Introduction to Using the HPRC Clusters

Ada & Terra

HIGH PERFORMANCE RESEARCH COMPUTING
TEXAS A&M UNIVERSITY

Fall 2019

Outline

- Usage Policies
- Hardware Overview of Ada and Terra
- Accessing Ada and Terra
- File Transfers
- File systems and User Directories
- Computing Environment
  - short break
- Development Environment
- Batch Processing
- Common Problems
- 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 Ada 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

Introduction

- Prerequisites:
  - Basic knowledge of UNIX commands
  - Slides from our UNIX short course are at:

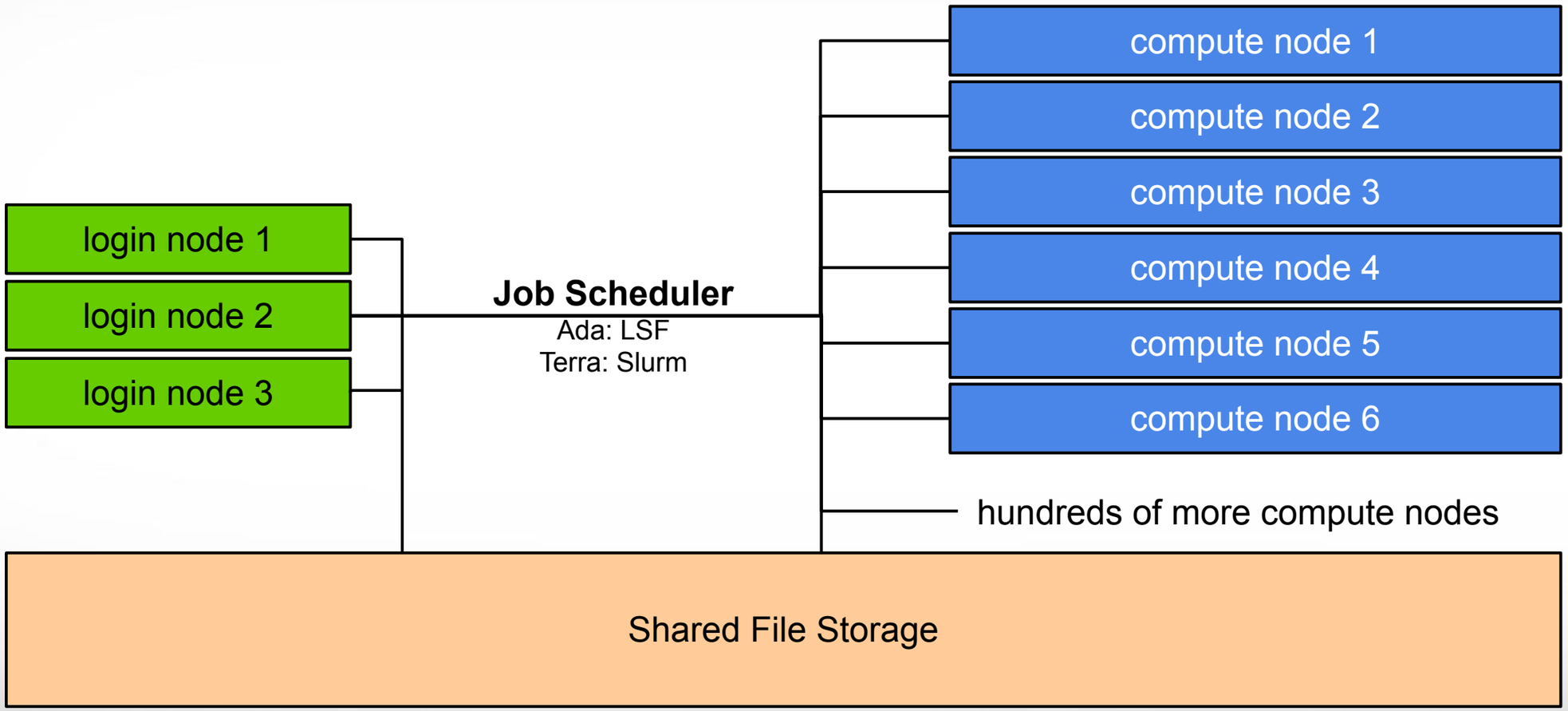
    hprc.tamu.edu/training/intro_linux.html
- Examples:
  - For **Ada**:
    - Available in /scratch/training/Intro-to-ada directory
    - Copy these files to your scratch directory
      - `cp -r /scratch/training/Intro-to-ada/batch_examples/ $SCRATCH`
  - For **Terra**:
    - Available in /scratch/training/Intro-to-terra directory
    - Copy these files to your scratch directory
      - `cp -r /scratch/training/Intro-to-terra/batch_examples/ $SCRATCH`

Laptops/Workstations vs HPC Clusters

	Laptops / Workstations	HPC Clusters
CPU Clock Rate	1.2 ~ 4 GHz	2.4 GHz
CPU Core Counts	4 ~ 12	20 ~ 40 / node
Memory Size	up to 10s GB	64GB ~ 2 TB / node
Node Counts	1 or a few	300 ~ 900
Storage Size	usually up to a few TB	a few PB (1 PB= 1000 TB)
Network or Interconnect Speed	usually <= 1 Gbps	40 ~ 100 Gbps
User Interface	GUI and Text	mostly Text; some GUI
Running jobs	Exclusive	Batch processing

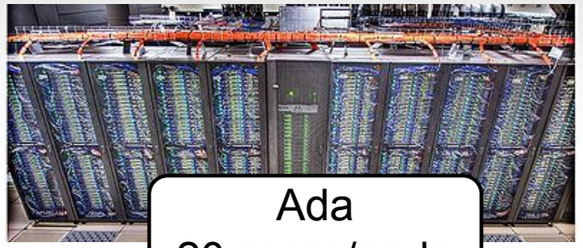
- When HPC clusters are more suitable
  - Problems are too big to fit in one laptop or workstation, due to limitation on memory, core count, or node count
  - Problems scale well with more CPU cores or memory
  - Single threaded problems with millions of permutations
  - Problems require large high speed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

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
Ada: LSF
Terra: Slurm
hundreds of more compute nodes
Shared File Storage

