# Running batch jobs at TACC

**Reservations**

Use our summer school ***reservation*** (**CoreNGS-Tue**) when submitting batch jobs to get higher priority on the **ls6** normal queue ***today***:

```
sbatch --reservation=CoreNGS-Tue <batch_file>.slurm
idev -m 180 -N 1 -A OTH21164 -r CoreNGS-Tue
```

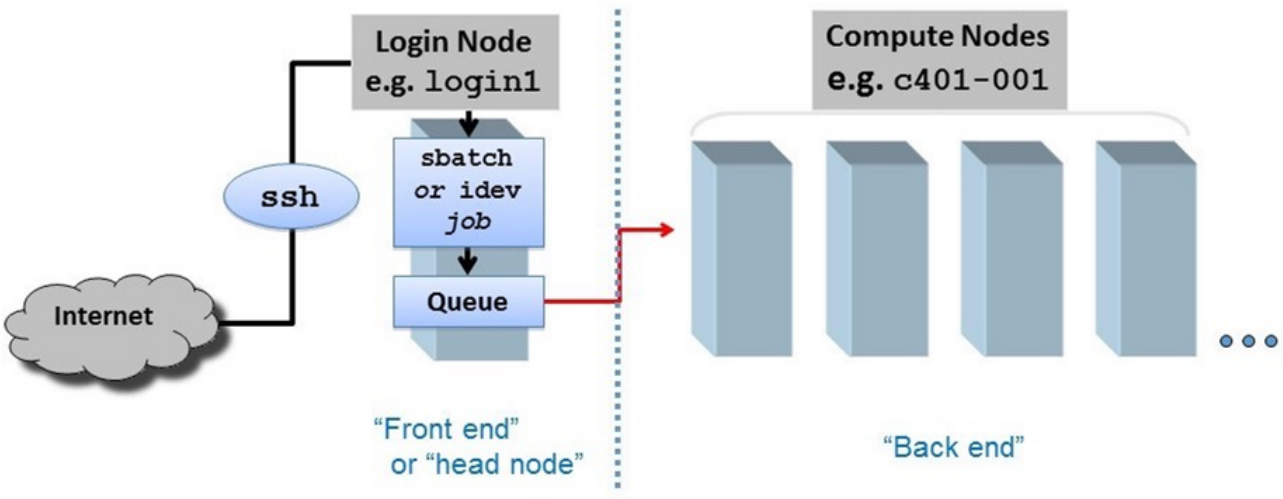
Note that the reservation name (**CoreNGS-Tue**) is different from the TACC allocation/project for this class, which is **OTH21164**.



## Compute cluster overview

When you SSH into **ls6**, your session is assigned to one of a small set of ***login nodes*** (also called ***head nodes***). These are separate from the ***cluster compute nodes*** that will run your jobs.

Think of a node as a computer, like your laptop, but probably with more cores and memory. Now multiply that computer a thousand or more, and you have a cluster.




The small set of login nodes are a shared resource (type the **users** command to see everyone currently logged in) and are ***not*** meant for running interactive programs – for that you submit a description of what you want done to a ***batch system***, which distributes the work to one or more compute nodes.

On the other hand, the login nodes *are* intended for copying files to and from TACC, so they have ***a lot*** of network bandwidth while compute nodes have limited network bandwidth.

So follow these guidelines:

- ***Do not perform substantial computation on the login nodes***.
  - They are closely monitored, and you will get warnings from the TACC admin folks!
  - Code is usually developed and tested somewhere other than TACC, and only moved over when pretty solid.
- ***Do not perform significant network access from your batch jobs***.
  - Instead, ***stage your data from a* login** node onto $SCRATCH before submitting your job.

## Lonestar6 and Stampede2 overview and comparison

Here is a comparison of the configurations and **ls6** and **stampede2**. As you can see, **stampede2** is the larger cluster, launched in 2017, but **ls6**, launched om 2022, has fewer but more powerful nodes.

| | **ls6** | **stampede2** |
|---|---|---|
| **login nodes** | 3<br><br>128 cores each<br>256 GB memory | 6<br><br>28 cores each<br>128 GB memory |
| **standard compute nodes** | 560 AMD Epyc Milan processors<br><br>128 cores per node<br>256 GB memory | 4,200 KNL (Knights Landing) processors<br><br>• 68 cores per node (272 virtual)<br>• 96 GB memory<br><br>1,736 SKX (Skylake) processors<br><br>• 48 cores per node (96 virtual)<br>• 192 GB memory |
| **GPU nodes** | 16 AMD Epyc Milan processors<br><br>128 cores per nod<br>256 GB memory<br><br>2x NVIDIA A100 GPUs<br>w/ 40GB RAM onboard | -- |
| **batch system** | **SLURM** | **SLURM** |
| **maximum job run time** | 48 hours, normal queue<br><br>2 hours, development queue | 96 hours on KNL nodes, normal queue<br><br>48 hours on SKX nodes, normal queue<br><br>2 hours, development queue |

User guides for **ls6** and **stampede2** can be found at:

- https://portal.tacc.utexas.edu/user-guides/lonestar6
- https://portal.tacc.utexas.edu/user-guides/stampede2

Unfortunately, the TACC user guides are aimed towards a different user community – the weather modelers and aerodynamic flow simulators who need very fast matrix manipulation and other High Performance Computing (HPC) features. The usage patterns for bioinformatics – generally running 3rd party tools on many different datasets – is rather a special case for HPC. TACC calls our type of processing "***parameter sweep jobs***" and has a special process for running them, using their **launcher** module.

