803877
               Requested SUs:   18218.666666667
```

- What to do if you need more SUs
  - Ask your PI to transfer SUs to your account
  - Apply for more SUs (if you are eligible, as a PI or permanent researcher)

hprc.tamu.edu/wiki/HPRC:CommonProblems#Q:_How_do_I_get_more_SUs.3F
hprc.tamu.edu/wiki/HPRC:AMS:Service_Unit
hprc.tamu.edu/wiki/HPRC:AMS:UI

Other Batch Job Examples

Slurm Job File (Serial Example)

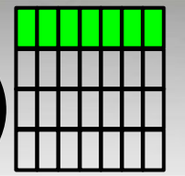


serial.job

```
#!/bin/bash

##NECESSARY JOB SPECIFICATIONS
#SBATCH --job-name=JobExample1       #Set the job name to "JobExample1"
#SBATCH --time=01:30:00              #Set the wall clock limit to 1hr and 30min
#SBATCH --ntasks=1                   #Request 1 task
#SBATCH --mem=2560M                  #Request 2560MB (2.5GB) per node
#SBATCH --output=Example1Out.%j      #Send stdout/err to "Example1Out.[jobID]"

##OPTIONAL JOB SPECIFICATIONS
##CHANGE ACCOUNT NUMBER AND EMAIL ADDRESS BEFORE USING
##SBATCH --account=123456             #Set billing account to 123456
##SBATCH --mail-type=ALL              #Send email on all job events
##SBATCH --mail-user=email_address    #Send all emails to email_address

# this intel toolchain is just an example.  recommended toolchain is TBD
module purge
module load intel/2017A

# run your program
./helloworld.omp.C.exe
```

SUs = 1.5

Slurm Job File (multi core, single node)



singlenode_multicore.job

```
#!/bin/bash

##NECESSARY JOB SPECIFICATIONS
#SBATCH --job-name=JobExample2          # Set the job name to "JobExample2"
#SBATCH --time=6:30:00                     # Set the wall clock limit to 6hr and 30min
#SBATCH --nodes=1                       # Request 1 node
#SBATCH --ntasks-per-node=8             # Request 8 tasks(cores) per node
#SBATCH --mem=8G                        # Request 8GB per node
#SBATCH --output=Example2Out.%j         # Send stdout/err to "Example2Out.[jobID]"

##OPTIONAL JOB SPECIFICATIONS
##CHANGE ACCOUNT NUMBER AND EMAIL ADDRESS BEFORE USING
##SBATCH --account=123456     # Set billing account to 123456  #find your account with "myproject"
##SBATCH --mail-type=ALL              # Send email on all job events
##SBATCH --mail-user=email_address    # Send all emails to email_address

# load required module(s)
module purge
module load intel/2017A

# run your program
mpirun ./helloworld.mpi.C.exe
```

SUs = 52

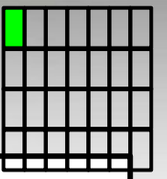
Slurm Job File (multi core, multi node)

multinode_multicore.job

```
#!/bin/bash

##NECESSARY JOB SPECIFICATIONS
#SBATCH --job-name=JobExample3          # Set the job name to "JobExample3"
#SBATCH --time=1-12:00:00               # Set the wall clock limit to 1 Day and 12hr
#SBATCH --ntasks=8                      # Request 8 tasks (cores)
#SBATCH --ntasks-per-node=2             # Request 2 tasks(cores) per node
#SBATCH --mem=4096M                     # Request 4096MB (4GB) per node
#SBATCH --output=Example3Out.%j         # Send stdout and stderr to "stdout.[jobID]"

##OPTIONAL JOB SPECIFICATIONS
##CHANGE ACCOUNT NUMBER AND EMAIL ADDRESS BEFORE USING
##SBATCH --account=123456      # Set billing account to 123456 #find your account with "myproject"
##SBATCH --mail-type=ALL               # Send email on all job events
##SBATCH --mail-user=email_address    # Send all emails to email_address

