HIGH PERFORMANCE RESEARCH COMPUTING

Using the Slurm Scheduler on Composable Resources

HPRC Training

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High Performance
Research Computing
DIVISION OF RESEARCH

Slurm Job Scheduling

- HPC Architecture
- SBATCH Parameters
- Single node jobs
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  - multi-core
  - Break
- Multi-node jobs
  - MPI jobs
  - TAMULauncher
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- Monitoring job resource usage
  - at runtime
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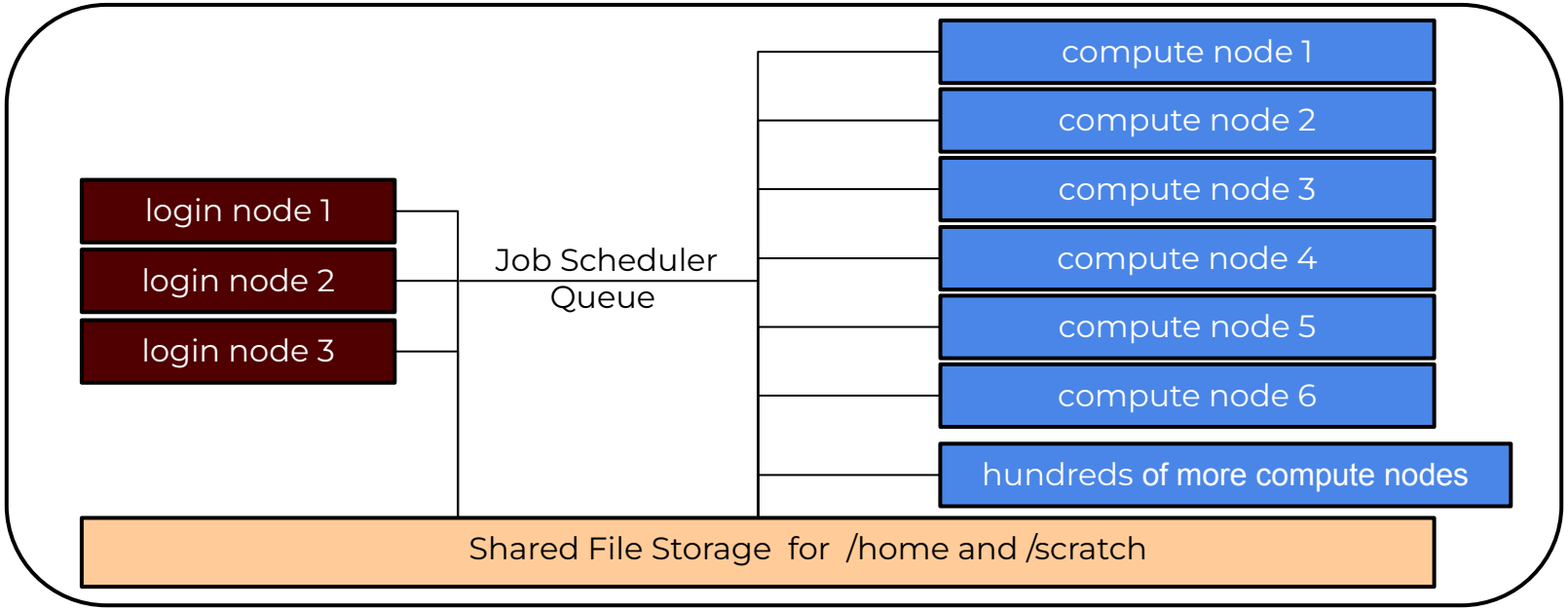
FASTER

- FASTER is a 184-node Intel cluster from Dell with an InfiniBand HDR-100 interconnect.
- A100 GPUs, A10 GPUs, A30 GPUs, A40 GPUs and T4 GPUs are distributed and composable via Liqid PCIe fabrics.
- All nodes are based on the Intel Ice Lake processor.

Nodes, Cores and Queues

- Node
  - one computer unit of an HPC cluster each containing memory and one or more CPUs. There are generally two classifications of HPC nodes; login and compute.
    - login node
      - this is where users first login to stage their job scripts and do file and directory manipulations with text file editors (vi, gedit, emacs, portal) and Unix commands.
    - compute node
      - These are often referred to as just nodes since jobs are only scheduled on the compute nodes.
      - some compute nodes contain GPUs.
      - can use one or more compute nodes for a job based on how you configure your job script
- Core
  - There are 64 cores (cpus) on the FASTER 256GB memory compute nodes (250GB avail)
  - can use one or all 64 cores in a job script
    - check to see that the software you use in your job script supports multi-core
- Queue
  - Ordered list of all scheduled jobs for all users both in the PENDING and RUNNING states
  - Individual queues are also termed Partition (Example partition names: gpu, cpu)
  - cpu partition is auto-assigned but you must specify gpu partition to use GPUs

HPC Diagram



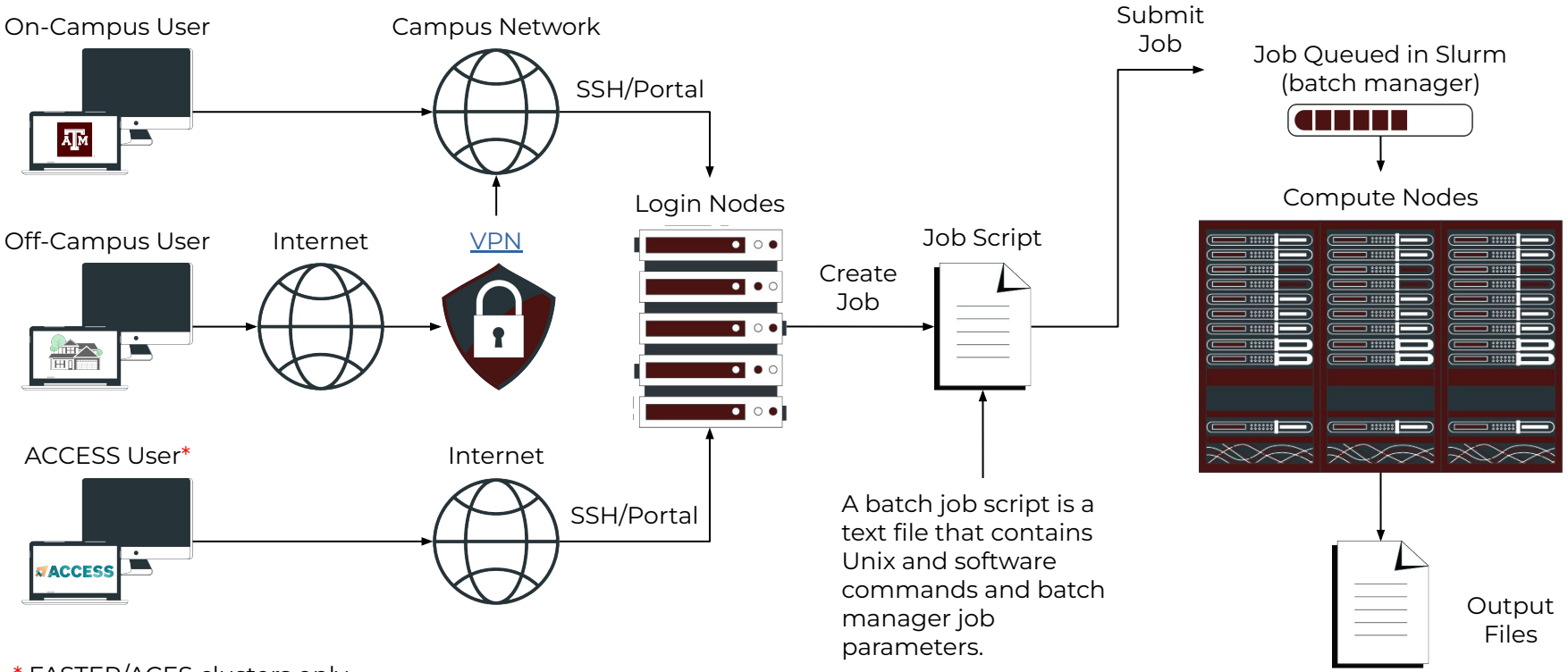
login nodes are for:

- file manipulation and job script preparation
- software installation and testing
- short tasks (< 60 minutes and max 8 cores)
  - also be aware of amount of memory utilized

compute nodes are for:

- computational jobs which can use up to 64 cores and/or up to 250GB memory per FASTER compute node.
- all jobs running > 60 minutes

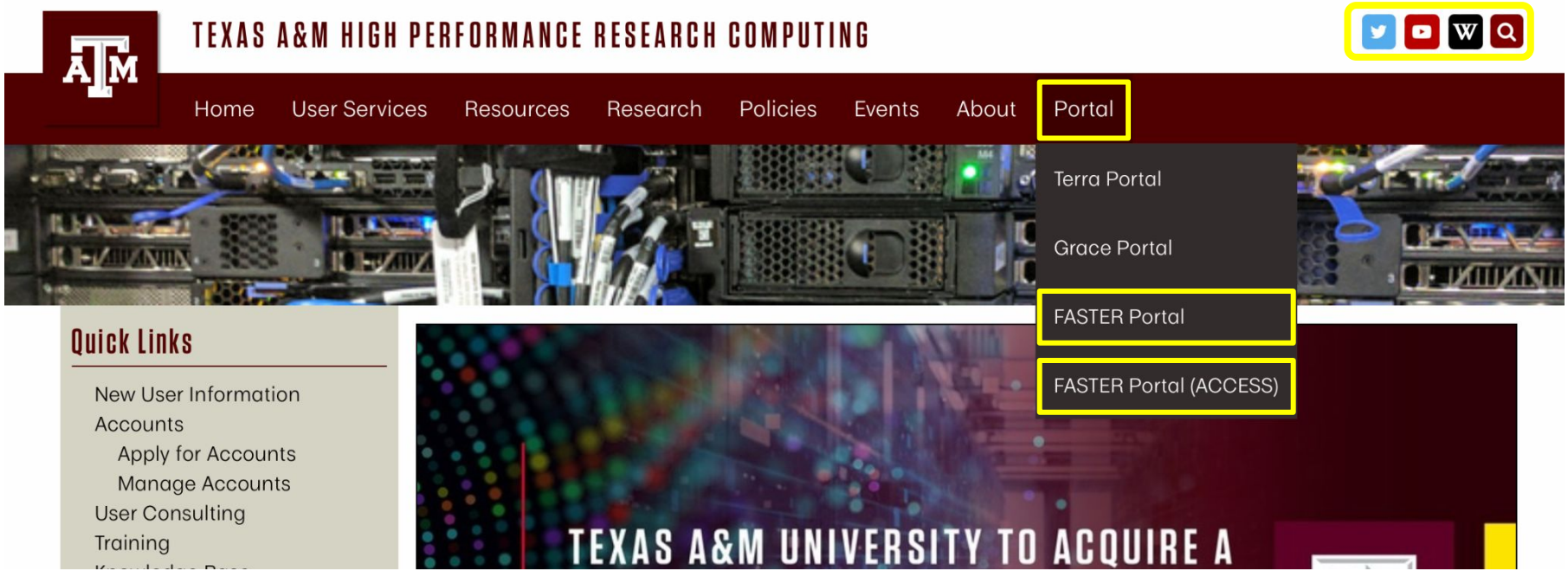
Batch Computing on HPRC Clusters



* FASTER/ACES clusters only

Accessing the HPRC Portal

- HPRC webpage: hprc.tamu.edu, Portal dropdown menu



Accessing FASTER via SSH

- SSH command is required for accessing FASTER:
  - On campus: **ssh userNetID@faster.hprc.tamu.edu**
  - Off campus:
    - Set up and start VPN (Virtual Private Network): u.tamu.edu/VPnetwork
    - Then: **ssh userNetID@faster.hprc.tamu.edu**
  - *Two-Factor Authentication* enabled for CAS, VPN, SSH
- SSH programs for Windows:
  - MobaXTerm (preferred, includes SSH and X11)
  - PuTTY SSH
  - Windows Subsystem for Linux
- https://portal-faster.hprc.tamu.edu
  - Select the "Clusters" tab and then ">_faster Shell Access"
- FASTER has 2 login nodes for TAMU users. Check the bash prompt.

  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 across all the login nodes!

  Do not use the sudo command.

  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
  - SSH/SFTP to HPRC clusters
- 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)
  - Putty for Windows
- SFTP clients work with Duo
  - scp/sftp command from Linux, macOS Terminal, Windows cmd
  - WinSCP for Windows
  - Cyberduck for macOS
- Not all software supports SSH+Duo: SFTP in MATLAB

Example: SSH login with Duo

```
$ ssh userNetID@faster.hprc.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

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

Hands-On Activity: 2 Minutes

1. Please try to login to FASTER now.

2. What message do you see when you log on?

3. On which login node did you land?

How Busy are the HPRC Clusters?

Check on the command line of a cluster using the sinfo command

sinfo

PARTITION	AVAIL	TIMELIMIT	JOB_SIZE	NODES(**A/I/O/T**)	CPUS(**A/I/O/T**)
cpu*	up	7-00:00:00	1-32	35/50/27/112	2058/3382/1728/7168
gpu	up	7-00:00:00	1-32	14/27/11/52	252/2372/704/3328
memverge	up	2-00:00:00	1-2	0/0/2/2	0/0/128/128
fpga	up	2-00:00:00	1-2	0/0/2/2	0/0/128/128
spr	up	2-00:00:00	1	0/1/0/1	0/112/0/112
atsp	up	2-00:00:00	1	0/8/2/10	0/512/128/640
staff	down	7-00:00:00	1-infinite	49/85/44/178	2310/6266/2816/11392

A/I/O/T

A = Active (in use by running jobs)
I = Idle (available for jobs)
O = Offline (unavailable for jobs)
T = Total

not all partitions are available to users

Checking GPU Availability on FASTER

See GPU configuration and current availability

```
gpuavail
```

```
    CONFIGURATION
NODE          NODE
TYPE          COUNT
-----------------
gpu:a100:4      3
gpu:a100:8      1
gpu:a10:2       1
gpu:a10:4       1
gpu:a30:2       2
gpu:a40:2       2
gpu:a40:4       1
gpu:t4:2        1
gpu:t4:4       29
gpu:t4:8       10
```

```
        AVAILABILITY
GPU       GPU      GPU      GPU
NODE      TYPE     COUNT    AVAIL*
-------------------------------
fc023      t4        2       2
fc070      t4        8       8
fc085      t4        4       4
fc096      a40       2       2
fc097      a40       2       2
fc098      a40       4       3
fc099      a10       2       2
fc101      t4        4       4
fc102      t4        4       4
fc121      t4        4       2
fc122      a10       4       4
fc123      a30       2       2
fc124      a30       2       2

* Some available GPUs may not be immediately
  available due to other jobs using all or most
  of the compute node memory
```

SBATCH Parameters

Slurm Job Script Example

```
#!/bin/bash
#SBATCH --job-name=spades       # keep job name short with no spaces
#SBATCH --time=1-00:00:00       # request 1 day; Format: days-hours:minutes:seconds
#SBATCH --nodes=1               # request 1 node (optional since default=1)
#SBATCH --ntasks-per-node=1     # request 1 task (command) per node
#SBATCH --cpus-per-task=1       # request 1 cpu (core, thread) per task
#SBATCH --mem=3G                # request 3GB total memory per node
#SBATCH --output=stdout.%x.%j   # save stdout to a file with job name and JobID appended to file name
#SBATCH --error=stderr.%x.%j    # save stdout to a file with job name and JobID appended to file name

