

# Introduction to HPC Resources and Linux

**Burak Himmetoglu**

Enterprise Technology Services &  
Center for Scientific Computing  
e-mail: [bhimmotoglu@ucsb.edu](mailto:bhimmetoglu@ucsb.edu)

**Paul Weakliem**

California Nanosystems Institute &  
Center for Scientific Computing  
e-mail: [weakliem@cnsi.ucsb.edu](mailto:weakliem@cnsi.ucsb.edu)

**Fuzzy Rogers**

Materials Research Laboratory &  
Center for Scientific Computing  
e-mail: [fuz@mrl.ucsb.edu](mailto:fuz@mrl.ucsb.edu)

<http://www.ets.ucsb.edu/services/supercomputing>

<http://csc.cnsi.ucsb.edu>



**CSC**

UNIVERSITY OF CALIFORNIA SANTA BARBARA  
CENTER FOR SCIENTIFIC COMPUTING

# Overview

- What is High Performance Computing (HPC)?

High Performance Computing (HPC) allows scientists and engineers to solve complex science, engineering, and business problems using applications that require high bandwidth, enhanced networking, and very high compute capabilities.

From: <https://aws.amazon.com/hpc/>

- Multiple computer nodes connected by a very fast interconnect
- Each node contains many CPU cores (around 12-32)
- Allows many users to run calculations simultaneously on nodes
- Allows a single user to use many CPU cores incorporating multiple nodes
- UCSB provide access and support for multiple HPC resources and educational/training/research support.

# Which resources do we have?

- UCSB Center for Scientific Computing (CSC) clusters
  - Access to all UCSB staff, free and condo clusters
- Extreme Science and Engineering Discovery Environment (XSEDE)
  - Project funded by NSF. Access to national resources. Free\*
- Triton Shared Computing Cluster (TSCC) at San Diego Supercomputing Center (SDSC)
  - Mostly used for education/training and class support

<http://csc.cnsi.ucsb.edu/resources>

# HPC systems at CSC

## **Campus available cluster Knot:**

- 110 node, ~1400 core system
- 4 ‘fat nodes’ (256/512 GB RAM)
- GPU nodes (12)
- Published papers should acknowledge CNSI and MRL

Request access: <http://csc.cnsi.ucsb.edu/acct>

## **Condo clusters:**

- Lattice (62 nodes)
- Guild (60 nodes)
- Braid (60 nodes, also has GPUs)

PIs buy nodes in the clusters, CSC handles infrastructure

# XSEDE

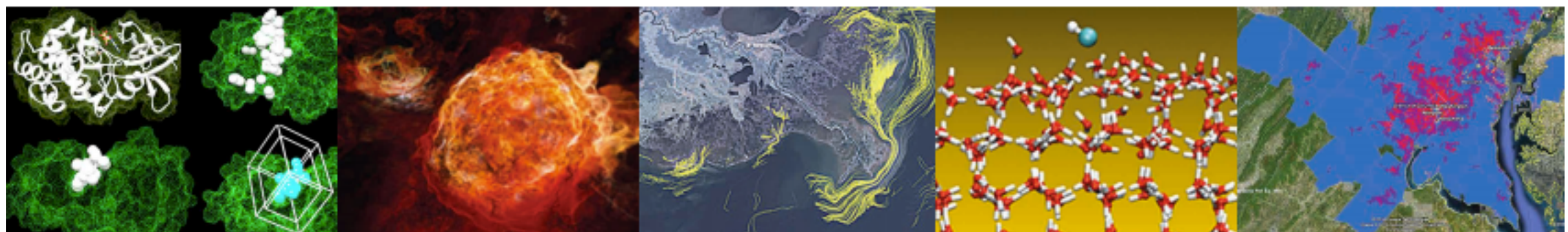
Extreme Science and Engineering  
Discovery Environment

XSEDE is an NSF sponsored service organization that provides access to computing resources.

<https://portal.xsede.org>

[www.xsede.org](http://www.xsede.org)









Currently XSEDE supports more than a dozen supercomputers and high-end visualization and data analysis resources.



