Accessing, Navigating, Running Jobs On Cyclone

Hands On Session

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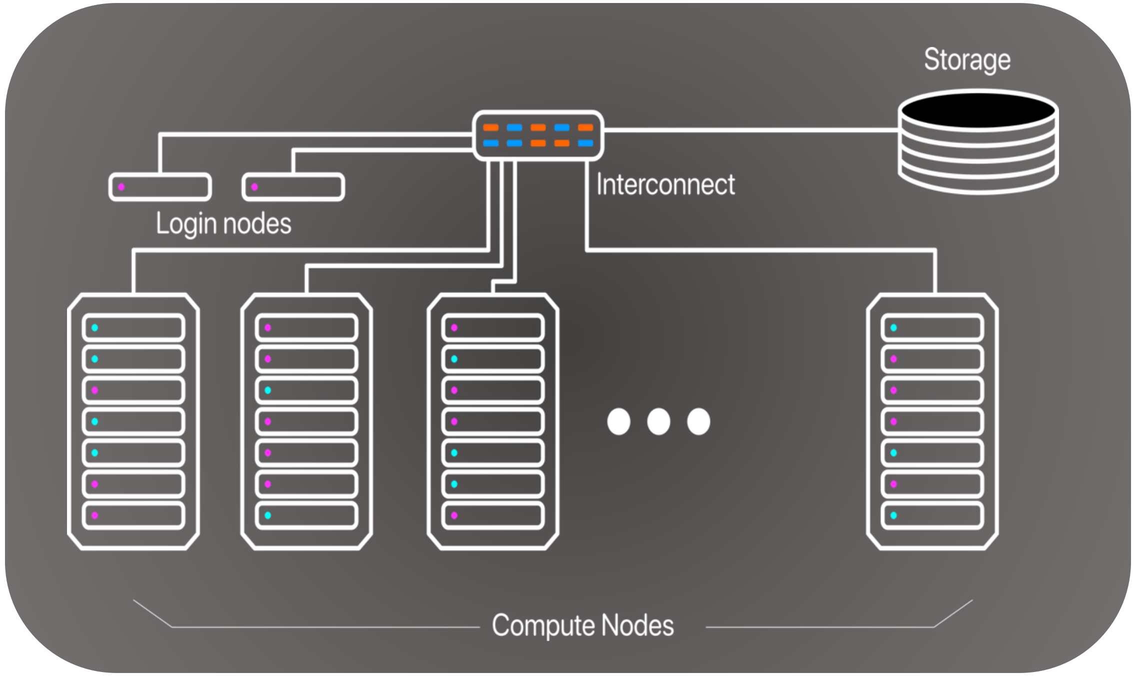
Outline

- Navigating an HPC Cluster
- Build Environment
- Submitting Jobs

- **Assumptions about this hands-on session**
  - Some familiarity with programming in Python
  - Familiarity with some common command-line tasks, e.g. navigating the file system
  - Can edit text files on a remote server, e.g. text-based (emacs or vim) or [VS Code Remote]

You can find the slides at: [https://github.com/CaSToRC-CyI/EuroCC-HPC-with-Python-2025]



- **Specific configuration of our local system**
- Part of a larger system with ~100 nodes
- 4 nodes reserved for this training
  - Hostnames: cn{04,07-08,15}
  - 2×20-core Intel Xeon
  - 186 GBytes RAM
  - 4×NVIDIA V100 GPUs with 32 GBytes Graphics memory each
- Common storage for our course: /nvme/scratch/edu27/

- Log in to a *login node* or *frontend node* –– login node in our case has hostname `front02`
- To run programs on *compute nodes*, a *job scheduler* is available
- Distinguish between *interactive* and *batch* jobs

SLURM job scheduler

- See currently running and waiting jobs: `squeue`
- Ask for an interactive job: `salloc`
- Submit a batch job: `sbatch`
- Run an executable: `srun`

Accessing the System

- To Log in, open a new terminal and type:

```
[localhost ~]$ ssh <username>@front02.hpcf.cyi.ac.cy
```

⚠ Should have gotten instructions how to get to this point before the training event!

⚠

- Type hostname. This tells you the name of the node you are currently logged into:

```
[cstyl@front02 ~]$ hostname
front02
```

this is the login node!