### About cores and hyperthreads

Note the use of the term ***virtual core*** on **stampede2**. Compute ***cores*** are standalone processors – mini CPUs, each of which can execute separate sets of instructions. However modern cores may also have ***hyperthreading*** enabled, where a single core can ***appear*** as more than one virtual processor to the operating system (see https://en.wikipedia.org/wiki/Hyper-threading). For example, **stampede2** nodes have 2 or 4 ***hyperthreads*** (***HTs***) per core. So KNL nodes with 4 HTs for each of the 68 physical cores, have a total of 272 ***virtual cores***.

***Threading*** is an operating system scheduling mechanism for allowing one CPU/core to execute multiple computations, ***seemingly*** in parallel.

The writer of a program that takes advantage of threading first identifies portions of code that can run in parallel because the computations are ***independen***. The programmer assigns some number of threads to that work (usually based on a command-line option) using specific thread and synchronization programming language constructs. An example is the the **samtools sort -@ N** option to specify **N** threads can be used for sorting independent sets of the input alignments.

If there are multiple cores/CPUs available, the operating system can assign a program thread to each of them for actual parallelism. But only "seeming" (or virtual) parallelism occurs if there are fewer cores than the number of threads specified.

Suppose there's only one core/CPU. The OS assigns program thread A to the core to run until the program performs an I/O operation that causes it to be "suspended" for the I/O operation to complete. During this time, when normally the CPU would be doing nothing but waiting on the I/O to complete, the OS assigns program thread B to the CPU and lets it do some work. This threading allows more efficient use of existing cores as long as the multiple program threads being assigned do some amount of I/O or other operations that cause them to suspend. But trying to run multiple compute-only, no-I/O programs using multiple threads on one CPU just causes "***thread thrashing***" -- OS scheduler overhead when threads are suspended for time, not just I/O.

The analogy is a grocery store where there are 5 customers (threads). If there are 5 checkout lines (cores), each customer (thread) can be serviced in a separate checkout line (core). But if there's only one checkout line (core) open, the customers (threads) will have to wait in line. To be a more accurate analogy, any checkout clerk would be able to handle some part of checkout for each customer, then while waiting for the customer to find and enter credit card information, the clerk could handle a part of a different customer's checkout.

***Hyperthreading*** is just a hardware implementation of OS scheduling. Each CPU offers some number of "virtual cores" (***hyperthreads***) that can "almost" act like separate cores using various hardware tricks. Still, if the work assigned to multiple hyperthreads on a single core does not pause from time to time, ***thread thrashing*** will occur.

# Software at TACC

## Programs and your $PATH

When you type in the name of an arbitrary program (**ls** for example), how does the shell know where to find that program? The answer is your **$PATH**. **$PATH** is a predefined environment variable whose value is a list of directories.The shell looks for program names in that list, in the order the directories appear.

To determine where the shell will find a particular program, use the **which** command. Note that **which** tells you where it looked if it cannot find the program.

**Using which to search $PATH**

```
which rsync
which cat

which bwa # not yet available to you
```

## The module system

The **module** system is an incredibly powerful way to have literally thousands of software packages available, some of which are incompatible with each other, without causing complete havoc. The TACC staff stages packages in well-known locations that are NOT on your **$PATH**. Then, when a module is loaded, its binaries are added to your **$PATH**.

For example, the following **module load** command makes the **singularity** container management system available to you:

**How module load affects $PATH**

```
# first type "singularity" to show that it is not present in your environment:
singularity
# it's not on your $PATH either:
which singularity

# now add biocontainers to your environment and try again:
module load biocontainers
# and see how singularity is now on your $PATH:
which singularity
# you can see the new directory at the front of $PATH
echo $PATH

# to remove it, use "unload"
module unload biocontainers
singularity
# gone from $PATH again...
which singularity
```

### TACC BioContainers modules

It is quite a large systems administration task to install software at TACC and configure it for the module system. As a result, TACC was always behind in making important bioinformatics software available. To address this problem, TACC moved to providing bioinformatics software via ***containers***, which are ***virtual machines*** like **VMware** and **Virtual Box**, but are lighter weight: they require less disk space because they rely more on the host's base Linux environment. Specifically, TACC (and many other **H**igh **P**erformance **C**omputing clusters) use **Singularity** containers, which are similar to **Docker** containers but are more suited to the HPC environment (in fact one can build a **Docker** container then easily convert it to **Singularity** for use at TACC).

TACC obtains its containers from **BioContainers** (https://biocontainers.pro/ and https://github.com/BioContainers/containers), a large public repository of bioinformatics tool **Singularity** containers. This has allowed TACC to easily provision thousands of such tools!

These **BioContainers** are not visible in TACC's "standard" module system, but only after the master **biocontainers** module is loaded. Once it has been loaded, you can search for your favorite bioinformatics program using **module spider**.

```
# Verify that samtools is not available
samtools
# and cannot be found in the standard module system
module spider samtools

# Load the BioContainers master module (this takes a while)
module load biocontainers

# Now look for these programs
module spider samtools
module spider Rstats
module spider kallisto
module spider bowtie2
module spider minimap2
module spider multiqc
module spider gatk
module spider velvet
```

Notice how the **BioContainers** module names have "**ctr**" in their names, version numbers, and other identifying information.