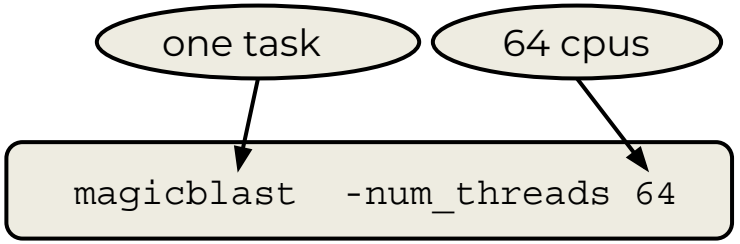
# unload any modules to start with a clean environment
module purge
# load software modules
module load GCC/11.2.0   SPAdes/3.15.3
# run commands
spades.py -1 s22_R1.fastq.gz -2 s22_R2.fastq.gz -o s22_out --threads 1
```

- Always include the first line exactly as it is; no trailing spaces or comments
- Slurm job parameters begin with **#SBATCH** and you can add comments afterwards as above
- Name the job script whatever you like but be consistent to make it easier to search for job scripts
  - **my_job_script.job**
  - **my_job_script.sbatch**
  - **run_program_project.sh**
  - **job_program_project.slurm**

Commonly Used Slurm SBATCH Parameters

- **`--nodes`**
  - number of nodes to use where a node is one computer unit of many in an HPC cluster
    - **`--nodes=1`** **`# request 1 node (optional since default=1)`**
  - used for multi-node jobs
    - **`--nodes=10`**
- if number of cpus per node is not specified then defaults to 1 cpu
- default is 1 node if --nodes not used & can use with --ntasks-per-node and --cpus-per-task
  - do not use `--nodes` with `--array`
- **`--ntasks`**
  - a task can be considered a command such as blastn, bwa, script.py, etc.
  - **`--ntasks=1`** **`# total tasks across all nodes where each task is scheduled a max of 1 cpu`**
- when using --ntasks > 1 without --nodes=1, the job may be scheduled on multiple compute nodes
- **`--ntasks-per-node`**
- use together with --cpus-per-task
  - **`--ntasks-per-node=1`**
- **`--cpus-per-task`**
  - number of CPUs (cores) for each task (command)
  - **`--cpus-per-task=64`**

either `--ntasks`, `--ntasks-per-node` or `--nodes` needs to be provided.



Commonly Used Slurm SBATCH Parameters

- **`--time`**
  - max runtime for job (*required*); format: days-hours:minutes:seconds (days- is optional)
  - **`--time=24:00:00`** **`# set max runtime 24 hours (same as --time=1-00:00:00)`**
  - **`--time=7-00:00:00`** **`# set max runtime 7 days`**
- **`--mem`**
  - total memory for each node (*required*)
  - **`--mem=250G`** **`# request 250GB total memory (max available for 256gb nodes)`**
- **`--job-name`**
  - set the job name, keep it short and concise without spaces (*optional but highly recommended*)
  - **`--job-name=myjob`**
- **`--output`**
  - save all stdout to a specified file (*optional but highly recommended for debugging*)
  - **`--output=stdout.%x.%j`** **`# saves stdout to a file named stdout.jobname.JobID`**
- **`--error`**
  - save all stderr to a specified file (*optional but highly recommended for debugging*)
  - **`--error=stderr.%x.%j`** **`# saves stderr to a file named stderr.jobname.JobID`**
  - use just --output to save stdout and stderr to the same output file: **`--output=output.%x.%j.log`**
- **`--partition`**
  - specify a partition (queue) to use (*optional, use as needed*)
  - partition is automatically assigned to short, medium, long.
    - need to specify **`--partition`** parameter to use gpu, memverge, fpga

Commonly Used Optional Slurm Parameters

- `--gres`
  - used for requesting 1 or 2 GPUs; use GPU type in lowercase
  - `--gres=gpu:t4:1  # request 1 T4 GPU; use replace :1 with :2 for two GPUs, etc`
  - `--partition=gpu  # also include this line when requesting GPUs`
- `--account`
  - specify which HPRC account to use; see your accounts with `myproject`
  - `--account=ACCOUNTNUMBER`
  - default account from `myproject` output is used if not specified
- `--mail-user`
  - send email to user
  - `--mail-user=myemail@tamu.edu`
- `--mail-type`
  - send email per job event: BEGIN, END, FAIL, ALL
  - `--mail-type=ALL`
- `--dependency`
  - schedule a job to start after a previous job successfully completes
  - `--dependency=afterok:JobID`
    - get the JobID of the previous job with `squeue -u $USER`

Submitting Slurm Jobs

- A job script is a text file of Unix commands with **#SBATCH** parameters
- **#SBATCH** parameters provide resource configuration request values
  - time, memory, nodes, cpus, output files, …
- Jobs can be submitted using a job script or directly on the command line
- Submit the job using sbatch command with the job script name
  - your job script provides a record of commands used for an analysis
  - `sbatch my_job_script.job`
- Submit command on the command line by specifying all necessary parameters
  - must rely on your bash history to see **#SBATCH** parameters used which is not reliable
  - `sbatch -t 01:00:00 -n 1 -J myjob --mem 3G -o stdout.%j commands.sh`
- You can start an interactive job on the command line which ends when you exit the terminal
  - do not to use more than the requested memory and CPUs when your job starts.
  - `srun --time=04:00:00 --mem=3G --ntasks=1 --cpus-per-task=1 --pty bash`

slurm.schedmd.com/sbatch.html

FASTER Service Unit Calculations

- For the FASTER 256GB memory nodes (250GB available), you are charged Service Units (SUs) based on one of the following values whichever is greater.
  - 1 SU per CPU per hour or 1 SU per 3GB (3700M) of requested memory per hour

Number of Cores	Total Memory per node (GB)	GPU count, type	Hours	SUs charged
1	3	0	1	1
1	4	0	1	2
1	250	0	1	64
64	250	0	1	64
1	3	1 gpu:a30:2	1	129
64	250	1 gpu:a30:2	1	320

charged for the second GPU which becomes unavailable for other jobs due to using all 64 cores

- Each T4 GPU would be an additional 64 SUs for one hour.
- Each A100, A10, A30, or A40 would be an addition 128 SUs for one hour.
- Unused SUs expire at the end of each fiscal year (Aug 31) and must be renewed

Single-Node Jobs

Single vs Multi-Core Jobs

- When to use single-core jobs
  - The software being used only supports commands utilizing a single-core
- When to use multi-core jobs
  - If the software supports multiple cores (--threads, --cpus, ...) then configure the job script and software command options to utilize all CPUs on a compute node to get the job done faster unless the software specifically recommends a limited number of cores
    - FASTER 256GB memory compute nodes
      - 64 CPUs (cores) per compute node
      - 250GB of available memory per compute node
  - Can group multiple single-core commands into a "multi-core" job using TAMULauncher on one or multiple nodes

Single-Node Single-Core Job Scripts

```
#!/bin/bash
#SBATCH --job-name=spades
#SBATCH --time=01:00:00
#SBATCH --nodes=1        # optional since default=1
#SBATCH --ntasks-per-node=1
#SBATCH --cpus-per-task=1
#SBATCH --mem=3G
#SBATCH --output=stdout.%x.%j
#SBATCH --error=stderr.%x.%j

module purge
module load GCC/11.2.0  SPAdes/3.15.3
spades.py -1 s1_R1 -2 s1_R2 -o outdir --threads 1
```

```
#!/bin/bash
#SBATCH --job-name=spades
#SBATCH --time=01:00:00
#SBATCH --nodes=1        # optional since default=1
#SBATCH --ntasks-per-node=1
#SBATCH --cpus-per-task=1
#SBATCH --mem=4G
#SBATCH --output=stdout.%x.%j
#SBATCH --error=stderr.%x.%j

module purge
module load GCC/11.2.0  SPAdes/3.15.3
spades.py -1 s1_R1 -2 s1_R2 -o outdir --threads 1
```

set number of threads to match SBATCH parameters

Example 1

1	Total CPUs requested	1
1	CPUs per node	1
3	total requested GB memory	4
1	SUs to start job	2

Example 2

any unused SUs charged for a job are automatically reimbursed a few minutes after the job completes

Slurm Parameter: --ntasks

