Ada

HPRC Clusters:

Ada Primer

Windows Users:

To follow along, please download Mobaxterm
(a free SSH client)

Google Search “Mobaxterm” or navigate to:
https://mobaxterm.mobatek.net/download.html

Download the “Installer edition” (green button)

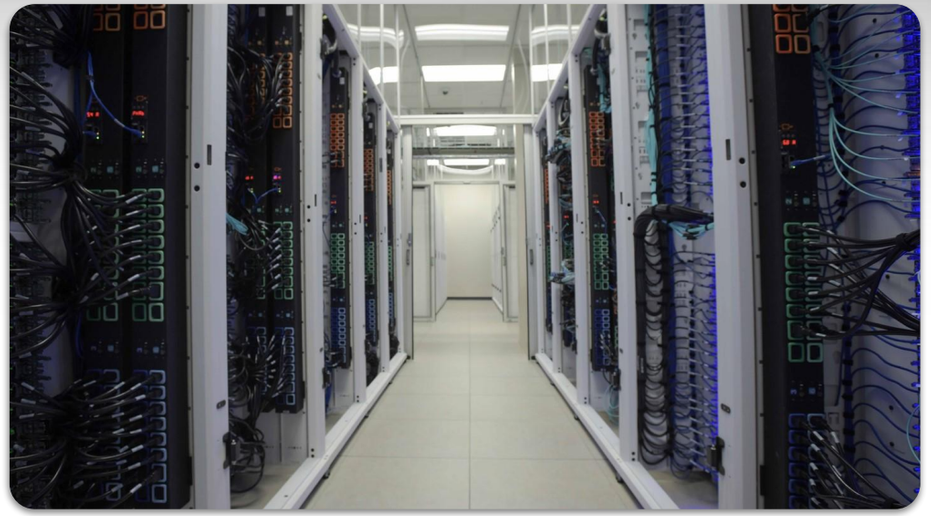
MobaXterm Home Edition v20.2
(Installer edition)

HIGH PERFORMANCE RESEARCH COMPUTING
TEXAS A&M UNIVERSITY

Spring 2020

HPRC's Newest Cluster

Grace is a 925-node Intel cluster from Dell with an InfiniBand HDR-100 interconnect, A100 GPUs, RTX 6000 GPUs and T4 GPUs. There are 925 nodes based on the Intel Cascade Lake processor.



Grace Status: Testing and Early user onboarding

Grace
3TB Large Memory-80 cores/nodes
Other Login Nodes-48 cores/node

Login Nodes	5
384GB memory general compute nodes	800
GPU - A100 nodes with 384GB memory	100
GPU - RTX 6000 nodes with 384GB memory	9
GPU - T4 nodes with 384GB memory	8
3TB Large Memory	8