The standard TACC module system has been phased out for bioinformatics programs, so always look for your application in **BioContainers**.

While it's great that there are now hundreds of programs available through **BioContainers**, the one drawback is that they can only be run on cluster compute nodes, not on login nodes. To test **BioContainer** program interactively, you will need to use TACC's **idev** command to obtain an interactive cluster node. More on this shortly...

### loading a biocontainer module

Once the **biocontainers** module has been loaded, you can just **module load** the desired tool, as with the **kallisto** pseudo-aligner program below.

```
# Load the Biocontainers master module
module load biocontainers

# Verify kallisto is not yet available
kallisto

# Load the default kallisto biocontainer
module load kallisto

# Verify kallisto is not available (although not on login nodes)
kallisto
```

Note that loading a **BioContainer** does not add anything to your **$PATH**. Instead, it defines an ***alias***, which is just a shortcut for executing the command. You can see the **alias** definition using the **type** command. And you can ensure the program is available using the **command -v** utility.

```
# Note that kallisto has not been added to your $PATH, but instead has an alias
which kallisto

# Ensure kallisto is available with command -v
command -v kallisto
```

### installing custom software

Even with all the tools available at TACC, inevitably you'll need something they don't have. In this case you can build the tool yourself and install it in a local TACC directory. While building 3rd party tools is beyond the scope of this course, it's really not that hard. The trick is keeping it all organized.

For one thing, remember that your **$HOME** directory quota is fairly small (10 GB on **ls6**), and that can fill up quickly if you install many programs. We recommend creating an installation area in your **$WORK** directory and installing programs there. You can then make symbolic links to the binaries you need in your **~/local/bin** directory (which was added to your **$PATH** in your **.bashrc**).

See how we used a similar trick to make the **launcher_creator.py** program available to you. Using the **ls -l** option shows you where symbolic links point to:

**Real location of launcher_creator.py**

```
ls -l ~/local/bin

# this will tell you the real location of the launcher_creator.py script is
# /work/projects/BioITeam/common/bin/launcher_creator.py
```

**$PATH caveat**

Remember that the order of locations in the **$PATH** environment variable is the order in which the locations will be searched.

# Job Execution

Job execution is controlled by the **SLURM** batch system on both **stampede2** and **ls6**.

To run a job you prepare 2 files:

1. a ***commands file*** file containing the commands to run, ***one task per line*** (**<job_name>.cmds**)
2. a ***job control file*** that describes how to run the job (**<job_name>.slurm**)

The process of running the job involves these steps:

1. Create a ***commands file*** containing ***exactly one task per line***.
2. Prepare a ***job control file*** for the commands file that describes how the job should be run.
3. You ***submit*** the ***job control file*** to the ***batch system***. The job is then said to be ***queued*** to run.
4. The batch system ***prioritizes*** the job based on the number of compute nodes needed and the job run time requested.
5. When compute nodes become available, the job tasks (command lines in the **<job_name>.cmds** file) are ***assigned*** to one or more compute nodes and ***begin to run*** in parallel.
6. The job ***completes*** when either:
    a. you ***cancel*** the job manually
    b. ***all job tasks complete*** (successfully or not!)
    c. the requested ***job run time has expired***

## SLURM at a glance

Here are the main components of the **SLURM** batch system.

| | **stampede2, ls5** |
|---|---|
| **batch system** | **SLURM** |
| **batch control file name** | **`<job_name>.slurm`** |
| **job submission command** | **`sbatch <job_name>.slurm`** |
| **job monitoring command** | **`showq -u`** |
| **job stop command** | **`scancel -n <job name>`** |

## Simple example

Let's go through a simple example. Execute the following commands to copy a pre-made **simple.cmds** commands file:

**Copy simple commands**

```
mkdir -p $SCRATCH/core_ngs/slurm/simple
cd $SCRATCH/core_ngs/slurm/simple
cp $CORENGS/tacc/simple.cmds .
```

What are the tasks we want to do? Each task corresponds to one line in the **simple.cmds** commands file, so let's take a look at it using the **cat** (con**cat**enat e) command that simply reads a file and writes each line of content to ***standard output*** (here, your **Terminal**):

**View simple commands**

```
cat simple.cmds
```

The tasks we want to perform look like this:

**simple.cmds commands file**

```
sleep 5; echo "Command 1 on `hostname` - `date`" > cmd1.log 2>&1
sleep 5; echo "Command 2 on `hostname` - `date`" > cmd2.log 2>&1
sleep 5; echo "Command 3 on `hostname` - `date`" > cmd3.log 2>&1
sleep 5; echo "Command 4 on `hostname` - `date`" > cmd4.log 2>&1
sleep 5; echo "Command 5 on `hostname` - `date`" > cmd5.log 2>&1
sleep 5; echo "Command 6 on `hostname` - `date`" > cmd6.log 2>&1
sleep 5; echo "Command 7 on `hostname` - `date`" > cmd7.log 2>&1
sleep 5; echo "Command 8 on `hostname` - `date`" > cmd8.log 2>&1
```

There are 8 tasks. Each task sleeps for 5 seconds, then uses the **echo** command to output a string containing the task number and date to a log file named for the task number. Notice that we can put two commands on one line if they are separated by a semicolon ( ; ).

Use the handy **launcher_creator.py** program to create the job control file.