```
#!/bin/bash
#SBATCH --job-name=myjob            # job name
#SBATCH --time=1:00:00              # set the wall clock limit to 1 hour
#SBATCH --ntasks=1                  # request 1 task (command) per node
#SBATCH --mem=3G                    # request 3GB of memory per node
#SBATCH --output=stdout.%x.%j       # create a file for stdout
#SBATCH --error=stderr.%x.%j        # create a file for stderr
```

When only `--ntasks` is used, `--cpus-per-task=1` and `--nodes` could be more than 1 if `--ntasks` is > 1

- **`--ntasks=1`**
  - NumNodes=1 NumCPUs=1 NumTasks=1 CPUs/Task=1
- **`--ntasks=48  # without –nodes=1 could result in multiple nodes`**
  - NumNodes=1 NumCPUs=48 NumTasks=48 CPUs/Task=1
  - NumNodes=48 NumCPUs=1 NumTasks=48 CPUs/Task=1

Requesting all CPUs and Available Memory on FASTER Compute Nodes

CPU only node

64 cores, 256 GB nodes (180 nodes available)

```
#SBATCH --ntasks-per-node=1
#SBATCH --cpus-per-task=64
#SBATCH --mem=250G
```

GPU node

64 cores, 256 GB memory and 4 x A100 GPUs

```
#SBATCH --gres=gpu:a100:4
#SBATCH --partition=gpu
#SBATCH --ntasks-per-node=1
#SBATCH --cpus-per-task=64
#SBATCH --mem=250G
```

use lowercase gpu types: t4, a100, a10, a30, a40

Requesting one GPU on FASTER Compute Nodes that have four GPUs

- Request ¼ or less of the available CPU and memory resources for a compute node that has 4 installed GPUs when you need 1 GPU so that someone else can use the other GPUs, unless you need more CPUs and memory resources for your job.
- If you request 1 GPU with 64 cores and 250GB memory, the other 3 GPUs on the compute node are unavailable for other jobs and you are charged for all 4 GPUs
- On FASTER each T4 GPU would be an additional 64 SUs for one hour and each A100, A10, A30, or A40 would be an addition 128 SUs for one hour.

gpuavail

```
     CONFIGURATION
NODE          NODE
TYPE          COUNT
-------------------
gpu:a100:4      3
```

```
      AVAILABILITY
GPU       GPU    GPU     GPU
NODE      TYPE   COUNT   AVAIL*
----------------------------
fc002     a100    4       1
fc026     a100    4       4
```

```
#SBATCH --gres=gpu:a100:1
#SBATCH --partition=gpu
#SBATCH --ntasks-per-node=1
#SBATCH --cpus-per-task=16
#SBATCH --mem=56G
#SBATCH --time=01:00:00
```

16 + 64 = 80 SUs per hour for fc026

How Many SUs?

- How many SUs are charged if your job is scheduled on GPU node fc026?
- On FASTER you are charged per CPU/memory plus GPU count
  - Each T4 GPU is charged an additional 64 SUs for one hour
  - Each A100, A10, A30, or A40 GPU is charged an addition 128 SUs for one hour.

gpuavail

```
     CONFIGURATION
NODE          NODE
TYPE          COUNT
-------------------
gpu:a100:4      3
```

```
      AVAILABILITY
GPU       GPU    GPU     GPU
NODE      TYPE   COUNT   AVAIL*
----------------------------
fc002     a100    4       1
fc026     a100    4       4
```

```
#SBATCH --gres=gpu:a100:1
#SBATCH --partition=gpu
#SBATCH --ntasks-per-node=1
#SBATCH --cpus-per-task=64
#SBATCH --mem=250G
#SBATCH --time=01:00:00
```

? + ? = ?? SUs per hour for fc026

Select GPU type on FASTER Cluster

```
#!/bin/bash
#SBATCH --job-name=my_gpu_job
#SBATCH --time=1-00:00:00       # request 1 day of time for the job
#SBATCH --ntasks=32             # request half of the total cores
#SBATCH --gres=gpu:a30:1        # request 1 A30 GPU; replace :1 with :2 for two GPUs
#SBATCH --partition=gpu         # use partition=gpu when selecting GPUs
#SBATCH --mem=115G              # request 3.7GB memory per core
#SBATCH --output=stdout.%x.%j
#SBATCH --error=stderr.%x.%j

# unload modules to start with a clean environment; then load required modules
module purge
module load CUDA/11.7.0
# run your gpu command
my_gpu_command
```

- There are five types of GPUs on FASTER compute nodes. Select the type and quantity with --gres
  - T4 **--gres=gpu:t4:N** (N can be 1 to 8) 200 x T4 on FASTER
  - A100 **--gres=gpu:a100:N** (N can be 1 to 12) 40 x A100 on FASTER
  - A10 **--gres=gpu:a10:N** (N can be 1 to 4) 8 x A10 on FASTER
  - A30 **--gres=gpu:a30:N** (N can be 1 to 2) 4 x A30 on FASTER
  - A40 **--gres=gpu:a40:N** (N can be 1 to 4) 8 x A40 on FASTER

Single-Node Multi-Core Job Scripts

```
#!/bin/bash
#SBATCH --job-name=spades
#SBATCH --time=1-00:00:00
#SBATCH --nodes=1     # optional since default=1
#SBATCH --ntasks-per-node=1
#SBATCH --cpus-per-task=32
#SBATCH --mem=250G
#SBATCH --output=stdout.%x.%j
#SBATCH --error=stderr.%x.%j

module purge
module load GCC/11.2.0  SPAdes/3.15.3
spades.py -1 s1_R1 -2 s1_R2 -o outdir --threads 32
```

```
#!/bin/bash
#SBATCH --job-name=spades
#SBATCH --time=1-00:00:00
#SBATCH --nodes=1     # optional since default=1
#SBATCH --ntasks-per-node=1
#SBATCH --cpus-per-task=64
#SBATCH --mem=250G
#SBATCH --output=stdout.%x.%j
#SBATCH --error=stderr.%x.%j

module purge
module load GCC/11.2.0  SPAdes/3.15.3
spades.py -1 s1_R1 -2 s1_R2 -o outdir --threads 64
```

specify number of threads to match SBATCH parameters

Example 1

32	Total CPUs requested	64
32	CPUs per node	64
250	total requested GB memory	250
1,536	SUs to start job	1,536

Example 2

It is best to request all cores and all memory if using the entire node

Slurm Environment Variables

```
#!/bin/bash
#SBATCH --job-name=spades
#SBATCH --time=1-00:00:00
#SBATCH --ntasks-per-node=1
#SBATCH --cpus-per-task=64
#SBATCH --mem=250G
#SBATCH --output=stdout.%x.%j
#SBATCH --error=stderr.%x.%j

module purge
module load GCC/11.2.0  SPAdes/3.15.3
spades.py -1 s1_R1 -2 s1_R2 -o outdir_s1 --threads $SLURM_CPUS_PER_TASK
spades.py -1 s2_R1 -2 s2_R2 -o outdir_s2 --threads $SLURM_CPUS_PER_TASK
```

$SLURM_CPUS_PER_TASK variable used in commands to match SBATCH parameters

You can use the environment variable **SLURM_CPUS_PER_TASK** to capture the value in the **#SBATCH --cpus-per-task** parameter so that you only need to adjust the cpus in one place

Multi-Node Jobs

Slurm Parameters: --nodes --ntasks-per-node

```
#!/bin/bash
#SBATCH --job-name=myjob              # job name
#SBATCH --time=1:00:00                # set the wall clock limit to 1 hour
#SBATCH --nodes=2                     # request 2 nodes
#SBATCH --ntasks-per-node=1           # request 1 task (command) per node
#SBATCH --cpus-per-task=64            # request 64 cores per task
#SBATCH --mem=250G                    # request 250GB of memory per node
#SBATCH --output=stdout.%x.%j         # create a file for stdout
#SBATCH --error=stderr.%x.%j          # create a file for stderr
```

It may be easier to scale jobs by using --nodes with --ntasks-per-node instead of with --ntasks.
If you use --nodes with --ntasks, you need to calculate total CPUs for all nodes as the --ntasks value

- **`--nodes=2 --ntasks-per-node=64`**
  - NumNodes=2 NumCPUs=128 NumTasks=128 CPUs/Task=1 mem=250G per node
- **`--nodes=2 --ntasks=128`**
  - NumNodes=2 NumCPUs=128 NumTasks=128 CPUs/Task=1 mem=250G per node
- **`--nodes=1 --ntasks=64`**
  - NumNodes=1 NumCPUs=64 NumTasks=64 CPUs/Task=1 mem=250G per node
- **`--nodes=2 --ntasks=64`**
  - will allocate 32 core on one node and 32 cores on a second node
- when --nodes is > 1, make sure the software you are using supports multi-node processing

MPI Multi-Node Multi-Core Job Script: Example 1