# Summary of XSEDE systems

## XSEDE Compute Resources

[Detail View](#)

Name	Status	Load	Jobs
Stampede   UT Austin 	Healthy		R: 677 Q: 624 O: 186
Comet   SDSC 	Healthy		R: 2327 Q: 217 O: 297
XStream   Stanford U 	Healthy		R: 50 Q: 286 O: 947
SuperMIC   LSU CCT 	Healthy		
Bridges Regular Memory   PSC 	Healthy		
Bridges Large Memory   PSC 	Healthy		
Jetstream   UT Austin 	Healthy		
Gordon Compute Cluster   SDSC 	Healthy		R: 179 Q: 0 O: 6
Wrangler   UT Austin 	Healthy		

Top 500

General purpose  
Big data

GPU

Small,  
general purpose

General purpose  
Big Data

Cloud (on demand)

General purpose  
Big data

High I/O  
data intensive



# XSEDE Campus Champions Program

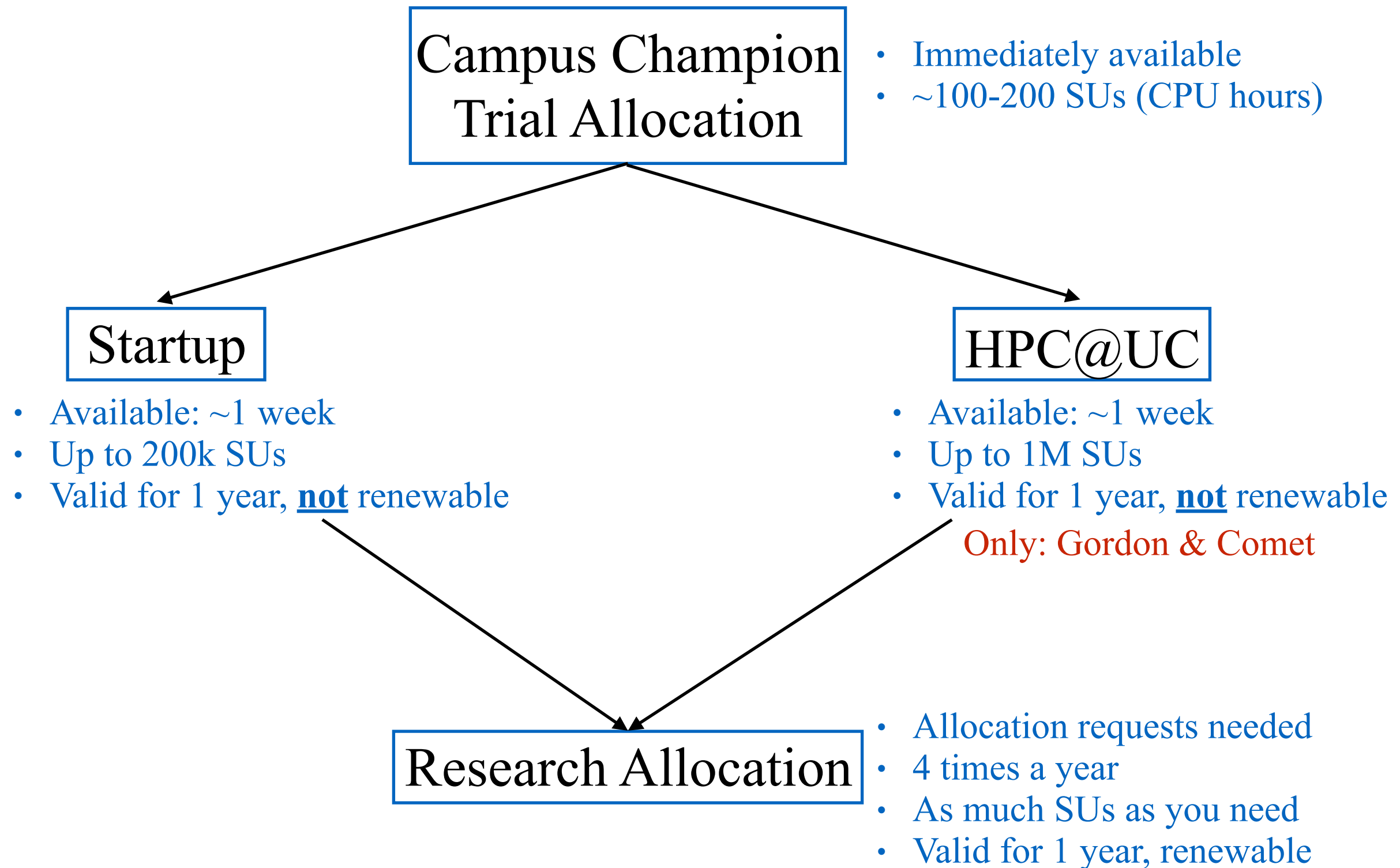
Campus Champion: Represents XSEDE on the campus

As a campus champion, I will help you:

- Understand the capabilities of HPC and get to include it as a part of your research and educational work.
- Get access to local, regional and national resources.
- Maintenance of accounts, allocations of computing time and technical expertise.
- Connect with the broader community of HPC users in your field

# How to get access?

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





# XSEDE Portal

Get access:

- Get a username from the portal
- Send me your username
- You will get limited trial time from any resource!