HPRC Clusters

Terra
28 cores/node



Ada
20 cores/node

Curie
16 cores/node

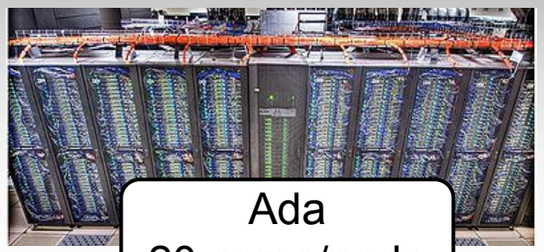
Nodes	307	864	72
Cores	8,512	17,596	1,152
CPU Architecture	*x86_64* Intel 14-core 2.4GHz *Broadwell*	*x86_64* Intel 10-core 2.5 GHz *IvyBridge*	*ppc64* IBM 8-core 4.2 GHz *Power7+*
Interconnect	Onmi-Path	FDR-10 Infiniband	10 Gbps Ethernet
Accelerator	48 nodes with Tesla K80	30 nodes with 2 Tesla K20 9 nodes with 2 *Phi* coprocessors 4 nodes with 2 Nvidia V100	N/A
Job Scheduler	Slurm	LSF	LSF (shared with Ada)
File System	GPFS; 3 PB raw	GPFS; 4 PB raw	GPFS (shared with Ada)
Production Date	Spring 2017	Sep 2014	May 2015

hprc.tamu.edu/resources

No SU charged on Curie

HPRC Clusters

Terra
28 cores/node



Ada
20 cores/node

Curie
16 cores/node

Login Nodes	3	8	2
64 GB memory compute nodes	256	792	-
PHI 64 GB memory compute nodes	-	9	-
KNL (Knights Landing) (no SUs charged)	16	-	-
K20 GPU 64 GB memory compute nodes	-	10	-
K80 GPU 128 GB memory compute nodes	48	-	-
K20 GPU 256 GB memory compute nodes	-	20	-
V100 192 GB memory compute nodes	-	4 (24 cores/node)	-
256 GB memory compute nodes	-	6	70
1 TB memory compute nodes	-	11 (40 cores/node)	-
2 TB memory compute nodes	-	4 (40 cores/node)	-

hprc.tamu.edu/resources

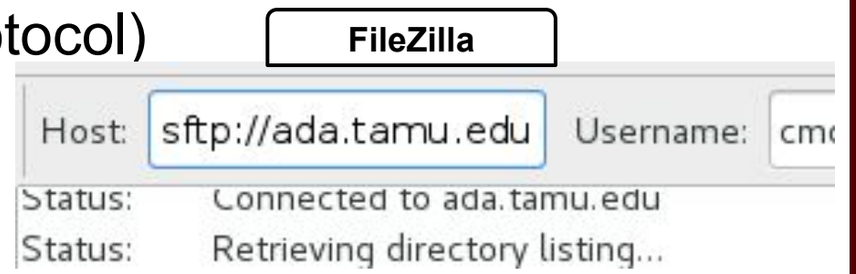
Accessing Ada and Terra

- SSH command is required for accessing Ada / Terra:
  - On campus: **`ssh NetID@ada.tamu.edu`** or **`ssh NetID@terra.tamu.edu`**
  - Off campus:
    - Set up and start VPN (Virtual Private Network): u.tamu.edu/VPnetwork
    - Then: **`ssh NetID@ada.tamu.edu`** or **`ssh NetID@terra.tamu.edu`**
- SSH programs for Windows:
  - MobaXTerm (preferred, includes SSH and X11)
  - PuTTY SSH
- Access through portal.hprc.tamu.edu (Menu “Clusters” => “Ada Shell Access”)
- Ada has 8 login nodes. Terra has 3 login nodes Check the bash prompt.
  - **`[NetID@ada1 ~]$`** **`[NetID@terra3 ~]$`**
- Login sessions that are idle for **60** minutes will be closed automatically
- Processes run longer than **60** minutes on login nodes will be killed automatically.
- **Do not use more than 8 cores on the login nodes!**
- **Do not use the sudo command.** Contact us for assistance installing software.

hprc.tamu.edu/wiki/HPRC:Access

File Transfers with **Ada** and **Terra**

- Simple File Transfers:
  - scp: command line (Linux, Mac)
  - rsync: command line (Linux, Mac); ***can resume transfer***
  - MobaXterm: GUI (Windows)
  - WinSCP: GUI (Windows)
  - FileZilla: GUI (Linux, Mac, Windows) (use sftp protocol)
  - Portal: portal.hprc.tamu.edu (through "Files" menu)



- Bulk data transfers:
  - Use fast transfer nodes
    - data transfer processes will not timeout at 60 minutes
    - on **Ada**: `ada-ftn1.tamu.edu` OR `ada-ftn2.tamu.edu`
    - on **Terra**: `terra-ftn.hprc.tamu.edu`
    - Globus Connect (hprc.tamu.edu/wiki/SW:GlobusConnect)
    - GridFTP

hprc.tamu.edu/wiki/HPRC:FileTransfers

File Systems and User Directories

Directory	Environment Variable	Space Limit	File Limit	Intended Use
/home/$USER	$HOME	10 GB	10,000	Small to modest amounts of processing.
/scratch/user/$USER	$SCRATCH	1 TB	50,000	Temporary storage of large files for on-going computations. Not intended to be a long-term storage area.
/tiered/user/$USER	$ARCHIVE	10 TB	50,000	Intended to hold valuable data files that are not frequently used **(on Ada/Curie only)**

- **`$HOME`** and **`$SCRATCH`** directories are not shared between Ada and Terra clusters.
- View usage and quota limits using the command: **`showquota`**
- Quota and file limit increases will only be considered for scratch and tiered directories
- Request a group directory for sharing files.
- Do not share your home, scratch, tiered directories.

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

Software

- See the Software wiki page for instructions and examples
  - hprc.tamu.edu/wiki/SW
  - hprc.tamu.edu/software/ada
  - hprc.tamu.edu/software/terra
  - hprc.tamu.edu/wiki/Bioinformatics
- 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

- Paths:
  - $PATH: for commands (eg. /bin:/usr/bin:/usr/local/sbin:/usr/sbin:/home/netid/bin)
  - $LD_LIBRARY_PATH: for libraries
  - See your $PATH variable with the command

```
echo $PATH
```

- There is a lot of software, many versions, and many paths to manage

  ..... How do you manage all these software versions?
- The solution (lmod) which 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 [Python-version]

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

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

Application Modules

- Installed applications are available as modules which are available to all users
  - (except for restricted modules)
- It's a good habit to purge 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`**

```
module avail                    # 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 boost             # case insensitive search for modules with 'boost' in name

module keyword graphics         # search module descriptions for keyword 'graphics'
                                # some graphics modules may be missed if
                                # keyword is not found in description (case insensitive)
```

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

The Case (in)sensitive spider command

The following commands will give you different results on **Ada** because the `module spider` command is not case sensitive unless it finds an exact match for the search term

```
module spider python
```

```
module spider Python
```

module spider python

---

python:

Description:
Python is a programming language that lets you work more quickly and integrate your systems more effectively. - Homepage: http://python.org/

Versions:
python/2.7.6-generic
python/2.7.6-ictce-7.1.2
python/2.7.10-intel-2015B.badSSL
python/2.7.10-intel-2015B
python/2.7.13-generic

Other possible modules matches:
Biopython IPython MySQL-python NGS-Python **Python** ScientificPython bx-python findpython myPython netcdf4-python ...

look for other possible modules

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

Module Loading Exercise

1. `module spider trinity` # search for available module names matching trinity
   # not case sensitive unless an exact match is found
2. `module load Trinity/2.5.1-GCCcore-6.3.0-Perl-5.24.0` # load specific module version
   # type Trinity/2.5 then hit tab key
3. `module list` # list all loaded modules
4. `module spider Bowtie2` # see which versions of Bowtie2 are available
5. `module swap Bowtie2 Bowtie2/2.3.4-GCCcore-6.3.0` # change the version of a loaded module
6. `module list` # list all loaded modules
7. `module purge` # remove all loaded modules

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/2017A iompi/2017A gompi/2017A
- Toolchains that contain MPI, MKL, and BLAS/FFTW/LAPACK
  - intel/2017A iomkl/2017A foss/2017A
- To load/use the current recommended Intel toolchain module

```
module load intel/2017A
```

- If you do not want to use GCC version in the intel/2017A 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

Modules and Toolchains

- Load modules with the same toolchains in your job scripts
- The **`2017A`** and **`GCCcore-6.3.0`** toolchain versions are recommended
    - `intel/2017A`
    - `iomkl/2017A`
    - `foss/2017A`
    - `GCCcore/6.3.0`
- Avoid loading modules in your .bashrc and .bash_profile files
- Avoid mixing toolchains if loading multiple modules in the same job script

```
module load HISAT2/2.0.4-foss-2016b
module load TopHat/2.1.1-intel-2017A-Python-2.7.12
module load Cufflinks/2.2.1-intel-2015B
```

- Same rule applies to compilers and libraries.