**Create batch submission script for simple commands**

```
launcher_creator.py -j simple.cmds -n simple -t 00:01:00 -a OTH21164 -q development
```

You should see output something like the following, and you should see a **simple.slurm** batch submission file in the current directory.

```
Project simple.
Using job file simple.cmds.
Using development queue.
For 00:01:00 time.
Using OTH21164 allocation.
Not sending start/stop email.
Launcher successfully created. Type "sbatch simple.slurm" to queue your job.
```

Submit your batch job then check the batch queue to see the job's status.

**Submit simple job to batch queue**

```
sbatch simple.slurm
showq -u

# Output looks something like this:
-------------------------------------------------------------
          Welcome to the Lonestar6 Supercomputer
-------------------------------------------------------------
--> Verifying valid submit host (login1)...OK
--> Verifying valid jobname...OK
--> Verifying valid ssh keys...OK
--> Verifying access to desired queue (normal)...OK
--> Checking available allocation (OTH21164)...OK
Submitted batch job 232542
```

The queue status will show your job as **ACTIVE** while its running, or **WAITING** if not.

```
SUMMARY OF JOBS FOR USER: <abattenh>

ACTIVE JOBS--------------------
JOBID     JOBNAME    USERNAME      STATE   NODES REMAINING STARTTIME
================================================================================
924965    simple     abattenh      Running 1      0:00:42  Sat Jun  3 21:33:31

WAITING JOBS------------------------
JOBID     JOBNAME    USERNAME      STATE   NODES WCLIMIT   QUEUETIME
================================================================================

Total Jobs: 1     Active Jobs: 1     Idle Jobs: 0     Blocked Jobs: 0
```

If you don't see your **simple** job in either the **ACTIVE** or **WAITING** sections of your queue, it probably already finished – it should only run for a few seconds!

Notice in my queue status, where the **STATE** is **Running**, there is only one node assigned. Why is this, since there were 8 tasks?

Every job, no matter how few tasks requested, will be assigned at least one node. Each **lonestar6** node has 128 physical cores, so each of the 8 tasks can be assigned to a different core.

**Exercise: What files were created by your job?**

**ls** should show you something like this:

```
cmd1.log  cmd3.log  cmd5.log  cmd7.log  simple.cmds     simple.o924965
cmd2.log  cmd4.log  cmd6.log  cmd8.log  simple.e924965  simple.slurm
```

The newly created files are the **.log** files, as well as error and output logs **simple.e924965** and **simple.o924965**.

**filename wildcarding**

You can look at one of the output log files like this:

```
cat cmd1.log
```

But here's a cute trick for viewing the contents all your output files at once, using the **cat** command and filename ***wildcarding***.

**Multi-character filename wildcarding**

```
cat cmd*.log
```

The **cat** command can take a list of one or more files. The **asterisk** ( ***** ) in **cmd*.log** is a ***multi-character wildcard*** that matches any filename starting with **cmd** then ending with **.log**.

You can also specify ***single-character matches*** inside brackets ( **[ ]** ) in either of the ways below, this time using the **ls** command so you can better see what is matching:

**Single character filename wildcarding**

```
ls cmd[1234].log
ls cmd[2-6].log
```

This technique is sometimes called ***filename globbing***, and the pattern a ***glob***. Don't ask me why – it's a Unix thing. ***Globbing*** – translating a glob pattern into a list of files – is one of the handy thing the **bash** shell does for you. (Read more about **Pathname wildcards**)

**Exercise: How would you list all files starting with "simple"?**

```
ls simple*
```

Here's what my **cat** output looks like. Notice the times are all nearly the same because all the tasks ran in parallel. That's the power of cluster computing!

```
Command 1 on c304-005.ls6.tacc.utexas.edu - Sat Jun  3 21:33:50 CDT 2023
Command 2 on c304-005.ls6.tacc.utexas.edu - Sat Jun  3 21:33:44 CDT 2023
Command 3 on c304-005.ls6.tacc.utexas.edu - Sat Jun  3 21:33:46 CDT 2023
Command 4 on c304-005.ls6.tacc.utexas.edu - Sat Jun  3 21:33:47 CDT 2023
Command 5 on c304-005.ls6.tacc.utexas.edu - Sat Jun  3 21:33:51 CDT 2023
Command 6 on c304-005.ls6.tacc.utexas.edu - Sat Jun  3 21:33:47 CDT 2023
Command 7 on c304-005.ls6.tacc.utexas.edu - Sat Jun  3 21:33:51 CDT 2023
Command 8 on c304-005.ls6.tacc.utexas.edu - Sat Jun  3 21:33:49 CDT 2023
```

**echo**

Lets take a closer look at a typical task in the **simple.cmds** file.

**A simple.cmds task line**

```
sleep 5; echo "Command 3 `date`" > cmd3.log 2>&1
```

The **echo** command is like a print statement in the **bash** shell. **echo** takes its arguments and writes them to ***standard output***. While not always required, it is a good idea to put **echo**'s output string in double quotes.

**backtick evaluation**

So what is this funny looking **`date`** bit doing? Well, **date** is just another Linux command (try just typing it in) that just displays the current date and time. Here we don't want the shell to put the string "date" in the output, we want it to ***execute*** the **date** command and put the ***result*** text into the output. The **backquotes** ( `` also called ***backticks***) around the **date** command tell the shell we want that command executed and its ***standard output*** substituted into the string. (Read more about **Quoting in the shell**.)