# this intel toolchain is just an example.  recommended toolchain is TBD
module purge
module load intel/2017A

# run program with MPI
mpirun ./helloworld.mpi.C.exe
```

SUs = 288

Slurm Job File (serial GPU)



serialgpu.job

```
#!/bin/bash

##NECESSARY JOB SPECIFICATIONS
#SBATCH --job-name=JobExample4          # Set the job name to "JobExample4"
#SBATCH --time=01:00:00                 # Set the wall clock limit to 1hr
#SBATCH --ntasks=1                      # Request 1 task (core)
#SBATCH --mem=2560M                     # Request 2560MB (2.5GB) per node
#SBATCH --output=Example4Out.%j         # Send stdout and stderr to "Example4Out.[jobID]"
#SBATCH --gres=gpu:1                    # Request 1 GPU
#SBATCH --partition=gpu                 # Request the GPU partition/queue

##OPTIONAL JOB SPECIFICATIONS
##CHANGE ACCOUNT NUMBER AND EMAIL ADDRESS BEFORE USING
##SBATCH --account=123456     # Set billing account to 123456  #find your account with "myproject"
##SBATCH --mail-type=ALL              # Send email on all job events
##SBATCH --mail-user=email_address    # Send all emails to email_address

# load required module(s)
module purge
module load intel/2017A CUDA/9.2.148.1

# run your program
./deviceQuery
```

SUs = 28

List Node Utilization: *lnu*

`lnu jobid`

lists the node utilization across all nodes for a running job.
to see more options use: `lnu -h`

Example:

```
lnu <jobid>
```

Note: Slurm updates the node information every few minutes

```
JOBID    NAME       USER       PARTITION    NODES    CPUS     STATE        TIME     TIME_LEFT        START_TIME
565849   somename   someuser   long         3        84       RUNNING      17:37    6-23:42:23       2018-01-25T15:19:55

HOSTNAMES     CPU_LOAD    FREE_MEM    MEMORY   CPUS(A/I/O/T)
tnxt-0703     26.99       53462       57344    28/0/0/28
tnxt-0704     26.93       52361       57344    28/0/0/28
tnxt-0705     26.95       47166       57344    28/0/0/28
```

Note: CPU_LOAD is not the same as % utilization

For the CPUS columns:
A = Active (in use by running jobs)
I = Idle (available for jobs)
O = Offline (unavailable for jobs)
T = Total

Monitor Compute Node Utilization: *pestat*

`pestat [-u username]`

lists the node utilization across all nodes for a running job.
to see more options use: `pestat -h`

Example:

```
pestat -u $USER
```

```
Hostname      Partition    Node  Num_CPU  CPUload  Memsize  Freemem  Joblist
                           State Use/Tot            (MB)     (MB)   JobId User ...
tnxt-0703         xlong    alloc  28   28   16.23*   57344    55506  565849 someuser
tnxt-0704         xlong    alloc  28   28   19.60*   57344    53408  565849 someuser
tnxt-0705         xlong    alloc  28   28   19.56*   57344    53408  565849 someuser
```

Low CPU load utilization highlighted in **Red**
(Freemem should also be noted)