The GCCcore Toolchain

- To minimize the number of software builds, the GCCcore-6.3.0 toolchain modules can be loaded alone or with any one of the following 2017A toolchains
  - `intel/2017A`
  - `iomkl/2017A`
  - `foss/2017A`
- Example of loading a GCCcore-6.3.0 module with a 2017A module

```
module load Bowtie2/2.3.3.1-GCCcore-6.3.0
module load TopHat/2.1.1-intel-2017A-Python-2.7.12
```

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

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

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

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  |
--------------------------------------------------------------------------------
```

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

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

A Service Unit (SU) on **Ada** is equivalent to one core or **2500** MB memory usage for one hour.

	Number of Cores	MB of memory per core	Total Memory (GB)	Hours	SUs charged
1.	1	2500	2.5	1	1
2.	1	2600	2.6	1	2
3.	1	50000	50	1	20
4.	20	2500	50	1	20

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

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.	1	2	2	1	1
2.	1	3	3	1	2
3.	1	56	56	1	28
4.	28	2	56	1	28

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

Batch Computing on HPRC Clusters

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

On-campus:

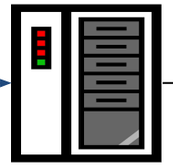
Campus Network

VPN

Internet

Off-campus:

SSH



Login nodes

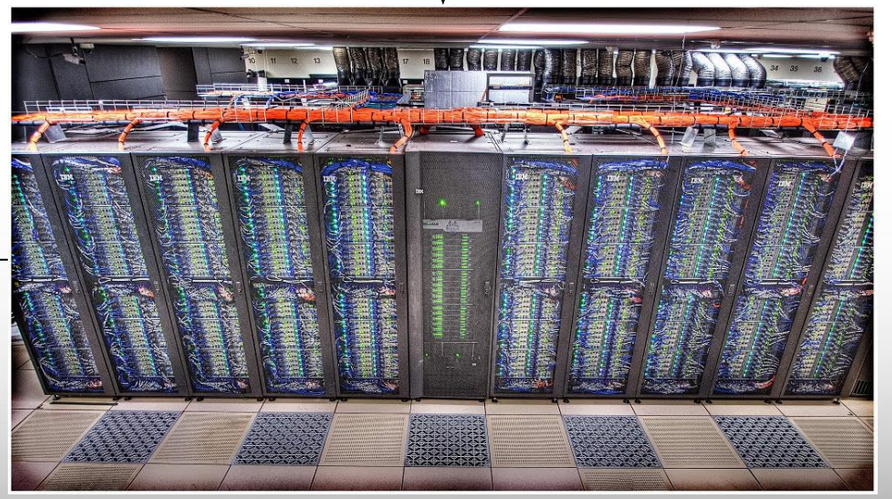
Create job

Job script file

Submit job

Batch manager:
LSF on Ada
Slurm on Terra

Queue



Cluster compute nodes

Output Files

Historical HPRC Cluster Usage

hprc.tamu.edu

Cluster Status

Terra

Nodes	228/315 (72%)
Cores	5889/9408 (63%)
Jobs	311R-1Q

Ada

Nodes	692/823 (84%)
Cores	12070/16740 (72%)
Jobs	318R-77Q

Curie

Nodes	41/57 (72%)
Cores	656/911 (72%)
Jobs	41R-5Q

Historical Status

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:
  - On **Ada**, if the 1TB or 2TB nodes are needed, use the xlarge queue
    ```
    #BSUB -q xlarge
    ```
  - Jobs that have special resource requirements are scheduled in the special queue (must request access to use this queue)
- Batch queue policies are used to manage the workload and may be adjusted periodically.

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

bqueues : Current Queues on **Ada**

```
[ user_netid@ada1 ~]$ bqueues
QUEUE_NAME      PRIO STATUS          MAX JL/U JL/P JL/H NJOBS  PEND   RUN  SUSP
staff            450  Open:Active       -    -    -    -     0     0     0     0
special          400  Open:Active       -    -    -    -  2080     0  2080     0
xlarge           100  Open:Active       -    -    -    -    80     0    80     0
vnc               90  Open:Active       -    -    -    -     2     0     2     0
sn_short          80  Open:Active       -    -    -    -     0     0     0     0
mn_short          80  Open:Active    2000    -    -    -     0     0     0     0
mn_large          80  Open:Active    8000    -    -    -  2500   720  1780     0
v100              80  Open:Active       -    -    -    -     0     0     0     0
general           50  Closed:Inact      0    -    -    -     0     0     0     0
sn_regular        50  Open:Active       -    -    -    -   846    31   815     0
sn_long           50  Open:Active       -    -    -    -   897     0   897     0
sn_xlong          50  Open:Active       -    -    -    -  2466    60  2406     0
mn_small          50  Open:Active    7000    -    -    -  3550    30  3520     0
mn_medium         50  Open:Active    6000    -    -    -  3784     0  3784     0
curie_devel       40  Open:Active       -    -    -    -     0     0     0     0
curie_medium      35  Open:Active       -    -    -    -     0     0     0     0
curie_long        30  Open:Active       -    -    -    -   765   301   464     0
curie_general     25  Closed:Inact      0    -    -    -     0     0     0     0
low_priority       1  Open:Active    2500  500    -    -     0     0     0     0
```

hprc.tamu.edu/wiki/Ada:Batch_Queues

Queue Limits on **Ada**

Queue	Min/Default/ Max Cores	Default/Max Walltime	Compute Node Types	Pre-Queue Limits	Aggregate Limits Across Queues	Per-User Limits Across Queues	Notes
sn_short	1 / 1 / 20	10 min / **1 hr**	64 GB nodes (811) 256 GB nodes (26)		Maximum of **7000** cores for all running jobs in the single-node (sn_*) queues.	Maximum of **1000 cores and 100 jobs per user** for all running jobs in the single node (sn_*) queues.	For jobs needing **only one compute node**.
sn_regular		1 hr / **1 day**					
sn_long		24 hr / **4 days**					
sn_xlong		4 days / **30 days**					
mn_short	2 / 2 / 200	10 min / **1 hr**		Maximum of **2000** cores for all running jobs in this queue.	Maximum of **12000** cores for all running jobs in the multi-node (mn_*) queues.	Maximum of **3000 cores and 150 jobs per user** for all running jobs in the multi-node (mn_*) queues.	For jobs needing **more than one compute node**.
mn_small	2 / 2 / 120	1 hr / **10 days**		Maximum of **7000** cores for all running jobs in this queue.			
mn_medium	121 / 121 / 600	1 hr / **7 days**		Maximum of **6000** cores for all running jobs in this queue.			
mn_large	600 / 601 / 2000	1 hr / **5 days**		Maximum of **8000** cores for all running jobs in this queue.			
xlarge	1 / 1 / 280	1 hr / **10 days**	1 TB nodes (11) 2 TB nodes (4)				For jobs needing **more than 256GB of memory per compute node**.
vnc	1 / 1 / 20	1 hr / **6 hr**	GPU nodes (30)				For remote visualization jobs.
special	None	1 hr / **7 days**	64 GB nodes (811) 256 GB nodes (26)				Requires permission to access this queue.
v100	1 / 1 / 96	1 hr / **2 days**	192 GB nodes dual 32 GB v100 (4)				

Run ***"blimits -w"*** to show how policies are applied to users and queues.

hprc.tamu.edu/wiki/Ada:Batch_Queues

sinfo : Current Queues on **Terra**

