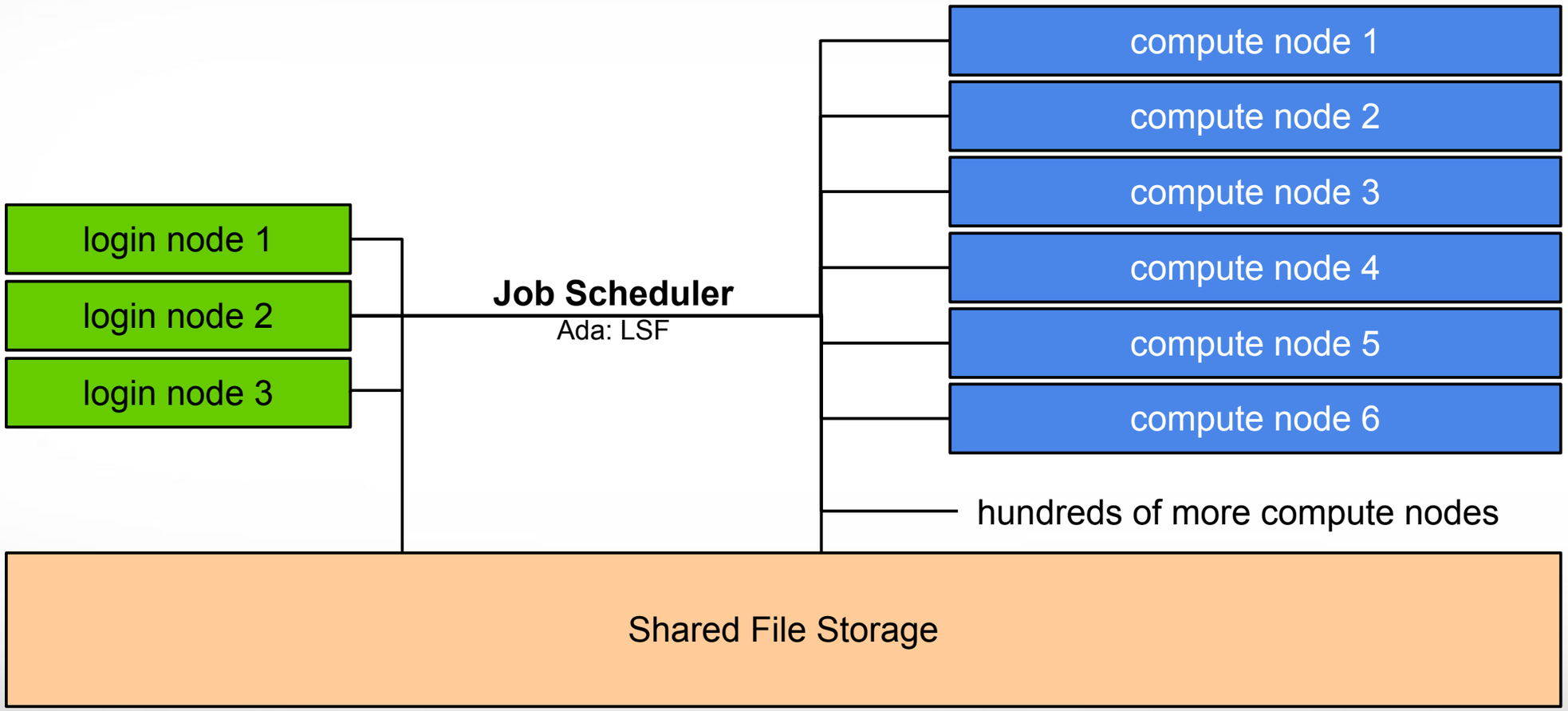
Ada

Using the LSF Job Scheduler on Ada

HIGH PERFORMANCE RESEARCH COMPUTING
TEXAS A&M UNIVERSITY

Fall 2020

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
hundreds of more compute nodes
Shared File Storage

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	$SCRATCH	1 TB	250,000	Temporary storage of large files for on-going computations. Not intended to be a long-term storage area.
/tiered/user/$USER	$ARCHIVE	10 TB	250,000	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`