Available late Spring 2021

For more information:
https://hprc.tamu.edu/wiki/Grace:Intro

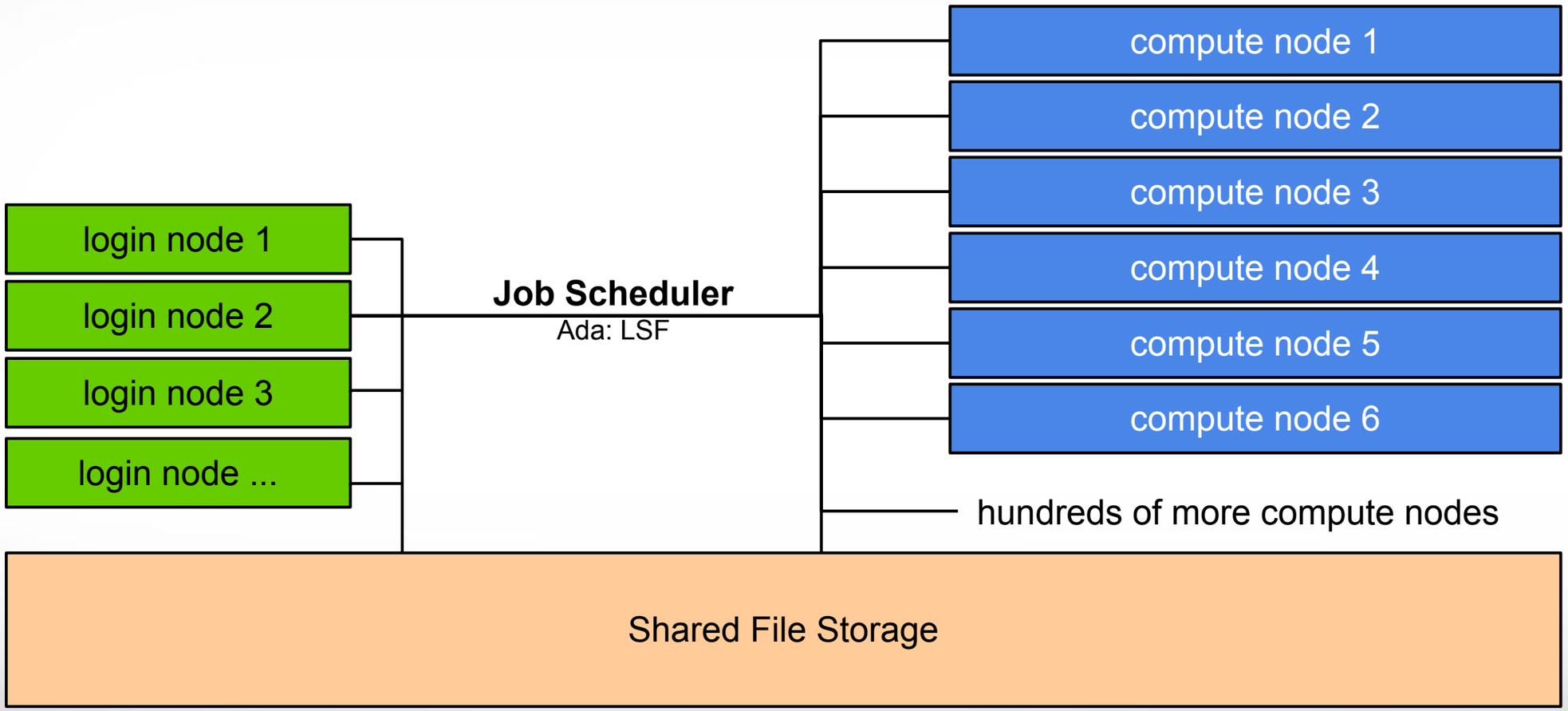
HPRC Clusters

Ada
20 cores/node

Login Nodes	8
64 GB memory compute nodes	792
PHI 64 GB memory compute nodes	9
K20 GPU 64 GB memory compute nodes	10
K20 GPU 256 GB memory compute nodes	20
V100 192 GB memory compute nodes	4 (24 cores/node)
256 GB memory compute nodes	6
1 TB memory compute nodes	11 (40 cores/node)
2 TB memory compute nodes	4 (40 cores/node)

hprc.tamu.edu/resources

Ada Cluster Diagram



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:

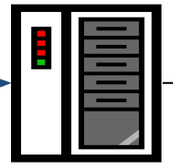
Campus Network

VPN

Internet

Off-campus:

SSH



Login nodes

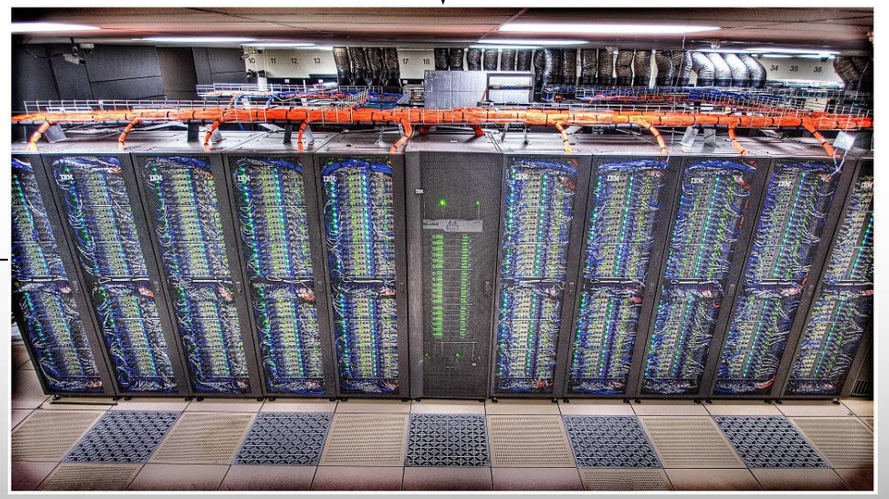
Create job

Job script file

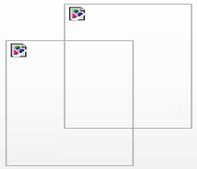
Submit job

Batch manager:
LSF on Ada

Queue



Cluster compute nodes



Output Files

Accessing Ada

Access

- On campus: **`ssh NetID@ada.tamu.edu`**
  - Off campus:
    - Set up and start VPN (Virtual Private Network): u.tamu.edu/VPnetwork
    - Then: **`ssh NetID@ada.tamu.edu`**
    - *Two-Factor Authentication* enabled
- SSH programs for Windows:
  - MobaXTerm (preferred, includes SSH and X11) or PuTTY SSH
- Access through portal.hprc.tamu.edu (Menu “Clusters” => “Ada Shell Access”)

Usage Policies

- Login sessions idle for **60** minutes, will be closed automatically
- Processes running longer than **60** minutes on login nodes will be killed automatically.
- **Please do not use more than 8 cores on the login nodes!**

hprc.tamu.edu/wiki/HPRC:Access

Two-Factor Authentication

- Duo NetID two-factor authentication to enhance security (it.tamu.edu/duo/)
  - All web login (howdy, portal.hprc.tamu.edu, Globus) through CAS
  - VPN to TAMU campus (since Oct 1st, 2018)
  - SSH/SFTP to HPRC clusters (since Nov 4th, 2019)

- See instructions in two-factor wiki page (hprc.tamu.edu/wiki/Two_Factor)
- SSH clients work with Duo
  - ssh command from Linux, macOS Terminal, Windows cmd
  - MobaXterm for Windows (click on "Session" icon or via local session: hit "enter" 3 times and wait for "Password:" prompt)

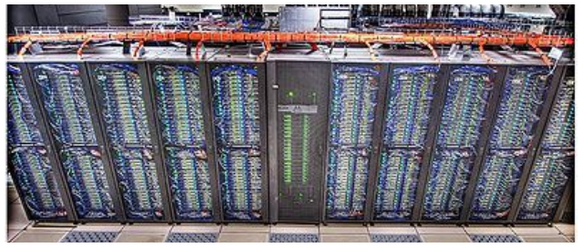
- SFTP clients work with Duo
  - scp/sftp command from Linux, macOS Terminal, Windows cmd
  - WinSCP for Windows
  - Cyberduck for macOS
  - FileZilla for Linux/macOS/Windows (but one file per authentication)
- Not all software supports SSH+Duo: SFTP in Matlab

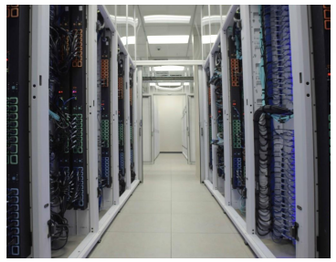
hprc.tamu.edu/wiki/Two_Factor

Example: SSH login with Duo

```
$ ssh ada.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...
```

Pop Quiz





Which one of the following is not an HPRC cluster?

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

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

Software

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

- Contact license owner to use restricted software

- Contact us for help with software installations
  - Users can install software in their home/scratch dir
  - Do not run the "*sudo*" command when installing software

Application Modules

- Installed applications are available as modules which are available to all users
  - (except for restricted modules)
- **Avoid loading modules in your `~/.bashrc`**

```
module list                          # list all loaded modules
module spider matlab                 # search for matlab
module load Matlab/R2019b            # load matlab R2019b
module list                          # list all loaded modules
module purge                         # remove all loaded modules
```

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

Modules and Toolchains

- Load modules with the same toolchains in your job scripts
- The **`2018b`** and **`GCCcore-7.3.0`** toolchain versions are recommended
  - `intel/2018b`
  - `iomkl/2018b`
  - `foss/2018b`
  - `GCCcore/7.3.0`
- 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.