```
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**

Queue Limits on Terra

Queue	Job Max Cores / Nodes	Job Max Walltime	Compute Node Types	Per-User Limits Across Queues	Notes
short	448 cores / 16 nodes	2 hrs	64 GB nodes (256) 128 GB nodes with GPUs (36)	1800 cores per user	
medium	1792 cores / 64 nodes	1 day			
long	896 cores / 32 nodes	7 days			
xlong	448 cores / 16 nodes	21 days	64 GB nodes (256)	448 cores per user	--partition xlong
gpu	1344 cores / 48 nodes	2 days	128 GB nodes with GPUs (48)		For jobs requiring GPUs.
vnc	28 cores / 1 node	12 hours	128 GB nodes with GPUs (48)		For remote visualization jobs
knl	68 cores / 8 nodes 72 cores / 8 nodes	7 days	96 GB nodes with KNL processors (16)		For jobs requiring a KNL processor

Batch Job Scripts

Sample Job Script Structure (Ada)

```
##NECESSARY JOB SPECIFICATIONS
#BSUB -L /bin/bash
#BSUB -J ExampleJob
#BSUB -W 24:00
#BSUB -n 1
#BSUB -R "span[ptile=1]"
#BSUB -R "rusage[mem=2500]"
#BSUB -M 2500
#BSUB -o stdout.%J
#BSUB -e stderr.%J

##OPTIONAL JOB SPECIFICATIONS
#BSUB -P 123456
#BSUB -u email_address
#BSUB -B -N

# load required module(s)
module load Python/3.5.2-intel-2017A

./my_program.py
```

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

Ada	Terra	Comment
`#BSUB -L /bin/bash`	`#SBATCH --export=NONE` `#SBATCH --get-user-env=L`	Initialize job environment.

`#BSUB -W HH:MM`
`or`
`#BSUB -W MM`
	`#SBATCH --time=HH:MM:SS`	Specifies the time limit for the job.
		Must specify seconds SS on Terra

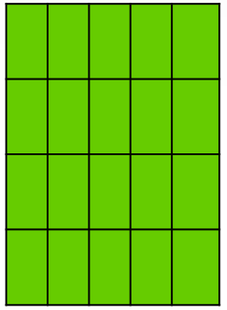
`#BSUB -n NNN`	`#SBATCH --ntasks=NNN`	Total number of tasks (cores) for the job.
`#BSUB -R "span[ptile=XX]"`	`#SBATCH --ntasks-per-node=XX`	Specifies the maximum number of tasks (cores) to allocate per node

`#BSUB -R "rusage[mem=nnnn]"`
`#BSUB -M nnnn`
`(memory per CORE)`
	`#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 **Ada**

A.

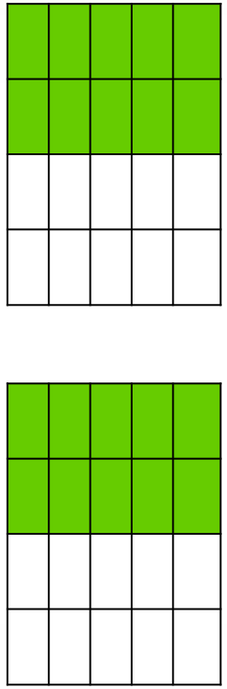


20 cores on
1 compute node

```
#BSUB -n 20
#BSUB -R “span[ptile=20]
```

Preferred Mapping
(if applicable)

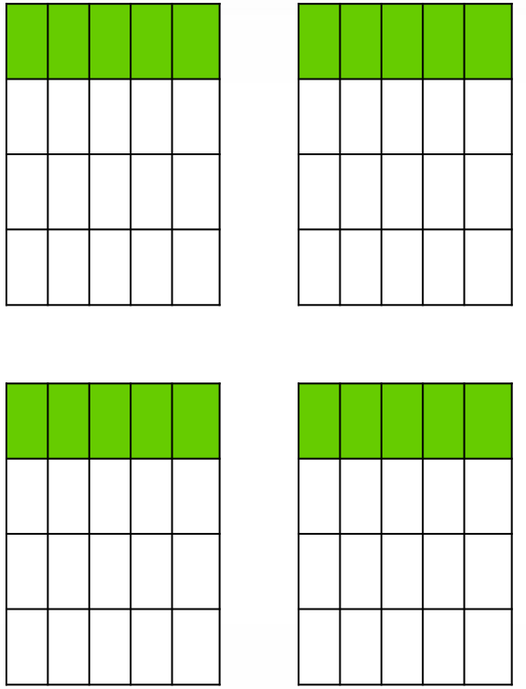
B.



20 cores on
2 compute nodes

```
#BSUB -n 20
#BSUB -R “span[ptile=10]
```

C.

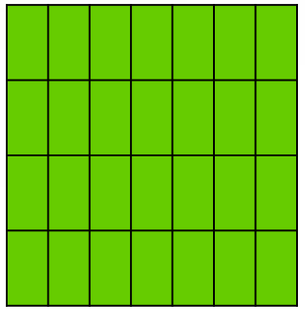


20 cores on
4 compute nodes

```
#BSUB -n 20
#BSUB -R “span[ptile=5]
```

Mapping Jobs to Cores per Node on Terra

A.

