Contents

1 Zeroo to Hero: XSEDE, PSC, and Bridges

1.1 Account setup

1.1.1 Creating account

If you do not already have an XSEDE account, you can create one here.

1.1.2 Requesting an allocation

TODO

1.1.3 Getting added to an allocation

To use compute resources, you will need to be added to an XSEDE allocation. Your PI and/or allocation manager can add you as a user to a specific project here.

1.2 Running your first job

1.2.1 Logging into Bridges2/PSC via `ssh`

Start by =ssh=ing into the bridges2 server at port 2222:

```
ssh -p 2222 <username>@bridges2.psc.edu
```

You will be prompted for your XSEDE credentials. Use your XSEDE User Portal password.

Tip: TODO Add tip about .bashrc etc.

Warning: TODO add warning about randomness when parallelizing

1.2.2 Creating a Slurm job script

Bridges-2 uses a job-scheduling system called "Slurm", providing a way for users like ourselves to request specific resources for our compute jobs and automatically launch jobs once said resources have become available.

Jobs are submitted using the `sbatch` command along with a **batch script** which we will create. These batch scripts take the following general form.

```
#!/bin/bash

### REQUEST RESOURCES ###
#SBATCH -arg1 argument1
#SBATCH -arg2 argument2
# .
# .
# .
#SBATCH -arg3 argument3

### LOAD MODULES ###
module load some_module

### RUN SCRIPTS ###
python myscript.py
Rscript myscript.R
```

1.2.3 Parallel computation

1. Python
2. R

1.3 Advanced

TODO