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:

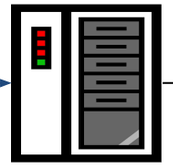
Campus Network

VPN

Internet

Off-campus:

SSH



Login nodes

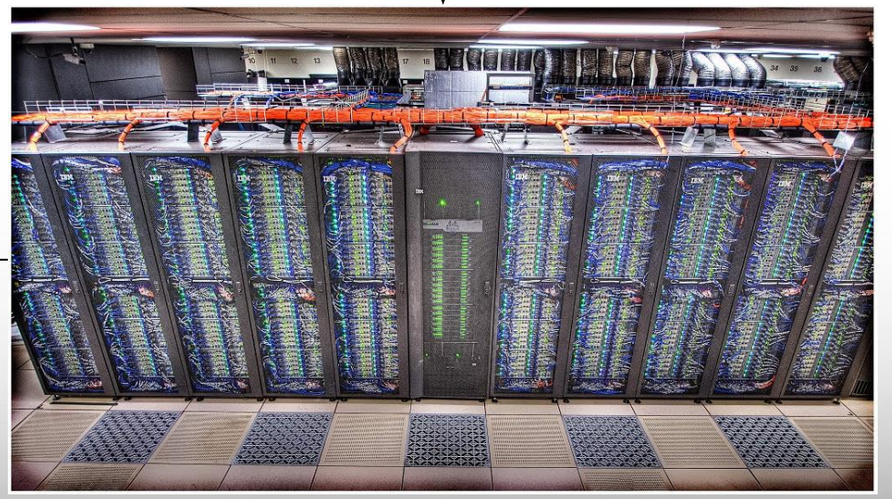
Create job

Job script file

Submit job

Batch manager:
LSF on Ada

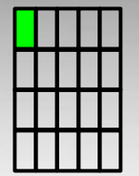
Queue



Cluster compute nodes

Output Files

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

Important Batch Job Parameters

Ada	Comment
`#BSUB -L /bin/bash`	Initialize job environment.

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

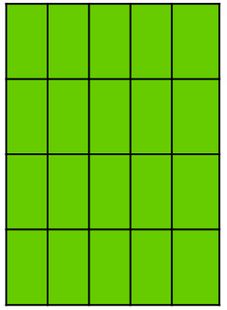
`#BSUB -n NNN`	Total number of tasks (cores) for the job.
`#BSUB -R "span[ptile=XX]"`	Specifies the maximum number of tasks (cores) to allocate per node

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

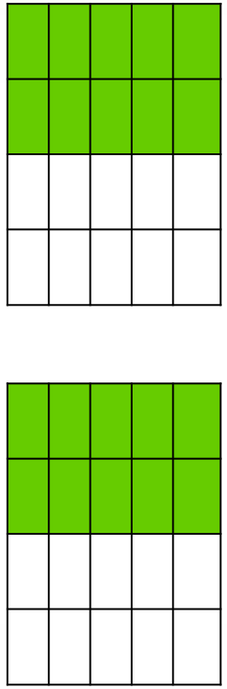


20 cores on
1 compute node

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

Preferred Mapping
(if applicable)

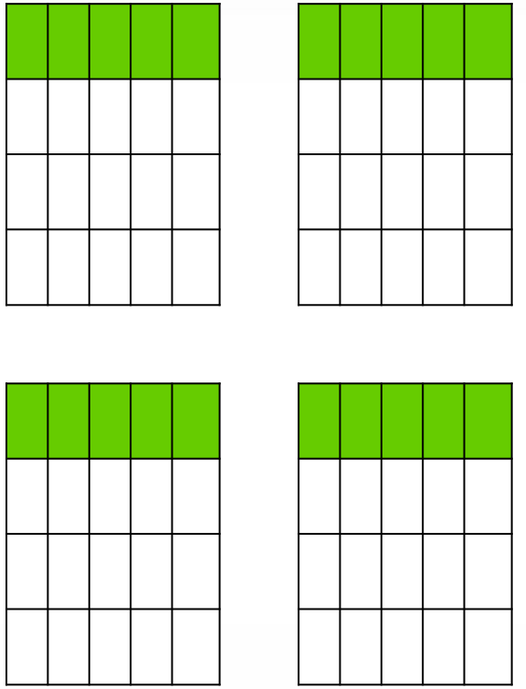
B.



