TUTORIAL 01:
CREATE THE WORKING ENVIRONEMENT

OBJECTIVES

- Review some basic instructions to **prepare the working environment**.
- Discover the CHPC **cluster** called LENGAU.
- Log onto the super-computer.
- Copy the CROCO and CROCO_TOOLS directories
- Test your working environment.

USEFUL DOCUMENTS

BASIC LINUX COMMANDS

Here is a list a commands and softwares we will use throughout the CROCO Training week.

1: Basic Linux commands

Linux command	Description	Linux command example
cd	Change director with a specific path	`cd lustre/croco; cd ..;`
clear	Clear the screen	`clear`
cp	Copy file(s)	`cp path1/file1 path2/file2`
diff	Compare the content of files	`diff file1 file2`
exit	Log out of Linux	`exit`
grep	Find a string of text in a file	`grep "NBPROCS" file1`
head	Display the heading of a file	`head file1`
ls	List contents of a directory	`ls path1/directory1`
ln	Create a symbolic link	`ln -sf /mnt/lustre lustre`
mv	Move file(s) or rename file(s)	`mv path1/file1 path2/file2`
mkdir	Create a directory	`mkdir directory`
rm	Delete file(s)	`rm file1`
rmdir	Remove an empty diectory	`rmdir directory`
tail	Display the end of a file	`tail file1`
tar	Store, list, or extract file in an archive	`tar file1`
scp	Copy file(s) from/to a distant machine	
ssh	Connect to a distant machine	`ssh login@lengau.chpc.ac.za`
vi	Edit file(s) with simple text editor	`vi file1`

2: List of useful softwares and how to execute them

→ Text editor: nedit
  ➥ Execute `nedit file1`

→ To pre- and post- process CROCO files: Matlab (https:// mathworks.com)
  ➥ Execute `matlab`

→ To display the header of a NetCDF file: NetCDF library
  ➥ Execute `ncdump -h my_NetCDF_file.nc`

→ To inspect a NetCDF file: Ncview
  ➥ Execute `ncview my_NetCDF_file.nc`

→ To manipulate NetCDF files: NCO tools
  ➥ Concatenate files: `ncrcat CROCO_avg*.nc My_CROCO_file.nc`
  ➥ Extract a variable: `ncks -v Myvar My_CROCO_file.nc My__CROCO_Myvar.nc`

LENGAU CLUSTER AT CHPC

The main system at the CHPC for high performance computing is a cluster supercomputer called Lengau — cheetah in seTswana. This peta-scale system consists of Dell servers, powered by Intel processors, using FDR InfiniBand by Mellanox and is managed by the Bright Cluster Manager.

1: The Cluster

→ The CHPC's Dell Linux cluster has been up and running since 2014.
  ➥ The system is a homogeneous cluster, comprising Intel 5th generation CPUs. As of March 2017 it has 1368 compute nodes with 24 cores and 128 GiB memory (360 nodes have only 64 GiB) each, and five large memory "fat" nodes with 56 cores and 1TiB each, all interconnected using FDR 56 Gb/s InfiniBand accessing 4 PB of shared storage over the Lustre filesystem.

→ The cluster has both NFS and the Lustre filesystems over Infiniband:

Mount Point	File System	Size	Quota	Backup
/home	NFS	80Tb	15GB	NO
/mnt/lustre/users	lustre	4PB	None ⚠	NO

2: The installed softwares/libraries

→ CHPC uses the GNU modules utility, which manipulates your environment, to provide access to the supported software in /apps/.
  ➥ Directly in your `.bashrc`, we will load the following modules to use the associated software/libraries: Matlab, Ncview, Intel Fortran Compilers, NCO tools, …

Command	Description
module purge	Remove all loaded modules
module avail	List of available modules
module list	List currently loaded modules
module help	Give information of a particular module file's operations

3: Job Scheduler

→ The CHPC cluster uses **PBSPro** as its job scheduler. With the exception of interactive jobs, all jobs are submitted to a batch queuing system and only execute when the requested resources become available. All batch jobs are queued according to priority. A user's priority is not static: the CHPC uses the "Fairshare" facility of PBSPro to modify priority based on activity. This is done to ensure the finite resources of the CHPC cluster are shared fairly amongst all users.

PBS Pro commands	Description	PBS command example
qsub [script file]	Job submission	`qsub run_croco.pbs`
qstat-u login	Job status (for user)	`qsub -u sillig` (or the alias `qs`)
qstat-f [job_id]	Extended job status	`qsub -f 10098976`
qdel [job_id]	Job deletion	`qdel 10098976`
qstat-Q	List of usable queues	

STEP 1: Logging onto the HPC cluster

- From a terminal/konsole:

```
ssh -X login@lengau.chpc.ac.za
```

- Practice some basic Linux commands: **`cd`** and **`ls`**
- If your lustre directory does not exist:

```
ln -sf /mnt/lustre/users/login lustre
```

STEP 2: Requesting some interactive nodes

- Replace your **.bashrc** file with mine:

```
cp /mnt/lustre/users/sillig/CROCO_TRAINING_Week1/
                3_Some_files/.bashrc ~
source ~/.bashrc
```

- Request one node with the alias command **qsubi1**

```
qsubi1
```

- Go back to your lustre directory.

STEP 3: Copying the source code of the CROCO model

- In your **lustre** directory, copy **CROCO** source code:

```
cp -r /mnt/lustre/users/sillig/CROCO_TRAINING_Week1/
      1_CROCO_code/croco .
```

- List the content of the **croco** directory:

```
cd croco; ls
```

- Go back to your lustre directory.

STEP 4: Copying the source code of the CROCO tools

- In your **lustre** directory, copy **CROCO_TOOLS** source code:

```
cp -r /mnt/lustre/users/sillig/CROCO_TRAINING_Week1/
      2_CROCO_tools/croco_tools .
```

- List the content of the **croco_tools** directory:

```
cd croco; ls
```

- Go back to your lustre directory.

STEP 5: Testing MATLAB Software

- Copy two files into your **lustre** directory:

```
cp /mnt/lustre/users/sillig/CROCO_TRAINING_Week1/
                    3_Some_files/TP0* .
```

- Start Matlab:

```
matlab -nodesktop
```

- Launch the test script:

```
TP0_test_script
```

STEP 6: Exiting

- Exit Matlab:

```
exit
```

- Give back the compute node:

```
exit
```

- Logoff the Lengau cluster:

```
exit
```