```
#!/bin/bash
#SBATCH --job-name=moose
#SBATCH --time=1-00:00:00
#SBATCH --nodes=10
#SBATCH --ntasks-per-node=1
#SBATCH --cpus-per-task=64
#SBATCH --mem=250G
#SBATCH --output=stdout.%x.%j
#SBATCH --error=stderr.%x.%j

module purge
module load MOOSE/e70fe56913
mpirun -np 640 -npernode 64 /path/to/moose-opt -i moose.i
```

640	Total CPUs requested
64	CPUs per node
250	Total requested GB memory per node
15,360	SUs to start job (nodes * cpus * hours)

MPI Multi-Node Multi-Core Job Script: Example 2

```
#!/bin/bash
#SBATCH --job-name=abyss-pe
#SBATCH --time=1-00:00:00
#SBATCH --nodes=10
#SBATCH --ntasks-per-node=1
#SBATCH --cpus-per-task=64
#SBATCH --mem=250G
#SBATCH --output=stdout.%x.%j
#SBATCH --error=stderr.%x.%j

module purge
module load GCC/8.3.0  OpenMPI/3.1.4 ABySS/2.1.5
abyss-pe np=640 j=64 lib='lib1' lib1='sample1_R1 sample1_R2'
```

640	Total CPUs requested
64	CPUs per node
250	Total requested GB memory per node
15,360	SUs to start job (nodes * cpus * hours)

TAMULauncher

- hprc.tamu.edu/wiki/SW:tamulauncher
- Use when you have hundreds or thousands of commands to run each utilizing a single-core or a few cores
  - tamulauncher keeps track of which commands completed successfully
    - to see the list of completed commands
      - `tamulauncher -status commands_file.txt`
    - if time runs out, tamulauncher can be restarted and it will know which was the last successfully completed command
  - submit tamulauncher as a batch job within your job script
  - can run tamulauncher interactively on login node; limited to 8 cores
  - you can check the --status on the command line from the working directory
- run a single command of your thousands to make sure the command is correct and to get an estimate of resource usage (CPUs, memory, time)
- request all cores and memory on the compute node(s) and configure your commands to use all available cores

TAMULauncher Multi-Node Single-Core Commands

commands.txt (500 lines for example)

```
spades.py -1 s1_R1.fastq.gz -2 s1_R2.fastq.gz -o s1_out --threads 1
spades.py -1 s2_R1.fastq.gz -2 s2_R2.fastq.gz -o s2_out --threads 1
spades.py -1 s3_R1.fastq.gz -2 s3_R2.fastq.gz -o s3_out --threads 1
spades.py -1 s4_R1.fastq.gz -2 s4_R2.fastq.gz -o s4_out --threads 1
spades.py -1 s5_R1.fastq.gz -2 s5_R2.fastq.gz -o s5_out --threads 1
spades.py -1 s6_R1.fastq.gz -2 s6_R2.fastq.gz -o s6_out --threads 1
spades.py -1 s7_R1.fastq.gz -2 s7_R2.fastq.gz -o s7_out --threads 1
spades.py -1 s8_R1.fastq.gz -2 s8_R2.fastq.gz -o s8_out --threads 1
spades.py -1 s9_R1.fastq.gz -2 s9_R2.fastq.gz -o s9_out --threads 1
spades.py -1 s10_R1.fastq.gz -2 s10_R2.fastq.gz -o s10_out --threads 1
spades.py -1 s11_R1.fastq.gz -2 s11_R2.fastq.gz -o s11_out --threads 1
spades.py -1 s12_R1.fastq.gz -2 s12_R2.fastq.gz -o s12_out --threads 1
spades.py -1 s13_R1.fastq.gz -2 s13_R2.fastq.gz -o s13_out --threads 1
spades.py -1 s14_R1.fastq.gz -2 s14_R2.fastq.gz -o s14_out --threads 1
spades.py -1 s15_R1.fastq.gz -2 s15_R2.fastq.gz -o s15_out --threads 1
spades.py -1 s16_R1.fastq.gz -2 s16_R2.fastq.gz -o s16_out --threads 1
spades.py -1 s17_R1.fastq.gz -2 s17_R2.fastq.gz -o s17_out --threads 1
spades.py -1 s18_R1.fastq.gz -2 s18_R2.fastq.gz -o s18_out --threads 1
spades.py -1 s19_R1.fastq.gz -2 s19_R2.fastq.gz -o s19_out --threads 1
spades.py -1 s20_R1.fastq.gz -2 s20_R2.fastq.gz -o s20_out --threads 1
spades.py -1 s21_R1.fastq.gz -2 s21_R2.fastq.gz -o s21_out --threads 1
spades.py -1 s22_R1.fastq.gz -2 s22_R2.fastq.gz -o s22_out --threads 1
```

run_spades_tamulauncher.sh

```
#!/bin/bash
#SBATCH --job-name=spades
#SBATCH --time=1-00:00:00
#SBATCH --nodes=2
#SBATCH --ntasks-per-node=64
#SBATCH --cpus-per-task=1
#SBATCH --mem=250G
#SBATCH --output=stdout.%x.%j
#SBATCH --error=stderr.%x.%j

module purge
module load GCC/11.2.0  SPAdes/3.15.3

tamulauncher commands.txt
```

run 64 spades.py commands per node with each command using 1 core.
Requesting all 64 cores on FASTER reserves entire node for your job

- run 64 single-core commands per node; useful when each command requires <= 3.7GB memory
- create a commands file (named whatever you want) to go with the the job script
- load the software module in the job script not the commands file

TAMULauncher Multi-Node Multi-Core Commands

commands.txt (500 lines for example)

```
spades.py -1 s1_R1.fastq.gz -2 s1_R2.fastq.gz -o s1_out --threads 4
spades.py -1 s2_R1.fastq.gz -2 s2_R2.fastq.gz -o s2_out --threads 4
spades.py -1 s3_R1.fastq.gz -2 s3_R2.fastq.gz -o s3_out --threads 4
spades.py -1 s4_R1.fastq.gz -2 s4_R2.fastq.gz -o s4_out --threads 4
spades.py -1 s5_R1.fastq.gz -2 s5_R2.fastq.gz -o s5_out --threads 4
spades.py -1 s6_R1.fastq.gz -2 s6_R2.fastq.gz -o s6_out --threads 4
spades.py -1 s7_R1.fastq.gz -2 s7_R2.fastq.gz -o s7_out --threads 4
spades.py -1 s8_R1.fastq.gz -2 s8_R2.fastq.gz -o s8_out --threads 4
spades.py -1 s9_R1.fastq.gz -2 s9_R2.fastq.gz -o s9_out --threads 4
spades.py -1 s10_R1.fastq.gz -2 s10_R2.fastq.gz -o s10_out --threads 4
spades.py -1 s11_R1.fastq.gz -2 s11_R2.fastq.gz -o s11_out --threads 4
spades.py -1 s12_R1.fastq.gz -2 s12_R2.fastq.gz -o s12_out --threads 4
spades.py -1 s13_R1.fastq.gz -2 s13_R2.fastq.gz -o s13_out --threads 4
spades.py -1 s14_R1.fastq.gz -2 s14_R2.fastq.gz -o s14_out --threads 4
spades.py -1 s15_R1.fastq.gz -2 s15_R2.fastq.gz -o s15_out --threads 4
spades.py -1 s16_R1.fastq.gz -2 s16_R2.fastq.gz -o s16_out --threads 4
spades.py -1 s17_R1.fastq.gz -2 s17_R2.fastq.gz -o s17_out --threads 4
spades.py -1 s18_R1.fastq.gz -2 s18_R2.fastq.gz -o s18_out --threads 4
spades.py -1 s19_R1.fastq.gz -2 s19_R2.fastq.gz -o s19_out --threads 4
spades.py -1 s20_R1.fastq.gz -2 s20_R2.fastq.gz -o s20_out --threads 4
spades.py -1 s21_R1.fastq.gz -2 s21_R2.fastq.gz -o s21_out --threads 4
spades.py -1 s22_R1.fastq.gz -2 s22_R2.fastq.gz -o s22_out --threads 4
```

run_spades_tamulauncher.sh