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]
```

Job Memory Requests

- 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.
- On 64GB nodes, usable memory is < **54 GB** (10 GB used by system).
  - Per-process memory limit < **2700 MB** for a 20-core job.
- For more memory, request a large memory nodes:
  - If under 256 GB (up to 20 cores per node):
    - **#BSUB -R “select[mem256gb]”**
  - For 1 or 2 TB of memory (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.

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

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
```

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

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

Submitting Your Job and Check Job Status

Submit job

```
bsub < example01.job
```

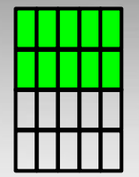
```
Verifying job submission parameters...
Verifying project account...
     Account to charge:   082792010838
         Balance (SUs):      4871.5983
         SUs to charge:         0.0333
Job <2470599> is submitted to default queue <sn_short>.
```

Check status

```
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
```

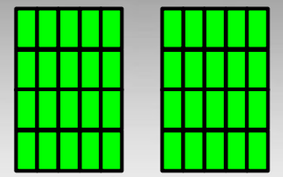
Ada Job File (multi core, single node)



```
##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

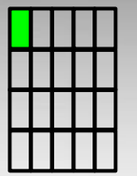
Ada Job File (multi core, multi node)



```
##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

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

Other Type of Jobs

- MPI and OpenMP
- Visualization:
  - portal.hprc.tamu.edu (visualization jobs can be run on both Ada and Terra)
- 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	Description
`bsub < jobfile1`	Submit jobfile1 to batch system
`bjobs [-u all or user_name] [[-l] job_id]`	List jobs
`bkill job_id`	Kill a job
`bhist [-l] job_id`	Show information for a job (can be when job is running or recently finished)
-	Show information for all of your jobs since YYYY-HH-MM
`lnu [-l] -j job_id`	Show resource usage for a job

hprc.tamu.edu/wiki/HPRC:Batch_Translation

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

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#`

- 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 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

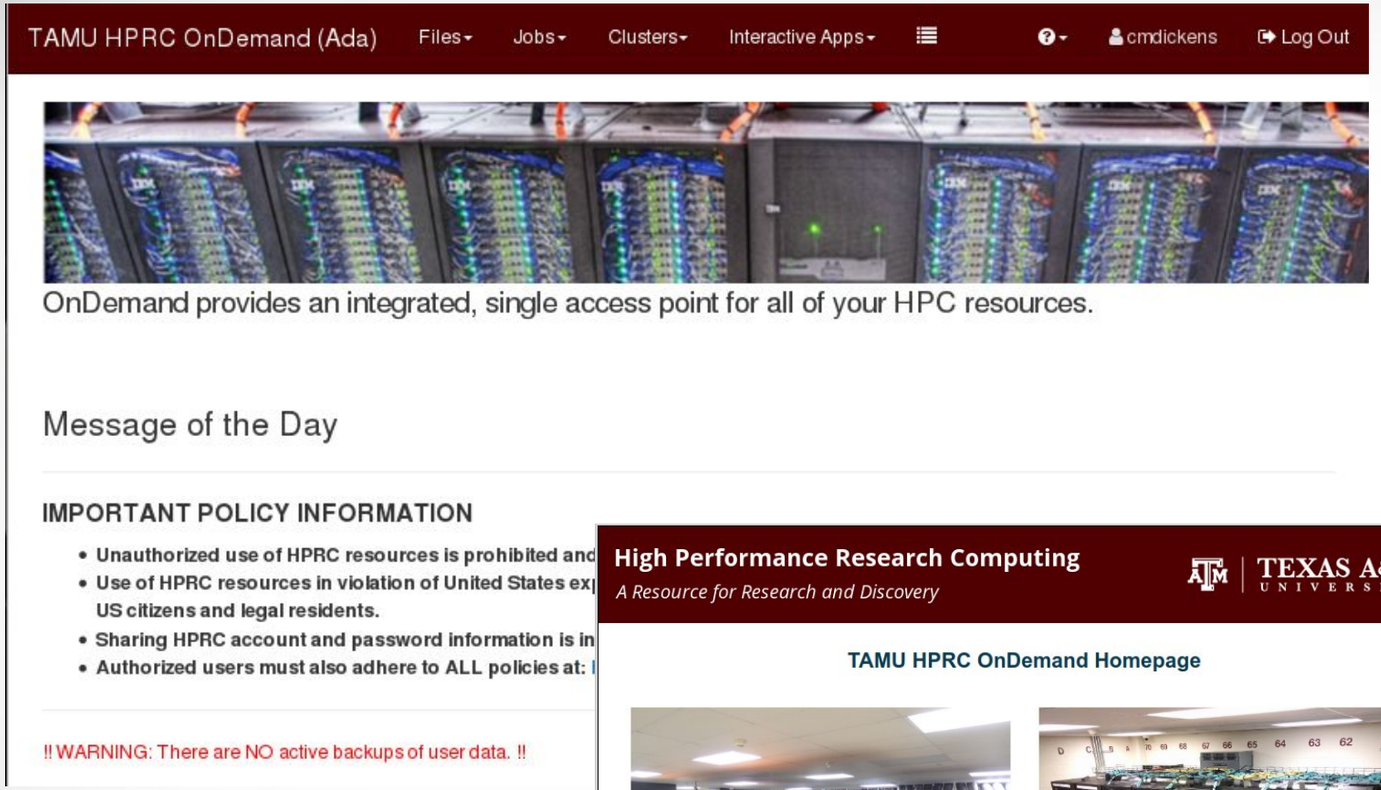
hprc.tamu.edu/wiki/Ada:Batch_Processing_LSF#Environment_Variables