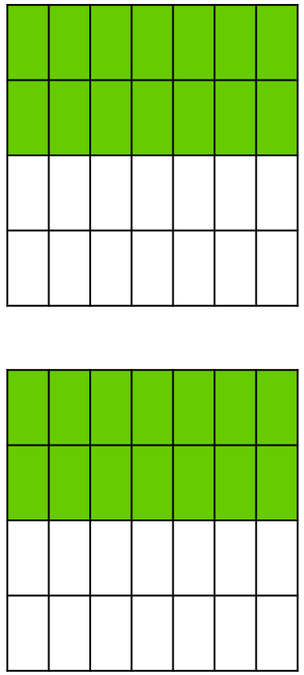


28 cores on
1 compute node

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

Preferred Mapping
(if applicable)

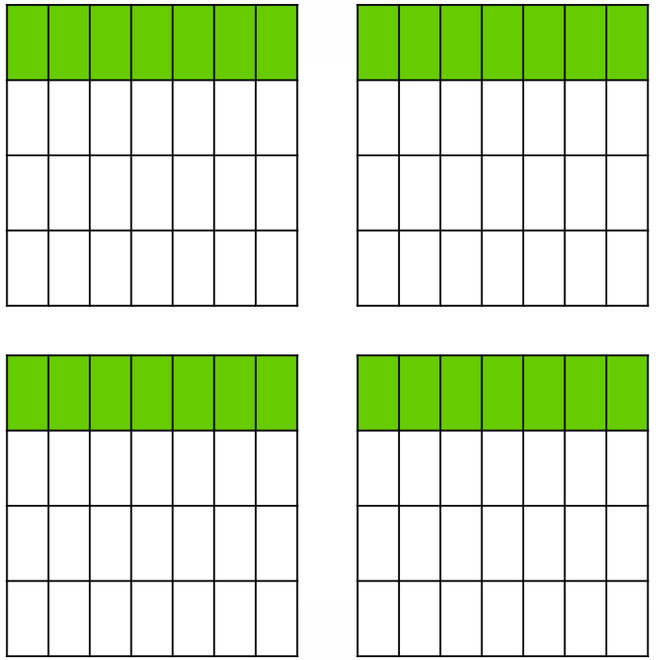
B.



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 **Ada**

- Must specify both parameters for requesting memory:

  #BSUB -R "rusage[mem=process_alloc_size]"

  #BSUB -M process_size_limit
- Default value of 2500 MB (2.5 GB) per job slot if -R/-M not specified, but it might cause memory contention when sharing a node with other jobs.
- On 64GB nodes, usable memory is at most **54 GB** (where 10 GB is used by the system).
  - The per-process memory limit should not exceed **2700 MB** for a 20-core job.
- If more memory is needed, request the large memory nodes:
  - If under 256 GB and up to 20 cores per node use:
    - **#BSUB -R "select[mem256gb]"**
  - If you need up to 1 or 2 TB of memory and up to 40 cores:
    - use the **-q xlarge** option with either **-R "select[mem1tb]"** or **-R "select[mem2tb]"**
    - The mem1tb and mem2tb nodes are accessible only via the *xlarge* queue.

Ada: Software for Large Memory Nodes

- The large memory nodes (1TB and 2TB) on Ada have their own separate modules
- To see the list of available large memory node modules use the following commands:

```
module load Westmere
module avail
```

- Look in the Westmere section:

```
--------------------------- /software/easybuild/Westmere/modules/all ------------------------------------
   ABINIT/8.0.8-intel-2016a                                      Tcl/8.6.3-foss-2015a
   ABySS/1.9.0-foss-2016a                                        Tcl/8.6.3-intel-2015B
   ABySS/1.9.0-intel-2015B-Python-2.7.10                  (D)    Tcl/8.6.4-foss-2016a
```

- Or type **module spider tool_name/version** to see if Westmere needs to be loaded

```
module spider Canu/1.7-intel-2017A-Perl-5.24.0
```

```
    You will need to load all module(s) on any one of the lines below before the
    "Canu/1.7-intel-2017A-Perl-5.24.0" module is available to load.

    Westmere/0.devel
    Westmere/1
```

- You can just load Westmere along with the other module(s)

```
module load Westmere
module load Canu/1.7-intel-2017A-Perl-5.24.0
```

Sample Job Script for 1TB Node on Ada

```
##NECESSARY JOB SPECIFICATIONS
#BSUB -L /bin/bash                    # Uses bash to initialize the job's execution environment.
#BSUB -J my_job_script                # Set the job name to "my_job_script"
#BSUB -W 24:00                        # Set the wall clock limit to 24hr
#BSUB -q xlarge                       # Request xlarge queue
#BSUB -R "select[mem1tb]"             # Request 1TB memory node
#BSUB -n 40                           # Request 40 core
#BSUB -R "span[ptile=40]"             # Request 40 core per node.
#BSUB -R "rusage[mem=24500]"          # Request 24500MB (24.5GB) per process (CPU) for the job
#BSUB -M 24500                        # Set the per process enforceable memory limit to 24500MB.
#BSUB -o stdout.%J                    # Send stdout to "stdout.[jobID]"
#BSUB -e stderr.%J                    # Send stderr to "stderr.[jobID]"
#BSUB -u email_address                # (optional) Send all emails to email_address
#BSUB -B -N                           # (optional) Send email on job begin (-B) and end (-N)

# load required module(s) for use on the large memory nodes
module load Westmere
module load Canu/1.7-intel-2017A-Perl-5.24.0

# run your commands
canu -assemble *fastq
```

Job Memory Requests on **Terra**

- Specify memory request based on memory per node:

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

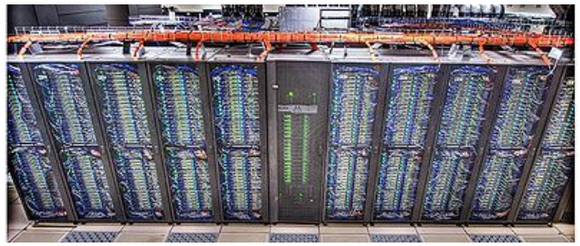
  or

  #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.

Pop Quiz

Pop Quiz



Which one of the following is not an HPRC cluster?

A. Ada
B. Bozo
C. Curie
D. Terra

Ada Pop Quiz

```
#BSUB -L /bin/bash
#BSUB -J stacks_S2
#BSUB -n 10
#BSUB -R "span[ptile=10]"
#BSUB -R "rusage[mem=2500]"
#BSUB -M 2500
#BSUB -W 36:00
#BSUB -o stdout.%J
#BSUB -e stderr.%J
```

How much total memory is requested for this job?

A. 2.5 GB
B. 2500 MB
C. 25 GB
D. 250 GB

Terra Pop Quiz

```
#SBATCH --export=NONE
#SBATCH --get-user-env=L
#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
```

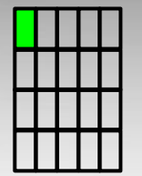
How many nodes is this job requesting?