```
#!/bin/bash
#SBATCH --job-name=spades
#SBATCH --time=1-00:00:00
#SBATCH --nodes=2
#SBATCH --ntasks-per-node=16
#SBATCH --cpus-per-task=4
#SBATCH --mem=250G
#SBATCH --output=stdout.%x.%j
#SBATCH --error=stderr.%x.%j

module purge
module load GCC/11.2.0  SPAdes/3.15.3

tamulauncher commands.txt
```

run 16 spades.py commands per node with each command using 4 cores. Requesting all 64 cores on FASTER reserves entire node for your job

- useful when each command requires more than 3.7GB but less than all available memory
- use OMP_NUM_THREADS if needed when running fewer commands than requested cores
  - add on the line before the tamulauncher command
  - **export OMP_NUM_THREADS=$SLURM_CPUS_PER_TASK**

Making a TAMULauncher Commands File Part 1

Input files are two files per sample and named: `s1_R1.fastq.gz` `s1_R2.fastq.gz`
Run this command to create the example files:

```
mkdir seqs && touch seqs/s{1..40}_R{1,2}.fastq.gz
```

Run the following commands to get familiar with useful shell commands for creating and manipulating variables

```
file=seqs/s1_R1.fastq.gz
echo $file
basename $file
sample=$(basename $file)
echo $sample
echo ${sample/_R1.fastq.gz}
echo ${sample/R1/R2}
```

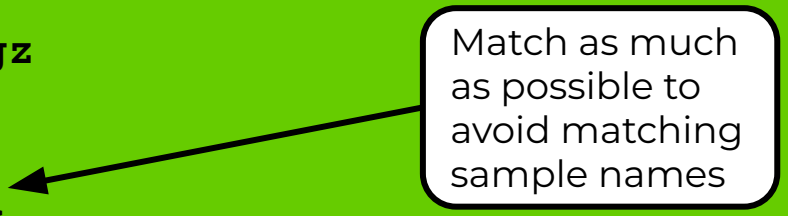
```
# create variable named file
# show contents of variable
# strip off path of variable
# create variable named sample
# show contents of variable
# strip off _R1.fastq.gz
# substitute R1 text with R2
```

Making a TAMULauncher Commands File Part 2

Input files are two files per sample and named: `s1_R1.fastq.gz` `s1_R2.fastq.gz`

- Run the following commands to loop through all R1 files in the reads directory and create the commands.txt
- Use just the R1 files because we only need to capture the sample names once.

```
for file in seqs/*_R1.*gz
do
read1=$file
read2=${read1/_R1./_R2.}
sample=$(basename ${read1/_R1.fastq.gz})
echo spades.py -1 $read1 -2 $read2 -o ${sample}_out --threads 1
done > commands.txt
```



Other Useful Unix Commands

```
${variable#*SubStr}    # will drop beginning of variable value up to first occurrence of 'SubStr'
${variable##*SubStr}   # will drop beginning of variable value up to last occurrence of 'SubStr'
${variable%SubStr*}    # will drop part of variable value from last occurrence of 'SubStr' to the end
${variable%%SubStr*}   # will drop part of variable value from first occurrence of 'SubStr' to the end
```

These are useful if the part of the filename for each sample that needs to be removed is not the same.

s1_S1_R1.fastq.gz **s2**_S2_R1.fastq.gz **s3**_S3_R1.fastq.gz

want to remove this part from each file name

Make a new directory and create a new set of files for this exercise.

```
mkdir seqs2
for i in {1..10}; do touch seqs2/s${i}_S${i}_R{1,2}.fastq.gz; done
```

Unix Command	Output
`file=seqs2/s1_S1_R1.fastq.gz`	
`echo $file`	`seqs2/s1_S1_R1.fastq.gz`
`echo ${file%_S*}`	`seqs2/s1`
`basename ${file%_S*}`	`s1`
`sample=$(basename ${file%_S*})`	
`echo $sample`	`s1`

Slurm Job Array Parameters and Runtime Environment Variables

- Array jobs are good to use when you have multiple samples each of which can utilize an entire compute node running software that supports multiple threads but does not support MPI
  - `--array=0-23` `# job array indexes 0-23`
  - `--array=1-24` `# job array indexes 1-24`
  - `--array=1,3,5,7` `# job array indexes 1,3,5,7`
  - `--array=1-7:2` `# job array indexes 1 to 7 with a step size of 2`
  - do not use `--nodes` with `--array`
- Use the index value to select which commands to run either from a text file of commands or as part of the input file name or parameter value
  - **`$SLURM_ARRAY_TASK_ID`** is the array index value
- stdout and stderr files can be saved per index value
  - **`--output=stdout.%x.%j.%A_%a`**
  - **`--error=stderr.%x.%j.%A_%a`**
- maximum array size is 1000 and max total pending and running jobs per user is 1000
- Limit the number of simultaneously running tasks
  - can help prevent reaching file and disk quotas due to many intermediate and temporary files
  - `--array=1-40%5` `# job array with indexes 1-40; max of 5 running array jobs`
  - as one job completes another array index is run on an available node

Slurm Job Array Example 1

```
#!/bin/bash
#SBATCH --job-name=bwa_array
#SBATCH --time=1-00:00:00
#SBATCH --array=1-40%5      # job array of indexes 1-40; max of 5 running array indexes
#SBATCH --ntasks-per-node=1
#SBATCH --cpus-per-task=64
#SBATCH --mem=250G
#SBATCH --output=stdout.%x.%j.%A_%a
#SBATCH --error=stderr.%x.%j.%A_%a

module purge
module load GCCcore/11.2.0  BWA/0.7.17
# get a line from commands.txt file into a variable named command
command=$(sed -n ${SLURM_ARRAY_TASK_ID}p commands.txt)
$command
```

- The sed command will print a specified line number from commands.txt based on the **$SLURM_ARRAY_TASK_ID**
- The number of lines in your commands.txt file should be the same as the number of array indexes
- Can use %5 to limit the array to a maximum of 5 nodes used simultaneously but you need enough SUs to cover entire number of array indexes in order to submit the job. May be useful to prevent creating too many temporary files.
- There are other ways to use **$SLURM_ARRAY_TASK_ID** but this example is useful because it has a file of all commands used in each array index
- Doesn't work when commands have redirection operators: | < >

Slurm Job Array Example 2

