

The Things I Wish I Had Known When I Started in HPC

Jorge Alarcón Ochoa

Department of Physics, Rensselaer Polytechnic Institute

- 1 Getting your Allocation
- 2 Access: Modules and Compiling
 - Logging In
 - Usage
- 3 Submitting Jobs
- 4 Programming
- 5 Open Sourcing

- 1 Getting your Allocation
- 2 Access: Modules and Compiling
 - Logging In
 - Usage
- 3 Submitting Jobs
- 4 Programming
- 5 Open Sourcing

Allocation Types

- **Education** : Workshops, courses, etc.
- Campus Champions : For small test (you need a campus champion near by).
- **Trial** : Within 1 business day you'll get about 1K SUs.
- **Startup** : Continually reviewed.
- **Research**

<https://portal.xsede.org/allocations-overview#types>

General Set Up for the Application

- Abstract
- Project Description
 - Tools you will use
 - **Have you done your benchmarking?**
- Request your machine
 - Calculations
 - Storage
 - Visualization

<https://www.xsede.org/resources/overview>

Keep in mind that there are limited resources, you have to justify your request and help XRC distribute the available resources.

- 1 Getting your Allocation
- 2 Access: Modules and Compiling
 - Logging In
 - Usage
- 3 Submitting Jobs
- 4 Programming
- 5 Open Sourcing

Logging In

On your terminal type:

```
ssh username@stampede.tacc.utexas.edu
```

or

```
ssh username@stampede.tacc.xsede.org
```

```
-----  
Welcome to the Stampede Supercomputer  
Texas Advanced Computing Center, The University of Texas at Austin  
-----
```

```
** Unauthorized use/access is prohibited. **
```

If you log on to this computer system, you acknowledge your awareness of and concurrence with the UT Austin Acceptable Use Policy. The University will prosecute violators to the full extent of the law.

TACC Usage Policies:
<http://www.tacc.utexas.edu/user-services/usage-policies/>

Questions and Problem Reports:

--> XD Projects: help@xsede.org (email)
--> TACC Projects: portal.tacc.utexas.edu (web)

Documentation: <http://www.tacc.utexas.edu/user-services/user-guides/>
User News: <http://www.tacc.utexas.edu/user-services/user-news/>

Welcome to Stampede, *please* read these important system notes:

The Others

Logging in to other machines is similar, simply type

```
ssh username@
```

followed by:

- ranch.tacc.xsede.org
- comet.sdsc.xsede.org
- supermic.cct-lsu.xsede.org

<https://portal.xsede.org/single-sign-on-hub>

Looking for Something?

For the random tip type on your terminal

```
module help tacc_tips
```

- `module spider` (beware of module avail) : Available packages
- `module keyword bio` : In case your looking for a 'bio' related package
- `module show "module"` : Useful for compiling new packages. Gives you all information about a package

- 1 Getting your Allocation
- 2 Access: Modules and Compiling
 - Logging In
 - Usage
- 3 Submitting Jobs
- 4 Programming
- 5 Open Sourcing

Slurm : Overview

- 1 Write your submission script
- 2 Sbatch your submission script (do not use login nodes to run jobs!)
- 3 Job will sit on queue waiting for resources
- 4 Get results.

Let's look at an example. We will run an nwchem calculation to obtain the Raman spectra of a carbon chain.

Examples files can be found here

<https://github.com/alejandrox1/HPC-howto>

Submitting

Run_blyp-pcs0.sh : Preprocessing

```
login1.stamped(8)$  
login1.stamped(8)$ bash run_blyp-pcs0.sh -N numbernodes -np numberoftasks -c inputstructure
```

Submit your job

```
sbatch -A TG-TRA140037 -p $partition -N $nodes -n $procs -J c${length} raman_run_blyp-pcs0.sh $procs > submit.txt  
id=$(awk 'END {print $NF}' submit.txt)  
sbatch -A TG-TRA140037 --dependency=afterok:${id} -p $partition -N $nodes -n $procs -J c${length} restart_raman.sh $procs
```

A Successful Submission Should Look Like This:

```
-----  
Welcome to the Stampede Supercomputer  
-----
```

```
--> Verifying valid submit host (login1)...OK  
--> Verifying valid jobname...OK  
--> Enforcing max jobs per user...OK  
--> Verifying availability of your home dir (/home1/03561/alarcj)...OK  
--> Verifying availability of your work dir (/work/03561/alarcj)...OK  
--> Verifying availability of your scratch dir (/scratch/03561/alarcj)...OK  
--> Verifying valid ssh keys...OK  
--> Verifying access to desired queue (normal)...OK  
--> Verifying job request is within current queue limits...OK  
--> Checking available allocation (TG-TRA140037)...OK  
Submitted batch job 7218770
```

job : raman_run_blyp-pcs0.sh

```
#!/bin/bash

#SBATCH --exclusive           # Individual nodes
#SBATCH -t 2-0                # Run time (hh:mm:ss)
#SBATCH -o slurm.%j.out
#SBATCH --mail-type=ALL
#SBATCH --mail-user=alarcj137@gmail.com

module load nwchem/6.5

# INPUT
n=$1

ibrun -np $n nwchem blyp-pcs0_acetylene.nw
```

For more info on Sbatch options, on your terminal type: `man sbatch`

checking up

On your terminal type: `squeue -u username`

```
login1.stampede(24)$ squeue -u hqj
```

JOBID	PARTITION	NAME	USER	ST	TIME	NODES	MODELIST(Reason)
7301151	serial	Mg_450GP	hqj	R	1:03:37	1	c558-803
7301187	serial	Mg_450GP	hqj	R	1:03:37	1	c558-902
7301277	serial	Mg_450GP	hqj	R	1:03:37	1	c558-203
7301852	serial	Mg_350GP	hqj	R	1:03:37	1	c559-203
7303336	serial	Mg_450GP	hqj	R	42:26	1	c559-002
7303333	serial	Mg_450GP	hqj	R	44:03	1	c558-004
7303332	serial	Mg_450GP	hqj	R	44:39	1	c559-003
7303330	serial	Mg_450GP	hqj	R	45:24	1	c558-303

For more info on `squeue`'s option, on your terminal type:
`man squeue`

For more info on `man`, on your terminal type: `man man`

- 1 Getting your Allocation
- 2 Access: Modules and Compiling
 - Logging In
 - Usage
- 3 Submitting Jobs
- 4 Programming
- 5 Open Sourcing

Some Tips

- Different tasks into different scripts
- Make your scripting read like a paper (that includes adding comments)
- Be as lazy as possible, but do not be disorganized!
- Begin line by line

Happy Computing!

```
echo $' $the_cow=""'>.cow; cowsay -f ./ .cow $'0 0\n\n\_/'; rm .cow
```

- 1 Getting your Allocation
- 2 Access: Modules and Compiling
 - Logging In
 - Usage
- 3 Submitting Jobs
- 4 Programming
- 5 Open Sourcing

Thank you

Special thanks to the XSEDE Scholar Program!