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

Example Batch Job Scripts

hprc.tamu.edu/wiki/Ada:Batch_Processing_LSF#Job_File_Examples

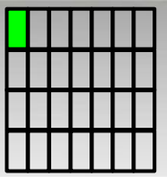
Ada Job File (Serial Example)



```
##NECESSARY JOB SPECIFICATIONS
#BSUB -L /bin/bash                    # Uses bash to initialize the job's execution environment.
#BSUB -J ExampleJob1                  # Set the job name to "ExampleJob1"
#BSUB -W 2:00                         # Set the wall clock limit to 2hr
#BSUB -n 1                            # Request 1 core
#BSUB -R "span[ptile=1]"              # Request 1 core per node.
#BSUB -R "rusage[mem=2500]"           # Request 2500MB per process (CPU) for the job
#BSUB -M 2500                         # Set the per process enforceable memory limit to 2500MB.
#BSUB -o stdout.%J                    # Send stdout to "stdout.[jobID]"
#BSUB -e stderr.%J                    # Send stderr to "stderr.[jobID]"

##OPTIONAL JOB SPECIFICATIONS
#BSUB -P 123456                       # Set billing account to 123456
#BSUB -u email_address                # Send all emails to email_address
#BSUB -B -N                           # Send email on job begin (-B) and end (-N)

# load required module(s)
module load Python/3.5.2-intel-2017A

# run your program
my_program.py
```

SUs = 2

Terra Job File (Serial Example)



```
#!/bin/bash
##ENVIRONMENT SETTINGS; CHANGE WITH CAUTION
#SBATCH --export=NONE                # Do not propagate environment
#SBATCH --get-user-env=L             # Replicate login environment

##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 (core)
#SBATCH --mem=2G                     # Request 2GB per node
#SBATCH --output=stdout.%j           # Send stdout and stderr to "stdout.[jobID]"

##OPTIONAL JOB SPECIFICATIONS
#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

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

# run your program
myprogram
```

SUs = 1.5

Submitting Your Job and Check Job Status

Submit job

```
cd $SCRATCH/Spring
```

Ada:

```
bsub < example01.job
```

```
Verifying job submission parameters...
Verifying project account...
     Account to charge:   082792010838
         Balance (SUs):      4871.5983
         SUs to charge:         0.0333
Job <2470599> is submitted to default queue <sn_short>.
```

Terra:

```
sbatch example01.job
```

```
Submitted batch job 161997
(from job_submit) your job is charged as below
                  Project Account: 122792016265
                  Account Balance: 1687.066160
                  Requested SUs:   3
```

Check status

(dash lower case `l` as in *list*)

Ada:

```
bjobs
```

```
JOBID   STAT USER        QUEUE     JOB_NAME  NEXEC_HOST SLOTS RUN_TIME     TIME_LEFT
2470599 RUN  tmarkhuang sn_short sample01  1          1     0 second(s)  0:5 L
```

Ada (more detailed):

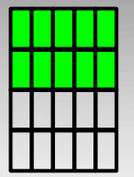
```
bjobs -l 2470599
```

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]
```

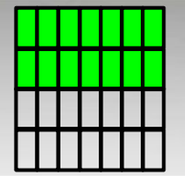
Ada Job File (multi core, single node)



```
##NECESSARY JOB SPECIFICATIONS
#BSUB -L /bin/bash                  # Use bashto initialize the job's execution environment.
#BSUB -J ExampleJob2                # Set the job name to "ExampleJob2"
#BSUB -W 6:30                       # Set the wall clock limit to 6hr and 30min
#BSUB -n 10                         # Request 10 cores total for the job
#BSUB -R "span[ptile=10]"           # Request 10 cores per node.
#BSUB -R "rusage[mem=2500]"         # Request 2500MB per process (CPU) for the job
#BSUB -M 2500                       # Set the per process enforceable memory limit to 2500MB.
#BSUB -o stdout.%J                  # Send stdout to "stdout.[jobID]"
#BSUB -e stderr.%J                  # Send stderr to "stderr.[jobID]"

##OPTIONAL JOB SPECIFICATIONS
#BSUB -P 123456           # Set billing account to 123456  #find your account with "myproject"
#BSUB -u email_address              # Send all emails to email_address
#BSUB -B -N                         # Send email on job begin (-B) and end (-N)

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

# run your program
my_multicore_program
```

SUs = 65

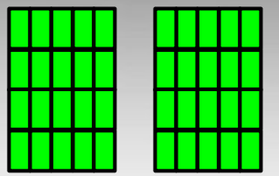
Terra Job File (multi core, single node)



```
#!/bin/bash
##ENVIRONMENT SETTINGS; CHANGE WITH CAUTION
#SBATCH --export=NONE                # Do not propagate environment
#SBATCH --get-user-env=L             # Replicate login environment

##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=14         # Request 14 tasks(cores) per node
#SBATCH --mem=28G                    # Request 28GB per node
#SBATCH --output=stdout.%j           # Send stdout to "stdout.[jobID]"
#SBATCH --error=stderr.%j            # Send stderr to "stderr.[jobID]"
##OPTIONAL JOB SPECIFICATIONS
#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 load intel/2017A

# run your program
my_multicore_program
```

SUs = 91

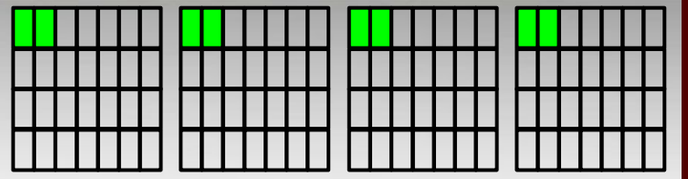
Ada Job File (multi core, multi node)



```
##NECESSARY JOB SPECIFICATIONS
#BSUB -J ExampleJob3                 # Set the job name to "ExampleJob3"
#BSUB -L /bin/bash                   # Use bash to initialize the job's execution environment.
#BSUB -W 24:00                       # Set the wall clock limit to 24hr
#BSUB -n 40                          # Request 40 cores total for the job
#BSUB -R "span[ptile=20]"            # Request 20 cores per node.
#BSUB -R "rusage[mem=2500]"          # Request 2500MB per process (CPU) for the job
#BSUB -M 2500                        # Set the per process enforceable memory limit to 2500MB.
#BSUB -o stdout.%J                   # Send stdout to "stdout.[jobID]"
#BSUB -e stderr.%J                   # Send stderr to "stderr.[jobID]"

##OPTIONAL JOB SPECIFICATIONS
#BSUB -P 123456                  # Set billing account to 123456 #find your account with " myproject"
#BSUB -u email_address           # Send all emails to email_address
#BSUB -B -N                      # Send email on job begin (-B) and end (-N)

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

# run your program
my_multicore_multinode_program
```

SUs = 960

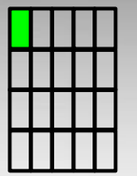
Terra Job File (multi core, multi node)



```
#!/bin/bash
##ENVIRONMENT SETTINGS; CHANGE WITH CAUTION
#SBATCH --export=NONE                # Do not propagate environment
#SBATCH --get-user-env=L             # Replicate login environment

##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=2.5G                   # Request 2.5 GB  per node
#SBATCH --output=stdout.%j           # Send stdout and stderr to "stdout.[jobID]"

##OPTIONAL JOB SPECIFICATIONS
#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 load intel/2017A

# run program with MPI
mpirun my_multicore_multinode_program
```

SUs = 288

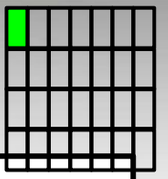
Ada Job File (serial GPU)