On the portal you will find:

- Documentation
- Help desk
- Training sessions broadcasted from the web
- Forums

The screenshot shows the XSEDE User Portal interface. At the top, there's a header with the XSEDE logo and 'USER PORTAL' text. Below the header is a navigation bar with links: MY XSEDE, RESOURCES, DOCUMENTATION, ALLOCATIONS, TRAINING, USER FORUMS, HELP, and ECSS. Under 'MY XSEDE', there's a sub-menu with links: Summary, Allocations/Usage, Accounts, Jobs, Profile, Publications, Tickets, Change Password, and Add User. A search bar is located in the top right corner. Below the navigation bar, there's a banner for 'XSEDE USER PORTAL ON THE GO' with images of the app on a smartphone and tablet. To the left of the banner, there's a user profile section with a photo of a man and text: 'Welcome, Burak!', 'Last login: Mon 10/26/15 at 09:52:16 AM CST'. Below the profile, there's a sidebar with icons for Profile, Allocations, Accounts, and Training, and a link to 'NEW! Share your XSEDE Science Achievements'. The main content area features a large pie chart titled 'In The Past 7 Days' showing 'XD SUS Charged: Total: by Field of Science'. The chart is divided into segments for various fields of science, with 'All 75 others' being the largest segment. To the right of the pie chart, there's a smaller pie chart and a bar chart. At the bottom, there's a section for 'My XSEDE Resources' with a table showing columns: Resource, Status, Load, Username, and My Jobs. A 'System Monitor' link is also present.

**XSEDE USER PORTAL**  
Extreme Science and Engineering Discovery Environment

Search XSEDE...

**MY XSEDE** RESOURCES DOCUMENTATION ALLOCATIONS TRAINING USER FORUMS HELP ECSS

Summary Allocations/Usage Accounts Jobs Profile Publications Tickets Change Password Add User

Share your feedback on XSEDE Extended Collaborative Support Services with a quick 5 question survey!

Welcome, Burak!  
Last login: Mon 10/26/15  
at 09:52:16 AM CST

Profile Allocations  
Accounts Training

NEW! Share your XSEDE Science Achievements

**In The Past 7 Days**

**XD SUS Charged: Total: by Field of Science**

Biophysics 15,496,525.0  
Materials Research 12,851,897.0  
Astronomical Sciences 7,212,089.0  
Fluid, Particulate, and Hydraulic Systems 6,234,052.0  
Molecular Biosciences 5,091,439.0  
Earth Sciences 4,802,351.0  
Gravitational Physics 3,786,288.0  
Extragalactic Astronomy and Cosmology 4,378,987.0  
Elementary Particle Physics 4,378,987.0

View Gallery

**My XSEDE Resources** System Monitor

Resource	Status	Load	Username	My Jobs
----------	--------	------	----------	---------