**Backtick evaluation**

```
# These are equivalent:
date
echo `date`

# But different from this:
echo date
```

**output redirection**

There's still more to learn from one of our simple tasks, something called ***output redirection***.

Every command and Unix program has three "built-in" streams: ***standard input***, ***standard output*** and ***standard error***, each with a name, a number, and a ***redirection*** syntax.


Normally **echo** writes its string to ***standard output***, but it could encounter an error and write an error message to ***standard error***. We want both ***standard output*** and ***standard error*** for each task stored in a log file named for the command number.

**A simple.cmds task line**

```
sleep 5; echo "Command 3 `date`" > cmd3.log 2>&1
```

So in the above example the first '**>**' says to redirect the ***standard output*** of the **echo** command to the **cmd3.log** file. The '**2>&1**' part says to redirect ***standard error*** to the same place. Technically, it says to redirect ***standard error*** (built-in Linux stream **2**) to the same place as ***standard output*** (built-in Linux stream **1**); and since ***standard output*** is going to **cmd3.log**, any ***standard error*** will go there also. (Read more about **Standard streams and redirection**)

When the TACC batch system runs a job, all outputs generated by tasks in the batch job are directed to one output and error file per job. Here they have names like **simple.e924965** and **simple.o924965**. **simple.o924965** contains all ***standard output*** and **simple.o924965** contains all ***standard error*** generated by your tasks that was not redirected elsewhere, as well as information relating to running your job and its tasks. For large jobs with complex tasks, it is not easy to troubleshoot execution problems using these files.

So a best practice is to ***separate the outputs*** of all our tasks into individual log files, one per task, as we do here. Why is this important? Suppose we run a job with 100 commands, each one a whole pipeline (alignment, for example). 88 finish fine but 12 do not. Just try figuring out which ones had the errors, and where the errors occurred, if all the ***standard output*** is in one intermingled file and all ***standard error*** in the other intermingled file!

## Job parameters

Now that we've executed a really simple job, let's take a look at some important job submission parameters. These correspond to arguments to the **launcher_creator.py** script.

A bit of background. Historically, TACC was set up to cater to researchers writing their own **C** or **Fortran** codes highly optimized to exploit parallelism (the HPC crowd). Much of TACC's documentation is aimed at this audience, which makes it difficult to pick out the important parts for us.

The kind of jobs we biologists generally run are relatively new to TACC. They even have a special name for them: "***parametric sweeps***", by which they mean the ***same program*** running on ***different data*** sets.

In fact there is a special software module required to run our jobs, called the **launcher** module. You don't need to worry about activating the launcher module – that's done by the **<job_name>.slurm** script created by **launcher_creator.py** like this:

```
module load launcher
```

The **launcher** module knows how to interpret various job parameters in the **<job_name>.slurm** batch **SLURM** submission script and use them to create your job and assign its tasks to compute nodes. Our **launcher_creator.py** program is a simple **Python** script that lets you specify job parameters and writes out a valid **<job_name>.slurm** submission script.

### launcher_creator.py

If you call **launcher_creator.py** with no arguments it gives you its usage description. Because it is a long help message, we may want to pipe the output to **more**, a ***pager*** that displays one screen of text at a time. Type the **spacebar** to advance to the next page, and **Ctrl-c** to exit from **more**.

**Get usage information for launcher_creator.py**

```
# Use spacebar to page forward; Ctrl-c to exit
launcher_creator.py | more
```

**launcher_creator.py usage**

```
usage: launcher_creator.py [-h] -n NAME -t TIME_REQUEST [-j JOB_FILE]
                           [-b SHELL_COMMANDS] [-B SHELL_COMMANDS_FILE]
                           [-q QUEUE] [-a [ALLOCATION]] [-m MODULES]
                           [-M MODULES_FILE] [-w WAYNESS] [-N NUM_NODES]
                           [-e [EMAIL]] [-l LAUNCHER] [-s]

Create launchers for TACC clusters. Report problems to rt-
other@ccbb.utexas.edu

optional arguments:
  -h, --help            show this help message and exit

Required:
  -n NAME, --name NAME  The name of your job.
  -t TIME_REQUEST, --time TIME_REQUEST
                        The time you want to give to your job. Format:
                        hh:mm:ss

Commands:
  You must use at least one of these options to submit your commands for TACC.

  -j JOB_FILE, --jobs JOB_FILE
                        The name of the job file containing your commands.
  -b SHELL_COMMANDS, --bash SHELL_COMMANDS
                        A string of shell (Bash, zsh, etc) commands that are
                        executed before any parametric jobs are launched.
  -B SHELL_COMMANDS_FILE, --bash_file SHELL_COMMANDS_FILE
                        A file containing shell (Bash, zsh, etc) commands that
                        are executed before any parametric jobs are launched.

Optional:
  -q QUEUE, --queue QUEUE
                        The TACC allocation for job submission.
                        Default="development"
  -a [ALLOCATION], -A [ALLOCATION], --allocation [ALLOCATION]
                        The TACC allocation for job submission. You can set a
                        default ALLOCATION environment variable.
  -m MODULES, --modules MODULES
                        A list of module commands. The "launcher" module is
                        always automatically included. Example: -m "module
                        swap intel gcc; module load bedtools"
  -M MODULES_FILE, --modules_file MODULES_FILE
                        A file containing module commands.
  -w WAYNESS, --wayness WAYNESS
                        Wayness: the number of commands you want to give each
                        node. The default is the number of cores per node.
  -N NUM_NODES, --num_nodes NUM_NODES
                        Number of nodes to request. You probably don't need
                        this option. Use wayness instead. You ONLY need it if
                        you want to run a job list that isn't defined at the
                        time you submit the launcher.
  -e [EMAIL], --email [EMAIL]
                        Your email address if you want to receive an email
                        from Lonestar when your job starts and ends. Without
                        an argument, it will use a default EMAIL_ADDRESS
                        environment variable.
  -l LAUNCHER, --launcher_name LAUNCHER
                        The name of the launcher script that will be created.
                        Default="<name>.slurm"
  -s                    Echoes the launcher filename to stdout.
```

