Cheatsheet – HPC services

HIGH PERFORMANCE COMPUTING

Structure

[id]@login.cx1.hpc.ic.ac.uk ..... container
[id]@login.cx1.hpc.ic.ac.uk:/$HOME ..... home dir.
/rds/general/user/[id]/home ..... $HOME

Connection

ssh container ..... Access to your cx1 container
scp [path1/file] [path2] ..... Copy file from path1 (local PC) to path2 (HPC server) or vice versa. [path2]=[id]@login.cx1.hpc.ic.ac.uk/copypath
scp -r [path1] [path2] . recursive copy for whole folders
quota -s ..... Check memory use

Module management

module avail ..... List modules available
module load [m] ..... Load module
module list ..... List loaded modules
module switch [m1] [m2] ..... Swap modules
module unload [m] ..... Unload module
module purge ..... Get rid of all loaded modules

Job script

-l select=1:ncpus=1:mem=1gb .... GPU specifications
-l walltime=HH:MM:SS ..... Walltime specification

```
#PBS -lwalltime=00:30:00
#PBS -lselect=1:ncpus=1:mem=32gb:ngpus=1
module load anaconda3/personal
source activate myvenv
python $HOME/path/mycode.py
```

Job management

qsub [job-script].sh ..... Submit job to system
qstat -s ..... Job status information
qstat -q ..... Queue information
qdel [xxx].cx1 ..... Delete job submission
cat [job-script].sh.o[xxx] .... Read output file obtained
cat [job-script].sh.e[xxx] ..... Read error file obtained

COMMAND LINE

Basics

cd [folder] ..... Go to directory
ls ..... List files and folder
pwd ..... Get path working directory
cp [file] [path/] ..... Copy file to path
mv [file] [path/] ..... Move file to path
mv [file1] [file2] ..... Rename file
rm [file1] ..... Remove file
rm -r [folder] ..... Remove folder
mkdir [folder] ..... Create new folder
cat [file] ..... Read file

Install Anaconda from HPC

module load anaconda3/personal .. Load anaconda in container. This should be done every time you login.
anaconda-setup ..... Install anaconda

Create virtual environment

conda create –n [name] python=[x.x] ..... Create env
source activate [name] ..... Activate environment
conda install [package] ..... Install packages
source deactivate ..... Deactivate environment
conda list ..... List loaded packages
conda env list ..... List virtualenv

Create scripts - Vim Editor

vim [name].sh ..... Create bashscript
"a" ..... Enable file editing
"Esc" ..... Exit editing mode
":x" ..... Quit file
":wq" ..... Save and quit file

GPU types

```
PBS [memory spec]:ngpus=1:gpu_type=GTXTITAN
PBS [memory spec]:ngpus=1:gpu_type=K80
PBS [memory spec]:ngpus=1:gpu_type=P100
```

GITHUB

Configure tooling

git config –global user.name "[name]" ... Config name
git config –global user.email "[email]" ... Config email
git config credential.helper store .... Store credentials

Create repository

git init [project-name] ..... Create local repository
git clone [url] ..... Download repository

Make changes

git add [file] ..... Add file to repository
git rm [file] ..... Remove file to repository
git reset [file] ..... Unstage file
git commit -m "[message]" ..... Commit modified files
git push ..... Push modifications
git pull ..... Pull modifications

Avoid conflict

git status ..... List modified files
git diff ..... Diff of modified files
git diff –staged ..... Diff staged files
git stash ..... Save modified/staged files
git reset –hard [commit] ... Rewrite from spec commit

USEFUL LINKS

```
Imperial College HPC website:
https://www.imperial.ac.uk/admin-services/
ict/self-service/research-support/rcs/
computing/
```