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

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

license_status -a

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

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

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
```

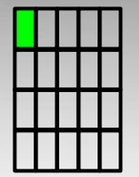
hprc.tamu.edu/wiki/Terra:Batch#Queues
hprc.tamu.edu/wiki/Ada:Batch_Queues

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

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

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

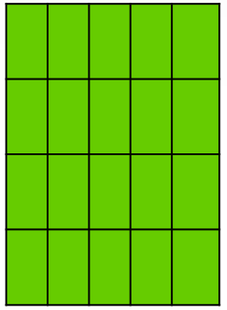
- To specify a project ID to charge in the job file
  - Ada: `#BSUB -P Account#`

- 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

Mapping Jobs to Cores per Node on **Ada**

A.

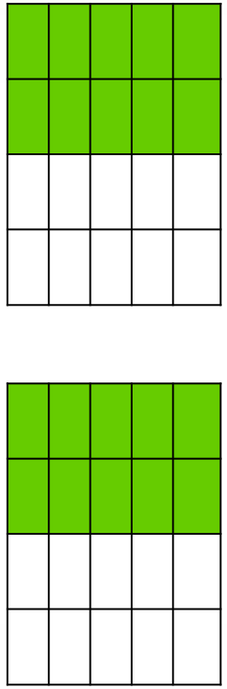


20 cores on
1 compute node

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

Preferred Mapping
(if applicable)

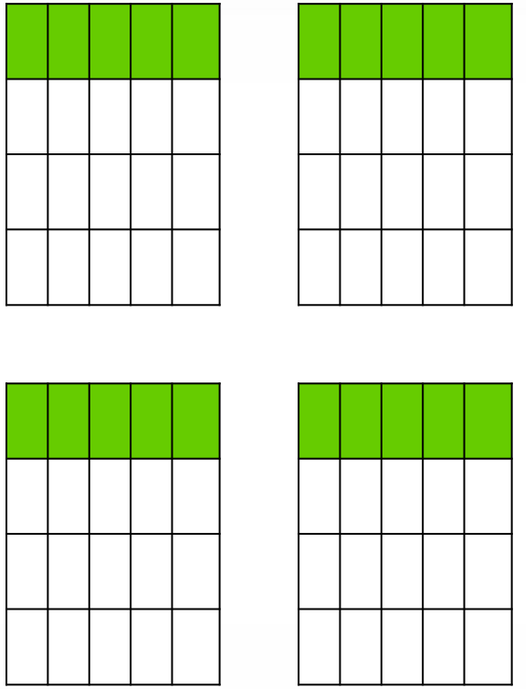
B.



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]
```

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

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
-	Show resource usage for a running job
-	Check CPU/memory efficiency for a job

hprc.tamu.edu/wiki/HPRC:Batch_Translation

Job submission issue: insufficient SUs

```
$ 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.
```

- 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

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

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.

Ada: Software for Large Memory Nodes

- The large memory nodes (1TB and 2TB) on Ada have their own separate modules

```
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
```

Submitting Your Job and Check Job Status

Submit job

```
cd $SCRATCH/batch_examples
```

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>.
```

Check status

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
```

HIGH PERFORMANCE RESEARCH COMPUTING

TEXAS A&M UNIVERSITY

Thank you.

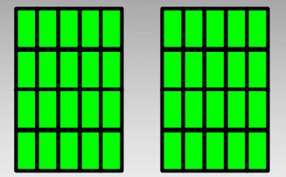
Any question?

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 `#SBATCH --time` or `#BSUB -W` parameter
- Insufficient memory specified in , `#SBATCH --mem` or `--mem-per-cpu` or `#BSUB -M` and `-R "rusage[mem=xxx]"` parameters
- No matching resource (`--mem` or `-R rusage[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
  - Or use Portal (portal.hprc.tamu.edu) `ssh -X user@ada.tamu.edu`

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

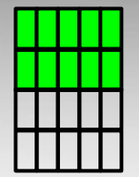
Ada Job File (multi core, multi node)



```
##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 (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

Continued Learning

Intro to HPRC Video Tutorial Series

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