The **launcher_creator.py** script does not handle every job control parameter you might ever want to set. For that, make a copy of the default script, found at **$LAUNCHER_DIR/extras/batch-scripts/launcher.slurm**, and edit it appropriately.

To read more about the **launcher** module:

```
module load launcher
module help launcher
more $LAUNCHER_DIR/README.md
```

### job name and commands file

Recall how the **simple.slurm** batch file was created:

**Create batch submission script for simple commands**

```
launcher_creator.py -j simple.cmds -n simple -t 00:01:00 -a OTH21164 -q development
```

- The name of your ***commands file*** is given with the **-j simple.cmds** option.
- Your desired ***job name*** is given with the **-n simple** option.
  - The **<job_name>** (here **simple**) is the ***job name*** you will see in your queue.
  - By default a corresponding **<job_name>.slurm** batch file is created for you.
    - It contains the name of the commands file that the batch system will execute.

### queues and runtime

TACC resources are partitioned into ***queues***: a named set of compute nodes with different characteristics. The main ones on **ls6** are listed below. Generally you use **development** (**-q development**) when you are writing and testing your code, then **normal** once you're sure your commands will execute properly.

| queue name | maximum runtime | purpose |
|---|---|---|
| **development** | 2 hrs | development/testing and short jobs (typically has short queue wait times) |
| **normal** | 48 hrs | normal jobs (queue waits are often long) |

- In **launcher_creator.py**, the queue is specified by the **-q** argument.
  - The default queue is **development**. Specify **-q normal** for **normal** queue jobs.
- The ***maximum runtime*** you are requesting for your job is specified by the **-t** argument.
  - Format is **hh:mm:ss**
  - Note that your job will be terminated ***without warning*** at the end of its time limit!

### allocation and SUs

You may be a member of a number of different projects, hence have a choice which resource ***allocation*** to run your job under.

- You specify that allocation name with the **-a** argument of **launcher_creator.py**.
- If you have set an **$ALLOCATION** environment variable to an allocation name, that allocation will be used.

The **.bashrc** login script you've installed for this course specifies the class's allocation as shown below. Note that this allocation will expire after the course, so you should change that setting appropriately at some point.

**ALLOCATION setting in .bashrc**

```
# This sets the default project allocation for launcher_creator.py
export ALLOCATION=OTH21164
```

- When you run a batch job, your project allocation gets "charged" for the time your job runs, in the currency of ***SUs*** (***System Units***).
- SUs are related in some way to node hours, usually 1 SU = 1 node hour.

**Jobs tasks should have similar expected runtimes**

Jobs should consist of tasks that will run for approximately the same length of time. This is because the total node hours for your job is calculated as the run time for your ***longest running*** task (the one that finishes last).

For example, if you specify 100 commands and 99 finish in 2 seconds but one runs for 24 hours, you'll be charged for 100 x 24 node hours even though the total amount of work performed was only ~24 hours.

### wayness (tasks per node)

One of the most confusing things in job submission is the parameter called ***wayness***, which controls ***how many tasks are run on each compute node***.

- Recall that there are 128 physical cores and 256 GB of memory on each compute node
  - so theoretically you could run up to 128 commands on a node, each with ~2 GB available memory
  - you usually run fewer tasks on a node, and when you do, each task gets more resources

| tasks per node (wayness) | cores available to each task | memory available to each task |
|---|---|---|
| **1** | 128 | ~256 GB |
| **2** | 64 | ~128 GB |
| **4** | 32 | ~64 GB |
| **8** | 16 | ~32 GB |
| **16** | 8 | ~16 GB |
| **32** | 4 | ~8 GB |
| **64** | 2 | ~4 GB |
| **128** | 1 | ~1 GB |

- In **launcher_creator.py**, ***wayness*** is specified by the **-w** argument.
  - the default is 128 (one task per core)
- A special case is when you have only 1 command in your job.
  - In that case, it doesn't matter what ***wayness*** you request.
  - Your job will run on one compute node, and have all cores available.

Your choice of the ***wayness*** parameter will depend on the nature of the work you are performing: its computational intensity, its memory requirements and its ability to take advantage of multi-processing/multi-threading (e.g. **bwa -t** option or **hisat2 -p** option).

Bioinformatics programs generally perform substantial I/O, require more memory and fewer cores, so you'll generally want to run only a few tasks per node.