```
pestat -u $USER
```

```
Hostname      Partition    Node  Num_CPU  CPUload  Memsize  Freemem  Joblist
                           State Use/Tot            (MB)     (MB)   JobId User ...
tnxt-0703         xlong    alloc  28   28   27.54    57344    55506  565849 someuser
tnxt-0704         xlong    alloc  28   28   27.50    57344    53408  565849 someuser
tnxt-0705         xlong    alloc  28   28   26.47*   57344    53408  565849 someuser
```

Good CPU load utilization highlighted in **Purple**
Ideal CPU load utilization displayed in White

Other Type of Jobs

- MPI and OpenMP
- Visualization:
  - portal.hprc.tamu.edu Interactive Apps > choose a visual application
- Large number of concurrent single core jobs
  - Check out ***tamulauncher***
    - hprc.tamu.edu/wiki/SW:tamulauncher
    - Useful for running many single core commands concurrently across multiple nodes within a job
    - Can be used with serial or multi-threaded programs
    - Distributes a set of commands from an input file to run on the cores assigned to a job
    - Can only be used in batch jobs
    - If a tamulauncher job gets killed, you can resubmit the same job to complete the unfinished commands in the input file

Need Help?

- Try these:
  - First check the FAQ hprc.tamu.edu/wiki/HPRC:CommonProblems
  - Also try the Terra User Guide hprc.tamu.edu/wiki/Terra
  - Email your questions to **help@hprc.tamu.edu**. (Managed by a ticketing system)
- Help us, help you -- we need more info
  - Which Cluster
  - UserID/NetID (*UIN is not needed!*)
  - Job id(s) if any
  - Location of your jobfile, input/output files
  - Application used if any
  - Module(s) loaded if any
  - Error messages
  - Steps you have taken, so we can reproduce the problem
- Or visit us @ 114A Henderson Hall (Making an appointment is recommended.)

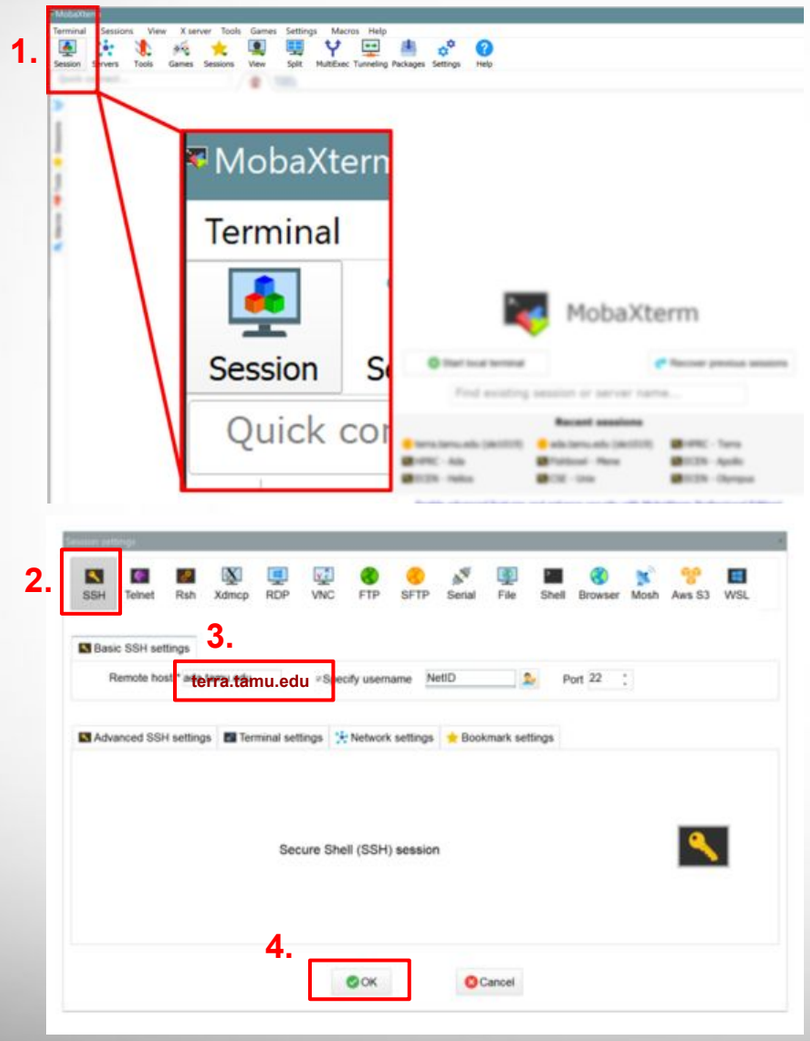
Thank you.

Questions?

Backups

MobaXterm with Duo

- Use “Session” icon



or

- Use local terminal (command line)

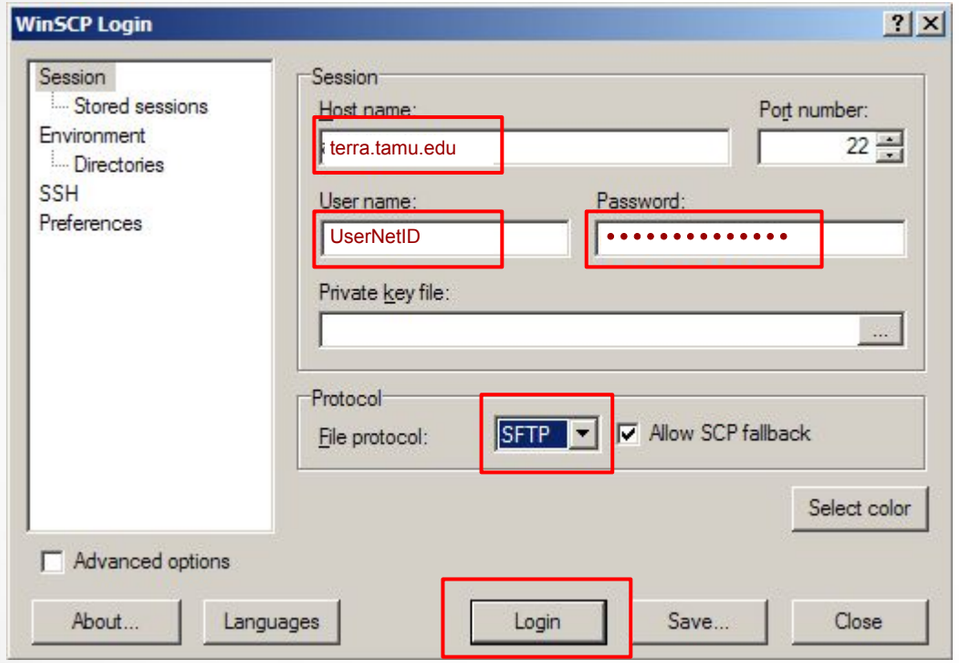
Connect to Terra from local terminal

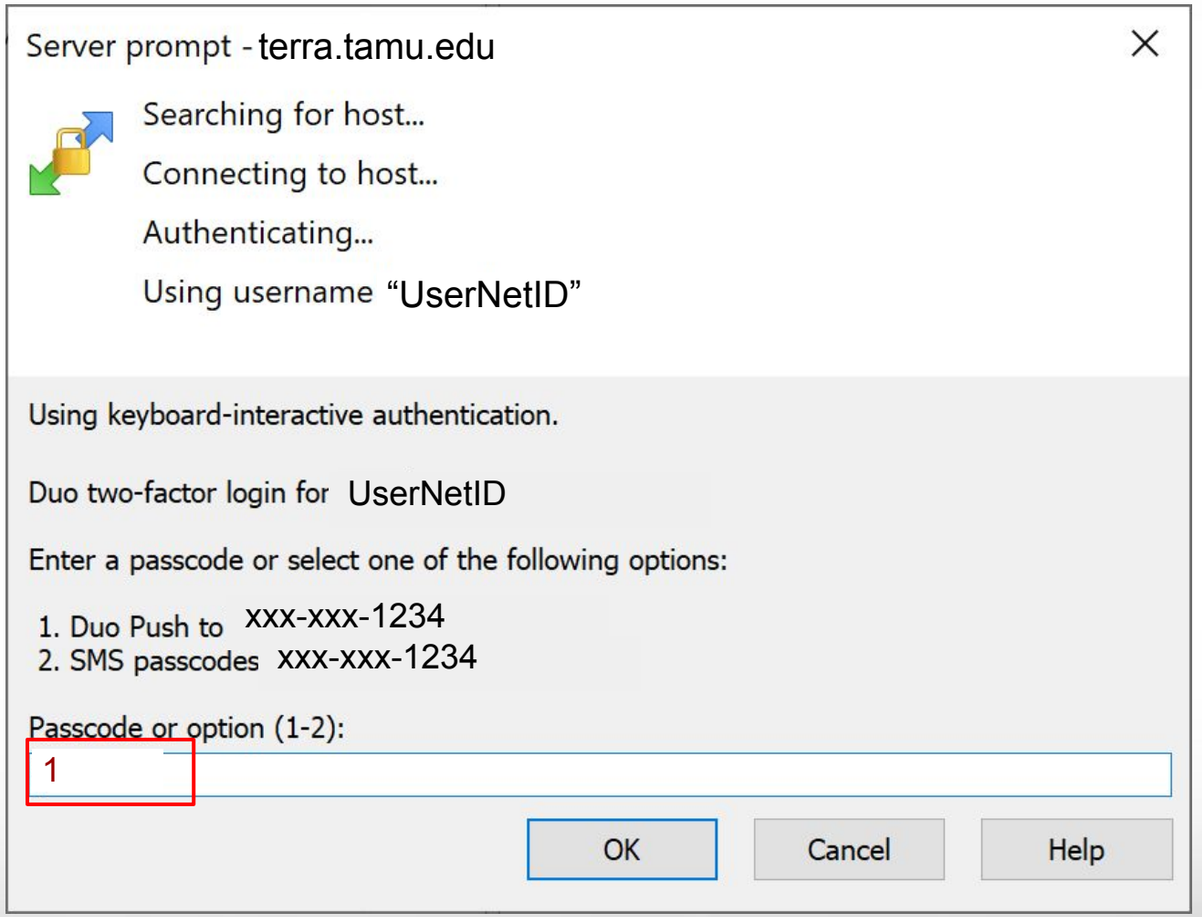
```
$ ssh UserNetID@terra.tamu.edu
************************************************************
…. warning message (snipped) …….
************************************************************