```
#!/bin/bash
#SBATCH --job-name=bwa_array
#SBATCH --time=1-00:00:00
#SBATCH --array=1-40          # run all 40 array indexes simultaneously using 40 nodes
#SBATCH --ntasks-per-node=1
#SBATCH --cpus-per-task=64
#SBATCH --mem=250G
#SBATCH --output=stdout.%x.%j.%A_%a
#SBATCH --error=stderr.%x.%j.%A_%a

module purge
module load GCCcore/11.2.0  BWA/0.7.17

bwa mem -M -t 64 -R '@RG\tID:\tLB:pe\tSM:DR34\tPL:ILLUMINA' genome.fasta \
sample_${SLURM_ARRAY_TASK_ID}_R1.fastq.gz  sample_${SLURM_ARRAY_TASK_ID}_R2.fastq.gz \
| samtools view -h -Sb - | samtools sort -o sample_${SLURM_ARRAY_TASK_ID}.out.bam \
-m 7G -@ 1 -T $TMPDIR/tmp4sort${SLURM_ARRAY_TASK_ID} -
```

- Lines ending with \ indicate the command continues on the next line
- do not put a space after \

- Can use **$SLURM_ARRAY_TASK_ID** if your commands only differ by a number in the file names
- The **$SLURM_ARRAY_TASK_ID** variable will be assigned the array index from 1 to 40 in this example
- Can use this approach when commands have redirection operators: | < >

Useful Slurm Runtime Environment Variables

- **$TMPDIR**
  - this is a temporary local disk space (3.84TB) created at runtime and is deleted when the job completes
  - the directory is mounted on the compute node and files created in $TMPDIR do not count against your file and disk quotas
  - **samtools sort -T $TMPDIR/sort**
- **$SLURM_CPUS_PER_TASK**
  - returns how many CPU cores were allocated on this node
  - can be used in your command to match requested #SBATCH cpus
    - **#SBATCH --cpus-per-task=64**
    - **samtools sort --threads $SLURM_CPUS_PER_TASK**
- **$SLURM_ARRAY_TASK_ID**
  - can be used to select or run one of many commands when using a job array
- **$SLURM_JOB_NAME**
  - populated by the `--job-name` parameter
  - **#SBATCH --job-name=bwa_array**
- **$SLURM_JOB_NODELIST**
  - can be used to get the list of nodes assigned at runtime
- **$SLURM_JOBID**
  - can be used to capture JobID at runtime

Useful Unix Environment Variables

- Type **`env`** to see all Unix environment variables for your login session
- **`$USER`**
  - This will be automatically populated with your NetID
    - **`echo $USER`**
- **`$SCRATCH`**
  - You can use this to change to your /scratch/user/netid directory
    - **`cd $SCRATCH`**
- **`$OMP_NUM_THREADS`**
  - used when software uses OpenMP for multithreading; default is 1
    - **`export OMP_NUM_THREADS=64`**
- **`$PWD`**
  - contains the full path of the current working directory

Finding NGS job template scripts using GCATemplates on HPRC clusters

```
mkdir $SCRATCH/slurm_class
```

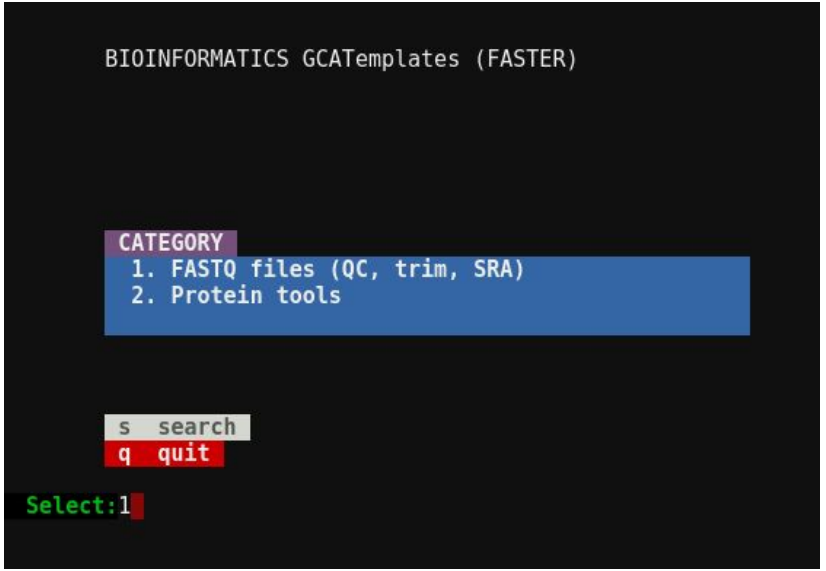
```
cd $SCRATCH/slurm_class
```

```
gcatemplates
```

For practice, we will copy a template file

- Enter 1 then continue through the menus to find the template that contains bbmap
  - or use the search to find bbmap
- Final step will save a template job script file to your current working directory

Genomic Computational Analysis Templates



Monitoring Job Resource Usage

Submit a Slurm Job

- Submit your job script
  - `sbatch run_bbmap_38.96_bbnorm_faster.sh`
- See status and JobID of all your submitted jobs
  - `squeue -u $USER`

```
  JOBID    PARTITION    NAME     USER      STATE    TIME   TIME_LIMIT   NODES NODELIST(REASON)
  119112   cpu          bbnorm   mynetid   RUNNING  3:54   1:00:00      1     fc083
```

- Can cancel (kill) a PENDING or RUNNING job using JOBID
  - `scancel JOBID`

Monitor CPU usage for a FASTER Running Job

- See CPU and memory usage of all your running jobs
  - `pestat -u $USER`
  - stats for pestat are updated every **3** minutes

```
Hostname   Partition   Node    Num_CPU  CPUload   Memsize   Freemem    Joblist
                       State   Use/Tot             (MB)      (MB)     JobId  User ...
fc162         cpu*      mix    64   64   63.56*   256000    253786   731601 netid
fc163         cpu*      mix    64   64   61.78*   256000    253404   731601 netid
fc164         gpu*      mix    56   64   25.65*   256000    253492   731601 netid
fc165         gpu*      mix    28   64   27.10*   256000    239764   731601 netid
fc166         gpu*      mix    28   64    0.01*   256000    238543   731601 netid
```

Low CPU load utilization highlighted in **Red**
Good CPU load utilization highlighted in **Purple**
Ideal CPU load utilization displayed in White
(Freemem should also be noted)

Monitor a Running Job

- See lots of info about your running or recently completed (~10 minutes) job

```
scontrol show job JobID
```

- can add this command at the beginning of your job script to capture job info into the stdout file

```
scontrol show job $SLURM_JOB_ID
```

example #SBATCH parameters

```
#!/bin/bash
#SBATCH --job-name=bbnorm
#SBATCH --time=01:00:00
#SBATCH --ntasks-per-node=1
#SBATCH --cpus-per-task=64
#SBATCH --mem=250G
#SBATCH --output=stdout.%x.%j
#SBATCH --error=stderr.%x.%j
```

```
JobId=119112 JobName=bbnorm
   UserId=mynetid(99999) GroupId=mynetid(99999) MCS_label=N/A
   Priority=22505 Nice=0 Account=hprc QOS=normal
   JobState=RUNNING Reason=None Dependency=(null)
   Requeue=1 Restarts=0 BatchFlag=1 Reboot=0 ExitCode=0:0
   RunTime=00:00:09 TimeLimit=01:00:00 TimeMin=N/A
   SubmitTime=2023-02-06T10:03:44 EligibleTime=2023-02-06T10:03:44
   AccrueTime=2023-02-06T10:03:44
   StartTime=2023-02-06T10:03:45 EndTime=2023-02-06T11:03:45 Deadline=N/A
   SuspendTime=None SecsPreSuspend=0 LastSchedEval=2023-02-06T10:03:45
Scheduler=Main
   Partition=cpu AllocNode:Sid=login2:513947
   ReqNodeList=(null) ExcNodeList=(null)
   NodeList=fc083
   BatchHost=fc083
   NumNodes=1 NumCPUs=64 NumTasks=1 CPUs/Task=64 ReqB:S:C:T=0:0:*:*
   TRES=cpu=64,mem=250G,node=1,billing=64
   Socks/Node=* NtasksPerN:B:S:C=1:0:*:* CoreSpec=*
   MinCPUsNode=64 MinMemoryNode=250G MinTmpDiskNode=0
   Features=(null) DelayBoot=00:00:00
   OverSubscribe=OK Contiguous=0 Licenses=(null) Network=(null)

Command=/scratch/user/mynetid/slurm_class/run_bbmap_38.96_bbnorm_faster.sh
   WorkDir=/scratch/user/mynetid/slurm_class
   StdErr=/scratch/user/mynetid/slurm_class/stderr.bbnorm.119112
   StdIn=/dev/null
   StdOut=/scratch/user/mynetid/slurm_class/stdout.bbnorm.119112
   Power=
```

See Completed Job Efficiency Stats

seff JobID

will show CPU and Memory efficiency based on selected resources