## Wayness example

Let's use **launcher_creator.py** to explore ***wayness*** options. First copy over the **wayness.cmds** commands file:

**Copy wayness commands**

```
# If $CORENGS is not defined:
export CORENGS=/work/projects/BioITeam/projects/courses/Core_NGS_Tools

cds
mkdir -p core_ngs/slurm/wayness
cd core_ngs/slurm/wayness
cp $CORENGS/tacc/wayness.cmds .
```

**Exercise: How many tasks are specified in the wayness.cmds file?**

**wc --help**
Find the number of lines in the **wayness.cmds** commands file using the **wc** (**w**ord **c**ount) command with the **-l** (**l**ines) option:

```
wc -l wayness.cmds
```

The file has 16 lines, representing 16 tasks.

The **wayness.cmds** commands file consists of a number of identical lines that look like this:

```
sleep 3; echo "Command $LAUNCHER_JID of $LAUNCHER_NJOBS ($LAUNCHER_PPN per node) ran on node `hostname` core
$LAUNCHER_TSK_ID" > cmd.$LAUNCHER_JID.log 2>&1
```

The ***wayness*** commands take advantage of a number of environment variables the **launcher** module system sets automatically for each task:

- **$LAUNCHER_JID** – the task number of the running task (from 1 to total number of tasks)
- **$LAUNCHER_NJOBS**– total number of tasks specified by the job
- **$LAUNCHER_TSK_ID** – number of the core running the task (0 to number of tasks - 1)
- **hostname** – Linux program that returns the name of the current compute node

For more information, see https://github.com/TACC/launcher

Create the batch submission script specifying a ***wayness*** of 4 (4 tasks per node), then submit the job and monitor the queue:

**Create batch submission script for wayness example**

```
launcher_creator.py -j wayness.cmds -n wayness -w 4 -t 00:02:00 -a OTH21164 -q development
sbatch wayness.slurm
showq -u
```

**Exercise: With 16 tasks requested and *wayness* of 4, how many nodes will this job require? How much memory will be available for each task?**

4 nodes (16 tasks x 1 node/4 tasks)
64 GB (256 GB/node * 1 node/4 tasks)

**Exercise: If you specified a *wayness* of 2, how many nodes would this job require? How much memory could each task use?**

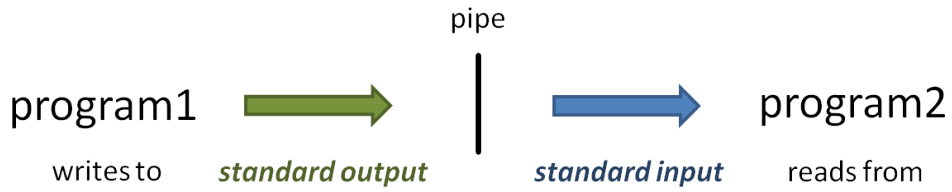
8 nodes (16 tasks x 1 node/2 tasks)
128 GB (256 GB/node * 1 node/2 tasks)

Look at the output file contents once the job is done.

```
cat cmd*log

# or, for a listing ordered by node name (the 11th field)
cat cmd*log | sort -k 11,11
```

The **vertical bar** ( **|** ) above is the ***pipe operator***, which connects one program's ***standard output*** to the next program's ***standard input***.




(Read more about the **sort** command at **Linux fundamentals: cut, sort, uniq**, and more about **Piping**)

You should see something like output below.

```
Command 1 of 16 (4 per node) ran on node c303-005.ls6.tacc.utexas.edu core 0
Command 10 of 16 (4 per node) ran on node c304-005.ls6.tacc.utexas.edu core 9
Command 11 of 16 (4 per node) ran on node c304-005.ls6.tacc.utexas.edu core 10
Command 12 of 16 (4 per node) ran on node c304-005.ls6.tacc.utexas.edu core 11
Command 13 of 16 (4 per node) ran on node c304-006.ls6.tacc.utexas.edu core 12
Command 14 of 16 (4 per node) ran on node c304-006.ls6.tacc.utexas.edu core 13
Command 15 of 16 (4 per node) ran on node c304-006.ls6.tacc.utexas.edu core 14
Command 16 of 16 (4 per node) ran on node c304-006.ls6.tacc.utexas.edu core 15
Command 2 of 16 (4 per node) ran on node c303-005.ls6.tacc.utexas.edu core 1
Command 3 of 16 (4 per node) ran on node c303-005.ls6.tacc.utexas.edu core 2
Command 4 of 16 (4 per node) ran on node c303-005.ls6.tacc.utexas.edu core 3
Command 5 of 16 (4 per node) ran on node c303-006.ls6.tacc.utexas.edu core 4
Command 6 of 16 (4 per node) ran on node c303-006.ls6.tacc.utexas.edu core 5
Command 7 of 16 (4 per node) ran on node c303-006.ls6.tacc.utexas.edu core 6
Command 8 of 16 (4 per node) ran on node c303-006.ls6.tacc.utexas.edu core 7
Command 9 of 16 (4 per node) ran on node c304-005.ls6.tacc.utexas.edu core 8
```

Notice that there are 4 different host names. This expression:

```
cat cmd*log | awk '{print $11}' | sort | uniq -c
```

should produce output something like this (read more about **piping commands to make a histogram**)

```
   4 c302-005.ls6.tacc.utexas.edu
   4 c302-006.ls6.tacc.utexas.edu
   4 c305-005.ls6.tacc.utexas.edu
   4 c305-006.ls6.tacc.utexas.edu
```

# Some best practices

## Redirect task output and error streams

We've already touched on the need to redirect ***standard output*** and ***standard error*** for each task. Just remember that funny redirection syntax:

**Redirect both standard output and standard error to a file**

```
my_program input_file1 output_file1 > file1.log 2>&1
```

## Combine serial workflows into scripts

Another really good way to work is to "bundle" a complex set of steps into a shell script that sets up its own environment, loads its own modules, then executes a series of program steps. You can then just call that script, probably with data-specific arguments, in your commands file. This multi-program script is sometimes termed a ***pipeline***, although complex pipelines may involve several such scripts.