UserNetID@terra.tamu.edu's password:
UserNetID@terra.tamu.edu's password:
UserNetID@terra.tamu.edu's password:
Password:
Duo two-factor login for UserNetID

Enter a passcode or select one of the following options:

 1. Duo Push to XXX-XXX-1234
 2. Phone call to XXX-XXX-1234
 3. SMS passcodes to XXX-XXX-1234 (next code starts with: 9)

Passcode or option (1-3): 1
Success. Logging you in...
```

1. Press “Enter” key 3 times
2. Enter your password
3. Enter Duo option

hprc.tamu.edu/wiki/Two_Factor#MobaXterm

WinSCP with Duo





hprc.tamu.edu/wiki/Two_Factor#WinSCP_.28Windows_only.29

Development Environment - Toolchains

- Intel toolchain (eg. software stack) is recommended
  - Intel C/C++/Fortran compilers (icc, icpc, ifort)
  - Intel Math Kernel Library
  - Intel MPI library
- For packages that require MPI but not MKL or BLAS/FFTW/LAPACK
  - iimpi/2018b iompi/2018b gompi/2018b
- Toolchains that contain MPI, MKL, and BLAS/FFTW/LAPACK
  - intel/2018b iomkl/2018b foss/2018b
- To load/use the current recommended Intel toolchain module

```
module load intel/2018b
```

- If you do not want to use GCC version in the intel/2018b toolchain, find available gcc versions for applications which must use gcc/g++

```
module spider GCC
```

hprc.tamu.edu/wiki/SW:Toolchains
hprc.tamu.edu/wiki/Ada:Compile:All#Getting_Started
hprc.tamu.edu/wiki/Terra:Compile:All#Getting_Started

The GCCcore Toolchain

- To minimize the number of software builds, the GCCcore-7.3.0 toolchain modules can be loaded alone or with any one of the following 2018b toolchains
  - `intel/2018b`
  - `iomkl/2018b`
  - `foss/2018b`
- Example of loading a GCCcore-7.3.0 module with a 2018b module

```
module load Bowtie2/2.3.4.3-intel-2018b
module load BCFtools/1.9-GCCcore-7.3.0
```

- See a short table of compatible toolchains

```
toolchains
```

hprc.tamu.edu/wiki/SW:Toolchains

Python-version-bare modules

- You need to load a non '-bare' Python version along with the -bare module
  - If you do not, then the older default OS Python version will be used
- Used in conjunction with GCCcore-6.3.0 builds in order to reduce the number of software modules built.

`intel/2017A` `iomkl/2017A` `foss/2017A`

Three different examples of loading GCCcore-6.3.0-Python-bare and a Python module with a 2017A toolchain

1.
```
module load Cython/0.25.2-GCCcore-6.3.0-Python-2.7.12-bare
module load Python/2.7.12-foss-2017A
```

2.
```
module load Cython/0.25.2-GCCcore-6.3.0-Python-2.7.12-bare
module load Python/2.7.12-iomkl-2017A
```

3.
```
module load Cython/0.25.2-GCCcore-6.3.0-Python-2.7.12-bare
module load HISAT2/2.1.0-intel-2017A-Python-2.7.12
```

Loads Python indirectly