Command Cheat Sheet

Web Resources

FASRC Documentation & tutorials
https://docs.rc.fas.harvard.edu/
        https://docs.rc.fas.harvard.edu/kb/running-jobs/ – use SLURM

The FASRC web interface
https://rcood.rc.fas.harvard.edu/
This provides access to the webapps, such as Jupyter

Monitor currently running SLURM jobs
https://portal.rc.fas.harvard.edu/login/?next=/jobs/

Browser-Shell
https://rcood.rc.fas.harvard.edu/pun/sys/shell/ssh/COMPUTE_NODE.rc.fas.harvard.edu
This opens a terminal in your browser to connect to a compute node. Replace
"COMPUTE_NODE" with an actual ID, such as, for example, "`holy7c24603`". This works only if
you have an (interactive) session running on the node you want to connect to.

GitHub repo with all workshop files
https://github.com/cga-harvard/python-workshop-gis-big-data

Google Drive repo with all datasets we'll work with
https://drive.google.com/drive/folders/1k6G9hu8IiaZmMt3MgDw-3vBTtLTpyqdK?usp=sharing

Connect to the Cluster

Open a SSH shell to the login node
`ssh USERNAME@login.rc.fas.harvard.edu`

Request a compute node and start an interactive session
`srun --pty -p test --mem 1000 -t 0-01:00 /bin/bash`
This gives you 1h on a test partition with 1GB or memory

Create, start and use Python environments

Load the Python module
```
module load Mambaforge/23.3.1-fasrc01
```

Create a python environment and install packages
```
mamba create -n workshop python=3.9 --file requirements.txt
```
This command expects a file "requirements.txt" in the same directory you call this command from. This file lists all packages one by one per line.

Activate this python environment
```
mamba activate workshop
```

Run a Python script
```
Python script.py
```

To run a Jupyter notebook on the command line, convert it to a python script first
```
jupytext --to py jupyter_notebook.ipynb
```
This creates a "jupyter_notebook.py" file in the same directory.

Monitor jobs and processes

List running SLURM jobs
```
squeue
```

Monitor the load on a system
```
htop
```

Working with Data

All datasets we'll work with are accessible from all nodes and all users at
```
/n/holyscratch01/cga/python-workshop-gis-big-data
```

To copy data to the cluster, you can use SCP
```
scp -r ./* USER@login.rc.fas.harvard.edu:/PATH/TO/DESTINATION/
```
Replace `USER` and `/PATH/TO/DESTINATION/`

Similarly, to copy data from the cluster to your local machine, you can use
```
scp -r USER@login.rc.fas.harvard.edu:/PATH/TO/SOURCE ./
```
Replace `USER` and `/PATH/TO/SOURCE/`

Create a sbatch file to submit as a SLURM job

The following is a template for a sbatch file to run a python script as a SLURM job. Save the following as, for example, "project_sbatch_job.sh", and adjust the parameters:

```bash
#!/bin/bash
# https://docs.rc.fas.harvard.edu/kb/running-jobs/#articleTOC_8

#SBATCH -c 2              # Number of cores (-c)
#SBATCH -t 0-00:10       # Runtime in D-HH:MM, minimum of 10 minutes
#SBATCH -p test          # Partition to submit to
#SBATCH --mem=16000      # Memory pool for all cores
#SBATCH -o /n/home01/USER/job_stdout_%j.out  # log STDOUT to file
#SBATCH -o /n/home01/USER/job_errout_%j.err  # log errors to file

# load modules
module load Mambaforge/23.3.1-fasrc01

# set python environmant
mamba activate workshop

# run code
python global_precipitation_sentiment.py
```

You can then simply run `sbatch project_sbatch_job.sh` to submit the job to SLURM. Caution: ensure your script saves results to a destination that is accessible to you after the job finished.