- Ask for one node (`-N 1`):

```
[cstyl@front02 ~]$ salloc -N 1 -p cpu --reservation=edu27 -A edu27
salloc: Granted job allocation 397828
salloc: Waiting for resource configuration
salloc: Nodes cn04 are ready for job
[cstyl@cn04 ~]$
```

- `-A edu27`: charge project with name `edu27`
- `--reservation=edu27`: use reservation `edu27` (reservation and project names need not be the same)
- `-p=cpu`: requests a node from the `cpu` partition –– the partition that includes all `cn[04,07-08,15]` nodes

- Type `hostname` again:

```
[cstyl@cn04 ~]$ hostname
cn04
```

`hostname` is the hostname of a compute node.

- Release the node (type `exit` or hit `ctrl-d`):

```
[cstyl@cn04 ~]$ exit
salloc: Relinquishing job allocation 397828
[cstyl@front02 ~]$
```

we're back on `front02`

⚠ Please **do not** hold nodes unnecessarily; when you have nodes `salloc`ed you may be blocking other users from using those nodes. ⚠

Submitting Jobs via SLURM

- Use `srun` instead of `salloc`:

```
[cstyl@front02 ~]$ srun -N 1 -p cpu -A edu27 --reservation=edu27 hostname
cn07
```

- Allocates a node, runs the specified command (in this case `hostname`), and then exits the node, releasing the allocation
- The output, `cn07`, reveals that we were allocated node `cn07` for this specific –– very short –– job!

Submitting Jobs via SLURM (2)

- Run multiple instances of `hostname` in parallel:

```
[cstyl@front02 ~]$ srun -N 1 -n 2 -p cpu -A edu27 --reservation=edu27 hostname
cn04
cn04
```

`-N 1`: use one node
`-n 2`: use two processes

- Run on **more than one node**:

```
[cstyl@front02 ~]$ srun -N 2 -n 2 -p cpu -A edu27 --reservation=edu27 hostname
cn04
cn07
```

runs one instance of `hostname` on each node.

- Try:

```
[cstyl@front02 ~]$ srun -N 2 -n 1 -p cpu -A edu27 --reservation=edu27 hostname
```

```
srun: Warning: can't run 1 processes on 2 nodes, setting nnodes to 1
cn04
```

- Make a directory. **List** it, see that it is there:

```
[cstyl@front02 ~]$ mkdir eurocc-training
[cstyl@front02 ~]$ ls
eurocc-training
```

- **Change** into it:

```
[cstyl@front02 ~]$ cd eurocc-training
[cstyl@front02 eurocc-training]$
```

- `pwd` will tell you where you are in the file system:

```
[cstyl@front02 eurocc-training]$ pwd
/nvme/h/cstyl/eurocc-training
```

- `/` is referred to as the *root* directory
- `.` is an alias for the *current* directory
- `..` is an alias for the directory one level above
- `~` is an alias for your home directory

E.g.:

```
[cstyl@front02 ~]$ cd ../../
[cstyl@front02 eurocc-training]$ pwd
/nvme/h
```

Navigating Directories (2)

- `cd` without any additional arguments takes you home (equivalent to `cd ~`)

```
[cstyl@front02 ~]$ cd
[cstyl@front02 ~]$ pwd
/nvme/h/cstyl
```

- Make a subdirectory under `eurocc-training` for our first Python program:

```
[cstyl@login02 ~]$ cd eurocc-training
[cstyl@login02 eurocc-training]$ mkdir 01
[cstyl@login02 eurocc-training]$ cd 01
```

- Copy the program from our shared space

```
[cstyl@login02 01]$ cp /nvme/scratch/edu27/Intro/01/prog-01.py .
```

- Use `emacs` or `vim` (or any other text editor you ‘re comfortable with) to inspect the program
- **E.g.:**

```
[cstyl@login02 01]$ vim prog-01.py
```

Running your First Program (1)

```python
import os # For getpid()
import socket # For gethostname()

def main():
    # Get the system's hostname (equivalent to gethostname() in C)
    hostname = socket.gethostname()

    # Get the current process ID (equivalent to getpid() in C)
    pid = os.getpid()

    # Print the hostname and process ID
    print(f"Hostname: {hostname}, pid: {pid}")

if __name__ == "__main__":
    main()
```