```
seff 119112

Job ID: 119112
Cluster: faster
User/Group: mynetid/mynetid
State: COMPLETED (exit code 0)
Nodes: 1
Cores per node: 64
CPU Utilized: 03:20:22
CPU Efficiency: 57.80% of 05:46:40
core-walltime
Job Wall-clock time: 00:05:25
Memory Utilized: 118.81 GB
Memory Efficiency: 47.52% of 250.00 GB
```

CPU load was at 100% for 57% of the run time or 37 cores were at 100% for the job time or some other combination

max memory utilized was 47% of requested memory

Monitor GPU and CPU usage for a Job

You can use the jobstats command to monitor resource usage and create graphs

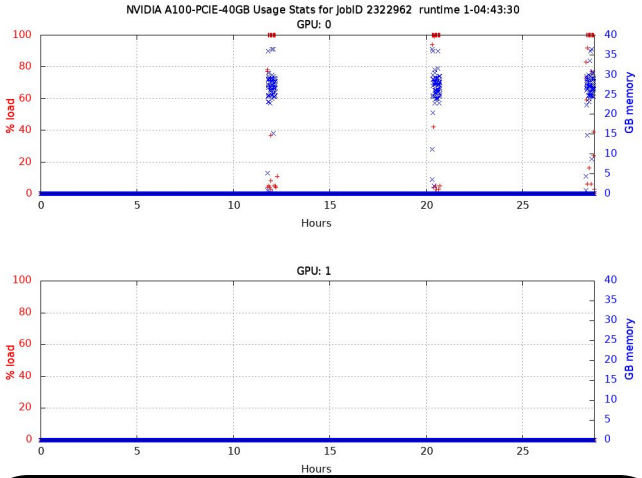
```
#!/bin/bash
#SBATCH --job-name=my_job
#SBATCH --time=2-00:00:00
#SBATCH --ntasks-per-node=1
#SBATCH --cpus-per-task=64
#SBATCH --mem=250G
#SBATCH --gres=gpu:a100:2
#SBATCH --partition=gpu
#SBATCH --output=stdout.%x.%j
#SBATCH --error=stderr.%x.%j

module purge
module load CUDA/11.7.0

# run jobstats in the background (&) to monitor resource usage
jobstats &

my_gpu_command

# run jobstats to create graphs of resource usage for this job
jobstats
```



- Notice that GPU: 1 was not used in this job.
- Next time configure job script to use just 1 GPU
  `--gres=gpu:a100:1`

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

See All Your Jobs for Current Fiscal Year

- `myproject -j all`
  - ProjectAccount
  - JobID
  - JobArrayIndex
  - SubmitTime
  - StartTime
  - EndTime
  - Walltime
  - TotalSlots
  - UsedSUs
  - Total Jobs
  - Total Usage (SUs)

It will take a few days for today's jobs to show up in the results

Debugging Job Submission

- The job was not scheduled
  - make sure the job CPU count and memory specification exist
    - ```
      sbatch: error: CPU count per node can not be satisfied
      sbatch: error: Batch job submission failed: Requested node configuration is not available
      ```
  - check your HPRC default account to see if you have enough SUs
    - **`myproject`**
    - ask your PI to allocate SUs to your account
    - Set or change your default account
      - **`myproject -d`** Account

```
[mynetid@faster2 bbnorm]$ myproject
run 'myproject -h' to see the other options.
================================================================================================
               List of mynetid's Project Accounts
------------------------------------------------------------------------------------------------
|  Account    |  FY  | Default | Allocation |Used & Pending SUs|   Balance    |       PI         |
------------------------------------------------------------------------------------------------
|123456789101|  2023|        Y|     5000.00|           4999.00|        1.00 |X, Reveille       |
------------------------------------------------------------------------------------------------
|123456789102|  2023|        N| 10000000.00|              0.00| 10000000.00 |X, Reveille       |
------------------------------------------------------------------------------------------------
```
```

PENDING Jobs

- If your job is in the PENDING state for a long time
  - check to see if the cluster is busy using `sinfo` or see hprc.tamu.edu
  - use `gpuavail` to see if the gpu partition is busy
  - check to see if your job walltime overlaps with a scheduled maintenance
    - `maintenance`

```
The scheduled 11 hour FASTER maintenance will start in:

  3 days   16 hours   41 minutes

Scheduled jobs will not start if they overlap with this maintenance window.
```

A 7-day job submitted at the time of the above message will remain queued and will not start until after the maintenance is complete

Debugging Slurm Jobs

- Look for an out of memory error message; could occur in only one index of a job array

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

  - Increase the amount of SBATCH memory in your job script and resubmit the job
- If you see an '*Out of disk space*' or '*No space left on device*' error
  - check your file and disk quotas using the showquota command
    - **`showquota`**
  - reduce the number of files you have generated
    - delete any nonessential or temporary files
    - use **`$TMPDIR`** in your command if software supports a temporary directory
    - create and download a .tar.gz package of completed projects and delete the original directory to free up disk space
  - request a temporary increase in file and/or disk quota for your project

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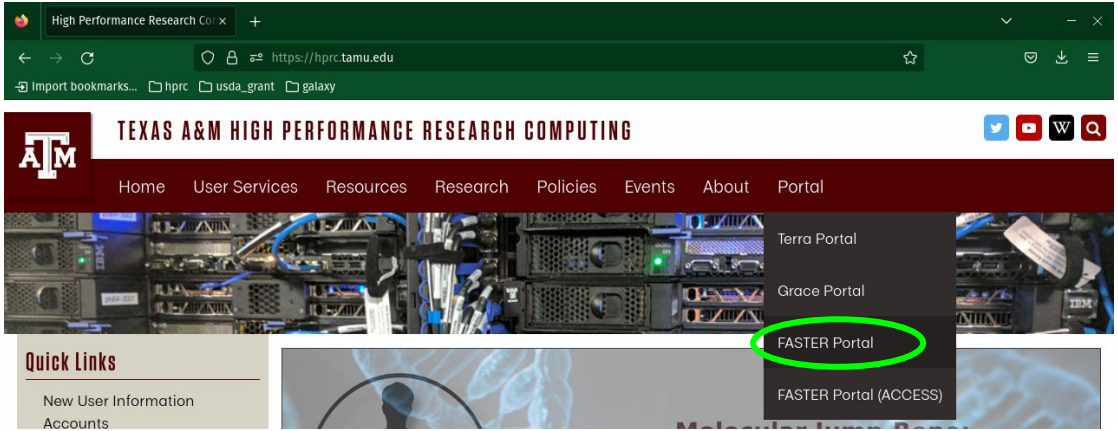
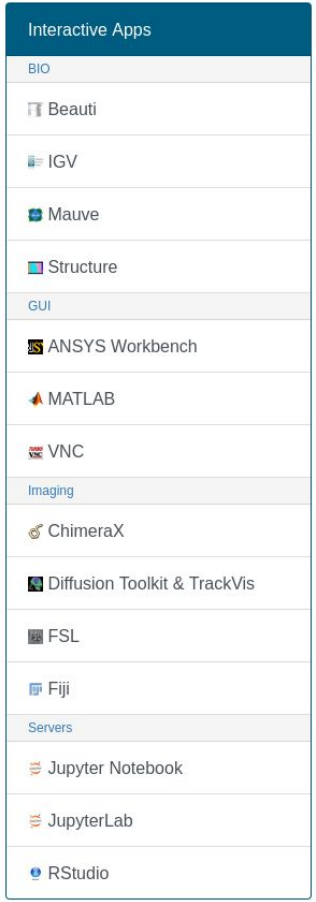
The HPRC portal allows users to do the following

- Browse files on the the FASTER filesystem
- Access the FASTER Unix command line
  - no SUs charged for using command line
  - SUs charged for jobs launched from command line
  - runs on login node; limit your processes to 8 cores
- Compose job scripts
- Launch interactive GUI apps (SUs charged)
- Monitor and stop running jobs and interactive sessions





Need Help?

First check the FAQ hprc.tamu.edu/wiki/HPRC:CommonProblems

- FASTER User Guide hprc.tamu.edu/wiki/FASTER
- Email your questions to help@hprc.tamu.edu

Help us, help you -- we need more info

- Which Cluster
- Username
- JobID(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

Let us know when the issue has been resolved so we can close the helpdesk ticket