# Using HPC Clusters and Basic Linux (examples on Knot)

<http://csc.cnsi.ucsb.edu/docs/getting-started>

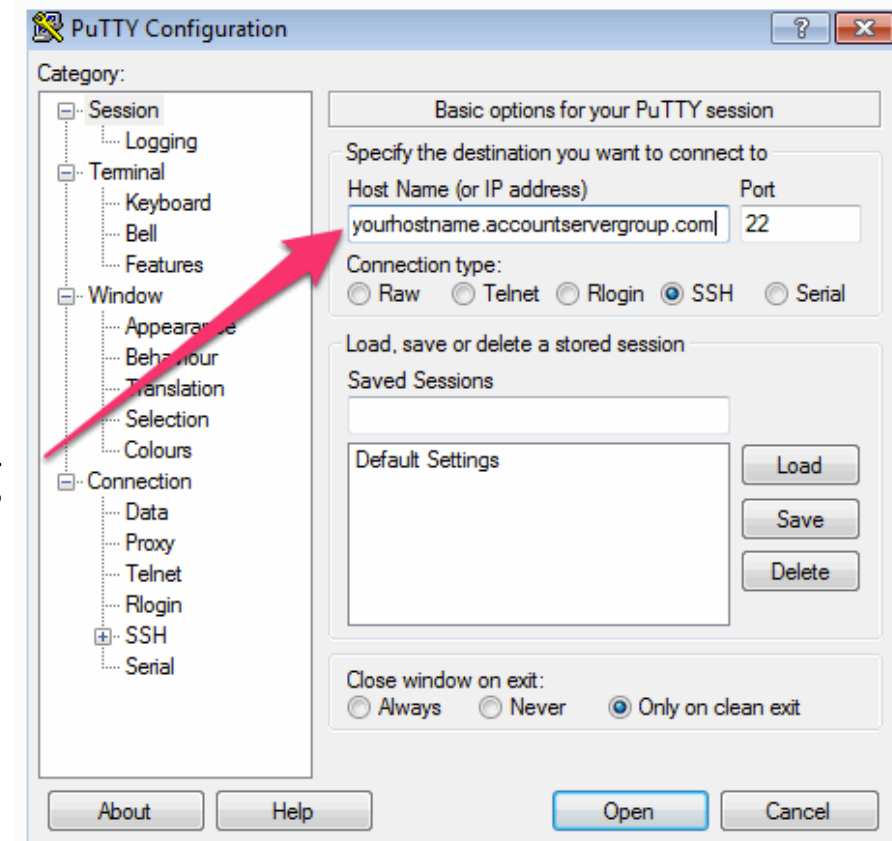
# Access

For Linux and Mac, open a terminal:

```
$ ssh username@knot.cnsi.ucsb.edu
```

For Windows, you will need a client (e.g. Putty, [www.putty.org](http://www.putty.org))

knot.cnsi.ucsb.org



Remote (non UCSB) login via VPN client:

<http://www.ets.ucsb.edu/services/campus-vpn/get-connected>

# File Transfer

For Linux and Mac, open a terminal, use `scp` or `rsync` commands:

E.g. Copy file.txt from your computer to your home directory on Knot

```
scp file.txt user@knot.cnsi.ucsb.edu:file_copy.txt
```

Windows users: Need a client to copy files. Usage is similar to Putty.

<https://filezilla-project.org/>

<https://winscp.net/eng/download.php>

Globus is another option (all operating systems). Preferred for large files transfers.

<http://csc.cnsi.ucsb.edu/docs/globus-online>

# Some useful commands

**ls [-option]** : list files

**mkdir** : make directory

**cd** : change directory

**man** : display manual for a command

**mv** : mv file/folder

**rm [-r]** : remove file. -r to remove folders

**pwd** : present working directory

**cat [file]** : view file

**less /more** : view file, one screen at a time

**grep [pattern] [file]** : Find matching patterns in a file

# Pipes and redirection

**command > file** : Redirect output of command to file

**command >> file** : Append output of command to file

**command < file1 > file2** : Get input from file1, write output to file2

**command1 | command2** : Join command1 & command2

# Common shortcuts

\* : Wildcard

~ : Home directory

. : Current directory

.. : One directory up

**TAB key:** Finish commands, good for typing fast



# Running Jobs

- When you login to Knot (or any other cluster), you are on the login node
- This node is NOT for running calculations!
- All jobs must be submitted to the queue
- Submission to the queue requires a script to be written

Example job submission script (submit.job):

```
#!/bin/bash
#PBS -l nodes=2:ppn=12
#PBS -l walltime=2:00:00
#PBS -N test

cd $PBS_O_WORKDIR

mpirun -machinefile $PBS_NODEFILE -np 24 ./run.x
```

\$ qsub submit.job

<http://csc.cnsi.ucsb.edu/docs/example-scripts-running-jobs>

# Running Jobs

Check status of the running jobs:      `$ showq -u $USER`  
   `$ qstat -u $USER`

Delete a running job:      `$ qdel job_id`

More options for PBS:

[https://www.olcf.ornl.gov/kb\\_articles/common-batch-options-to-pbs/](https://www.olcf.ornl.gov/kb_articles/common-batch-options-to-pbs/)

Available queues:

- Short queue: `$ qsub -q short submit.job`
- Large memory queues : `$ qsub -q (x)largemem submit.job`
- GPU queue: `$ qsub -q gpuq submit.job`

# Creating/Extracting Archives

Suppose you have an archive: `package.tar.gz`

Extract: `$ tar -xzvf package.tar.gz`

Suppose you have files you want to collect together: file1, ..., file10

`$ tar czf file1 file2 .. file10 package.tar.gz`