```
##NECESSARY JOB SPECIFICATIONS
#BSUB -J ExampleJob4           # Set the job name to "ExampleJob4"
#BSUB -L /bin/bash             # Use bash login shell to initialize the job's execution environment.
#BSUB -W 2:00                  # Set the wall clock limit to 2hr
#BSUB -n 1                     # Request 1 core total for the job
#BSUB -R "span[ptile=1]"       # Request 1 core per node.
#BSUB -R "rusage[mem=2500]"    # Request 2500MB per process (CPU) for the job
#BSUB -M 2500                  # Set the per process enforceable memory limit to 2500MB.
#BSUB -o stdout.%J             # Send stdout to "stdout.[jobID]"
#BSUB -e stderr.%J             # Send stderr to "stderr.[jobID]"

#BSUB -R "select[gpu]"         # Request a node with a GPU
##OPTIONAL JOB SPECIFICATIONS
#BSUB -P 123456                # Set billing account to 123456 #find your account with "myproject"
#BSUB -u email_address         # Send all emails to email_address
#BSUB -B -N                    # Send email on job begin (-B) and end (-N)

# load required module(s)
module load CUDA/9.2.148.1

# run your program
my_gpu_program
```

SUs = 1

Terra Job File (serial GPU)



```
#!/bin/bash
##ENVIRONMENT SETTINGS; CHANGE WITH CAUTION
#SBATCH --export=NONE                # Do not propagate environment
#SBATCH --get-user-env=L             # Replicate login environment

##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=2G                     # Request 2GB per node
#SBATCH --output=stdout.%j           # Send stdout and stderr to "stdout.[jobID]"
#SBATCH --gres=gpu:1                 # Request 1 GPU
#SBATCH --partition=gpu              # Request the GPU partition/queue

##OPTIONAL JOB SPECIFICATIONS
#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 load intel/2017A
module load CUDA/9.2.148.1

# run your program
my_gpu_program
```

SUs = 28

Other Type of Jobs

- MPI and OpenMP
- Visualization:
  - portal.hprc.tamu.edu (visualization jobs can be run on both Ada and Terra; more details in later slide)
- 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

Job Submission and Tracking

Ada	Terra	Description
`bsub < jobfile1`	`sbatch jobfile1`	Submit jobfile1 to batch system
`bjobs [-u all or user_name] [[-l] job_id]`	`squeue [-u user_name] [-j job_id]`	List jobs
`bkill job_id`	`scancel job_id`	Kill a job
`bhist [-l] job_id`	`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 [-l] -j job_id`	`lnu job_id`	Show resource usage for a job
-	`pestat -u $USER`	Show resource usage for a running job

hprc.tamu.edu/wiki/HPRC:Batch_Translation

Debug job failures

```
cd $SCRATCH/batch_examples
```

- Debug job failures using the stdout and stderr files

```
bsub < example03.python_memory.job
```

```
cat output.ex03.python_mem.2447336
```

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

Ada: `#BSUB -o output.ex03.python_mem.%J`

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

Ada:

```
TERM_MEMLIMIT: job killed after reaching LSF memory usage limit.
Exited with signal termination: Killed.

Resource usage summary:

    CPU time :                                   1.42 sec.
    Max Memory :                                 10 MB
    Average Memory :                             6.50 MB
    Total Requested Memory :                     10.00 MB
    Delta Memory :                               0.00 MB
    Max Processes :                              5
    Max Threads :                                6
```

Terra:

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

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

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
  - Ada: `#BSUB -P Account#`
  - 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

Ada:

```
$ bsub < myjob
Verifying job submission parameters...
Verifying project account...
     Account to charge:   082792010838
         Balance (SUs):       342.5322
         SUs to charge:       480.0000
         ------------------------------------------------------------------------
        |ERROR! Your project account does not have sufficient balance to submit your job! |
         ------------------------------------------------------------------------
Request aborted by esub. Job not submitted.
```

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

List Node Utilization on **Ada**: *lnu*

```
lnu [-h] [-l] -j jobid
```

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

Example with a multi-node job (4 nodes):

```
lnu -l -j 795375
```

```
Job           User                    Queue         Status Node  Cpus
795375        jomber23                medium                R    4    80
   HOST_NAME    status  r15s   r1m  r15m   ut    pg  ls    it   tmp   swp   mem  Assigned Cores
   nxt1417          ok  20.0  21.0  21.0  97%   0.0   0 94976  366M  3.7G 41.6G     20
   nxt1764 (L)      ok  19.7  20.0  20.0  95%   0.0   0 95040  366M  3.7G 41.5G     20
   nxt2111          ok  20.0  20.0  20.0  98%   0.0   0 91712  370M  4.2G 41.5G     20
   nxt2112          ok  20.0  21.1  21.0  97%   0.0   0 91712  370M  4.2G 41.6G     20
================================================================================
```

The % utilization (**ut**) in conjunction with Assigned Cores is the most useful.
Note that the **tmp**, **swp**, and **mem** refer to available amounts respectively and not usage.
See "*man lsload*" for explanations on labels.

hprc.tamu.edu/wiki/Ada:Batch_Processing_LSF#Job_Tracking

List Node Utilization on **Terra**: *lnu*

```
lnu jobid
```

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

Example:

```
lnu 565849
```

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 Note Utilization on Terra: *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

Job Environment Variables

- **Ada:**
  - **$LSB_JOBID** = job id
  - **$LS_SUBCWD** = directory where job was submitted from
  - **$SCRATCH** = /scratch/user/NetID
  - **$TMPDIR** = /work/$LSB_JOBID.tmpdir
    - $TMPDIR is local to each assigned compute node for the job and is about 750 GB
    - Use of $TMPDIR is recommended for jobs that use many small temporary files
    - Do not use $TMPDIR for software that has checkpoints to restart where it left off
- **Terra:**
  - **$SLURM_JOBID** = job id
  - **$SLURM_SUBMIT_DIR** = directory where job was submitted from
  - **$SCRATCH** = /scratch/user/NetID
  - **$TMPDIR** = /work/job.$SLURM_JOBID
    - $TMPDIR is local to each assigned compute node for the job and is about 850GB

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

Common Job Problems

- Control characters (`^M`) in job files or data files edited with Windows editor
  - remove the `^M` characters with: `dos2unix my_job_file`
- Did not load the required module(s)
- Insufficient walltime specified in `#BSUB -W` or `#SBATCH --time` parameter
- Insufficient memory specified in `#BSUB -M` and `-R "rusage[mem=xxx]"`, or `#SBATCH --mem` or `--mem-per-cpu` parameters
- No matching resource (`-R rusage[mem]` or `--mem` too large)
- Running OpenMP jobs across nodes
- Insufficient SU: See your SU balance: `myproject`
- Insufficient disk or file quotas: check quota with `showquota`
- Using GUI-based software without setting up X11 forwarding
  - Enable X11 forwarding at login `ssh -X user@ada.tamu.edu`
  - Or use VNC
- Software license availability

`license_status -a`

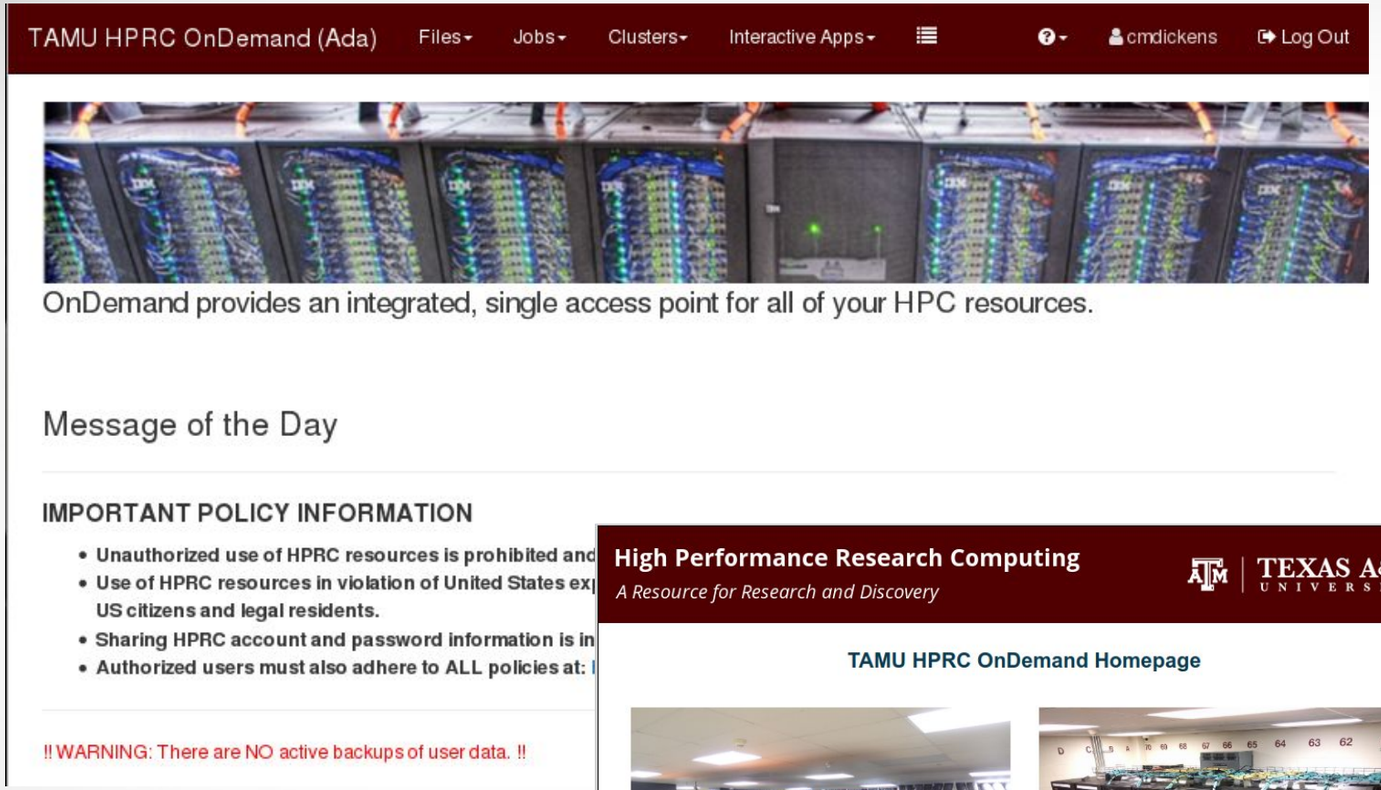
FAQ: hprc.tamu.edu/wiki/HPRC:CommonProblems

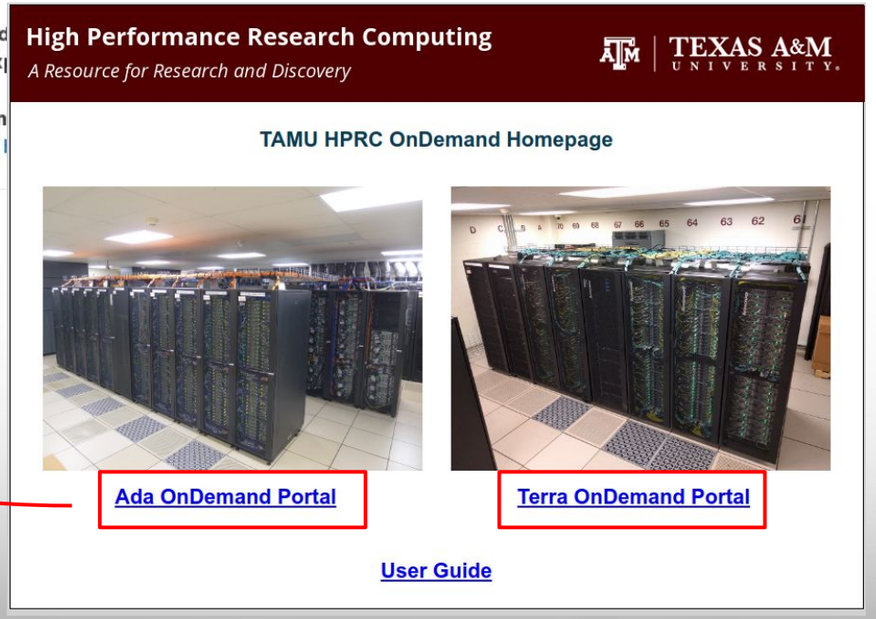
CRLF Line Terminators

Windows editors such as Notepad will add hidden Carriage Return Line Feed (CRLF) characters that will cause problems with many applications

```
cd $SCRATCH/batch_examples
file dos_text.txt                    # use file command to check
dos_text.txt: ASCII English text, with CRLF line terminators
cat -v dos_text.txt                  # use cat command to see CRLF characters
dos2unix dos_text.txt                # use dos2unix command to correct
file dos_text.txt
dos_text.txt: ASCII English text
```

portal.hprc.tamu.edu





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

The HPRC portal allows users to do the following

- Browse files on the Ada (Curie), Terra filesystem
- Access the Ada, Terra, Curie Unix command line
  - no SUs charged for using command line
  - running on login node; please limit to 8 cores
- Launch jobs
  - SUs charged when launching jobs
- Compose job scripts
- Launch interactive GUI apps (SUs charged) on Ada such as
  - ANSYS Workbench
  - Abaqus/CAE
  - IGV
  - LS-PREPOST
  - MATLAB
  - ParaView
  - VNC
  - Galaxy
  - Jupyter Notebook
  - RStudio
- On Terra
  - ANSYS Workbench
  - Abaqus/CAE
  - JBrowse
  - LS-PREPOST
  - MATLAB
  - ParaView
  - VNC
  - Jupyter Notebook
  - BEAUti, Tracer
  - FigTree
- Monitor and stop running jobs and interactive sessions

Need Help?

- First check the FAQ hprc.tamu.edu/wiki/HPRC:CommonProblems
  - Ada User Guide hprc.tamu.edu/wiki/Ada
    - Exercises hprc.tamu.edu/wiki/Ada:Exercises
  - Terra User Guide hprc.tamu.edu/wiki/Terra
    - Exercises hprc.tamu.edu/wiki/Terra:Exercises
- 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.)

HIGH PERFORMANCE RESEARCH COMPUTING

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Thank you.

Any question?