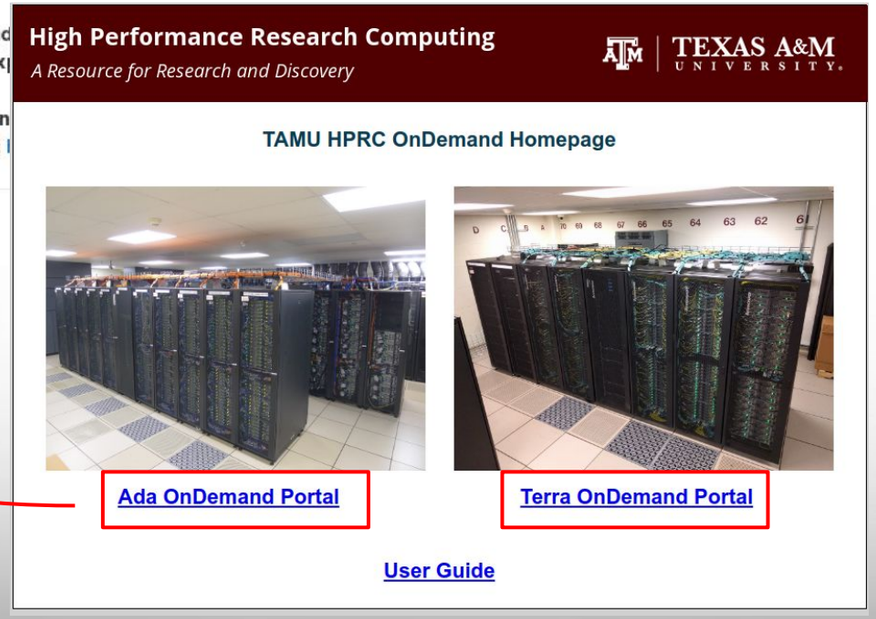
Jobs using tamubatch

Automatic batch job script that submits jobs for the user without the need of writing a full batch script on the cluster

Access help with: `tamubatch --help`

portal.hprc.tamu.edu





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

The HPRC portal allows users to do the following

- Browse files on the filesystem
- Access the Ada, Terra, Unix command line
- Launch jobs
- Compose job scripts
- Launch interactive GUI apps (SUs charged)

HIGH PERFORMANCE RESEARCH COMPUTING

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Thank you.

Any questions?