For example, you might have a script called **align_bwa.sh** (a **bash** script) or **align_bowtie2.py** (written in **Python**) that performs multiple steps needed during the alignment process:

- quality checking the input **FASTQ** file
- trimming or removing adapters from the sequences
- performing the alignment step(s) to create a **BAM** file
- sort the **BAM** file
- index the **BAM** file
- gather alignment statistics from the **BAM** file

The BioITeam maintains a set of such scripts in the **/work/projects/BioITeam/common/script** directory. Take a look at some of them after you feel more comfortable with initial NGS processing steps. They can be executed by anyone with a TACC account.

## Use one directory per job

You may have noticed that all the files involved in our job were in one directory – the batch submissions file, commands file, log files our tasks wrote, and the launcher job output and error files. Of course you'll probably need input files too as well as output files 😉.

Because a single job can create a lot of files, it is a good idea to ***use a different directory*** for each job or set of closely related jobs, maybe with a name similar to the job being performed. This will help you stay organized.

Here's an example directory structure

```
$SCRATCH/my_project
             /original      # contains or links to original fastq files
             /fastq_prep    # run fastq QC and trimming jobs here
             /alignment     # run alignment jobs here
             /gene_counts   # analyze gene overlap here
             /test1         # play around with stuff here
             /test2         # play around with other stuff here
```

Command files in each directory can refer to files in other directories using relative path syntax, e.g.:

**Relative path syntax**

```
cd $SCRATCH/my_project/fastq_prep
ls ../original/my_raw_sequences.fastq.gz
```

Or create a symbolic link to the directory and refer to it as a sub-directory:

**Symbolic link to relative path**

```
cd $SCRATCH/my_project/fastq_prep
ln -s ../original fq
ls ./fq/my_raw_sequences.fastq.gz
```

**relative path syntax**

As we have seen, there are several special "directory names" the **bash** shell understands:

- ***dot directory*** ( **.** ) refers to "here" or "the current directory"
- ***dot dot directory*** ( **..** ) refers to "one directory up"
- ***tilde directory*** ( **~** ) refers to your **Home** directory

Try these relative path examples:

**Relative path exercise**

```
# navigate through the symbolic link in your Home directory
cd ~scratch/core_ngs/slurm/simple
ls ../wayness
ls ../..
ls -l ~/.bashrc
```

(Read more about **Absolute and relative pathname syntax**)

## Interactive sessions (idev)

So we've explored the TACC batch system. What if you want to do some interactive-style testing of your workflow?

Interactive sessions are available through the **idev** command as shown below. **idev** sessions are configured with similar parameters to batch jobs.

**Start an idev session**

```
idev -m 60 -N 1 -A OTH21164 -p normal -r CoreNGS-Tue
```

***Notes:***

- **-p normal** requests nodes on the **normal** queue
  - this is the default for our reservation, while the **development** queue is the normal default
- **-m 60** asks for a 60 minute session
- **-A OTH21164** specifies the TACC allocation/project to use
- **-N 1** asks for 1 node

- **--reservation=CoreNGS-Tue** gives us priority access to TACC nodes for the class. You normally won't use this option.

When you ask for an **idev** session, you'll see output as shown below. Note that the process may repeat the "job status:  PD" (pending) step while it waits for an available node.

```
  -> Checking on the status of development queue. OK

 -> Defaults file    : ~/.idevrc
 -> System           : ls6
 -> Queue            : development    (cmd line: -p        )
 -> Nodes            : 1              (cmd line: -N        )
 -> Tasks per Node   : 128            (Queue default       )
 -> Time (minutes)   : 60             (cmd line: -m        )
 -> Project          : OTH21164       (cmd line: -A        )

----------------------------------------------------------------
          Welcome to the Lonestar6 Supercomputer
----------------------------------------------------------------

--> Verifying valid submit host (login1)...OK
--> Verifying valid jobname...OK
--> Verifying valid ssh keys...OK
--> Verifying access to desired queue (development)...OK
--> Checking available allocation (OTH21164)...OK
Submitted batch job 235465

 -> After your idev job begins to run, a command prompt will appear,
 -> and you can begin your interactive development session.
 -> We will report the job status every 4 seconds: (PD=pending, R=running).

 -> job status:  PD
 -> job status:  R

 -> Job is now running on masternode= c302-005...OK
 -> Sleeping for 7 seconds...OK
 -> Checking to make sure your job has initialized an env for you....OK
 -> Creating interactive terminal session (login) on master node c302-005.
 -> ssh -Y  -o "StrictHostKeyChecking no" c302-005
```

Once the **idev** session has started, it looks quite similar to a login node environment, except for these differences:

- the **hostname** command on a login node will return a ***login server*** name like **login3.ls6.tacc.utexas.edu**
    - while in an **idev** session **hostname** returns a ***compute node*** name like **c303-006.ls6.tacc.utexas.edu**
- you cannot submit a batch job from inside an **idev** session, only from a login node
- your **idev** session will end when the requested time has expired
    - or you can just type **exit** to return to a login node session