

Kua Research Lab: Getting Started

0. Resources

<http://home.sandiego.edu/~jkua>

Kua Research Lab Website Login is *kualab* (with the same password!)

1. Your HPC Account

USD has a High Performance Computing (HPC) cluster located in a special server room on campus. You have an individual account on this machine as part of my research group. If you're off-campus (i.e. not connecting through USD's *eduroam* wifi on campus), you must first connect to USD through VPN. (We can set you up with VPN if needed through ITS.)

Your *username* and *password* are the same as your USDOne username and password.

To connect to the HPC from the client machine, open a Terminal window (Mac) or a PowerShell window (Windows PC), then type:

```
ssh username@saber3.sandiego.edu
```

Aliases and shortcuts can be found in the **.bashrc** file of your home directory. (For example, a common alias we use for the program Jaguar is **jrun**)

2. Learning Unix/Linux

In the Unix folder on the Kua Group website:

- Go through the Unix Introduction and the tutorials
- Learn how to use the text editor vi
- Read the two short entries "setting up shortcuts" & "ssh and scp". You'll be using scp (or WinSCP) to copy files between your laptop and saber3.

3. General Guidelines about Running Calculations/Jobs

Instructions for specific programs will be provided depending on your project.

- To check the status of your job, type: the command **squeue -u username**
- You can type **squeue** to see *all* the jobs running on the HPC, not just yours.
- To kill one of your jobs, type **scancel JobID** (use **squeue** to find the JobID).

You will generate a lot of files in the course of your research. Give some thought to your filenames, your folders, and the organization of your data. Believe me, it will be VERY hard to find stuff midway through the semester if you are not organized.

4. End of Day. Log out of saber3 when you're done with the command **logout**. Note that if your machine goes to sleep or loses its internet connection or the VPN, if you're ssh-ed into a machine, your terminal will freeze.