Running your First Program (2)

- Time to *execute* the program.
- It is common on HPC systems, as is the case for this system, to have multiple versions and releases of software installed
- This is also the case for ***build environments***, i.e. various versions of interpreters, compilers, linkers, debuggers, and libraries
- The user can select the version that is available to them in each session via a so-called ***modules*** *system*
- List all available modules (long listing truncated in this slide)

```
[cstyl@front02 01]$ module avail
------------------------------------------------------------------ /eb/modules/all ------------------------------------------------
ABAQUS/2024                                          attr/2.5.1-GCCcore-11.3.0
ANTLR/2.7.7-GCCcore-8.3.0-Java-11                    binutils/2.32-GCCcore-8.3.0
...
Use "module spider" to find all possible modules and extensions.
Use "module keyword key1 key2 ..." to search for all possible modules matching any of the "keys".
```

- `module list` should show the currently loaded modules. In a fresh environment with no modules loaded, you should see:

```
[cstyl@front02 01]$ module list
No modules loaded
```

- `module purge` will unload all modules!

- We will be using the `Python` module to load the Python Interpreter. See info:

```
[cstyl@front02 01]$ module show Python
…
```

- Now let's load the module before running the program:

```
[cstyl@front02 01]$ module load Python
[cstyl@front02 01]$ module list
Currently Loaded Modules:
  1) GCCcore/13.3.0                 4) bzip2/1.0.8-GCCcore-13.3.0       7) Tcl/8.6.14-GCCcore-13.3.0        10) libffi/3.4.5-GCCcore-13.3.0
  2) zlib/1.3.1-GCCcore-13.3.0      5) ncurses/6.5-GCCcore-13.3.0       8) SQLite/3.45.3-GCCcore-13.3.0     11) OpenSSL/3
  3) binutils/2.42-GCCcore-13.3.0   6) libreadline/8.2-GCCcore-13.3.0   9) XZ/5.4.5-GCCcore-13.3.0          12) Python/3.12.3-GCCcore-13.3.0
```

- Type `ls` to make sure the program is in the correct directory. Then run it on the frontend node:

```
[cstyl@front02 01]$ ls
prog-01.py
[cstyl @front02 01]$ python prog-01.py
Hostname: front02, pid: 14848
```

Running your First Program (5)

- Run the program using `srun` on two nodes with two processes each:

```
[cstyl@front02 01]$ srun -N 2 -n 4 -p cpu --reservation=edu27 -A
edu27 python prog-01.py
Hostname: cn04, pid: 129145
Hostname: cn07, pid: 241544
Hostname: cn07, pid: 241543
Hostname: cn07, pid: 241545
[cstyl@front02 01]$
```

1 process ran on `cn04` and 3 processes ran **in parallel** on `cn07`

The Fletcher 32 Checksum – Setting Up

- Time for step 2 –– a simple program to compute the Fletcher 32 checksum of several files
- First, make a new directory under `~/eurocc-training/.`

```
[cstyl@front02 01]$ cd ../
[cstyl @front02 eurocc-training]$ mkdir 02
[cstyl @front02 eurocc-training]$ cd 02/
[cstyl @front02 02]$
```

- Copy the program `fletcher32.py` from `/nvme/scratch/edu27/Intro/02/fletcher32.py`

```
[cstyl @front02 02]$ cp /nvme/scratch/edu27/Intro/02/fletcher32.py .
```

- Inspect `fletcher32.py`, e.g.:

```
[cstyl @front02 02]$ vim fletcher32.py .
```

The Fletcher 32 Checksum – Frontend Run

- To run on the frontend:

```
[cstyl@front02 02]$ python fletcher32.py
Usage: python fletcher32.py FNAME
```

- Requires as argument the filename to compute the checksum over. There are 10 files you can use under `/nvme/scratch/edu27/Intro/data/`

```
[cstyl@front02 02]$ ls -1 /nvme/scratch/edu27/Intro/data/
00.txt
01.txt
02.txt
03.txt
04.txt
05.txt
06.txt
07.txt
[cstyl@front02 02]$
```

- For example:

```
[cstyl@front02 02]$ python fletcher32.py /nvme/scratch/edu27/Intro/data/03.txt
/nvme/scratch/edu27/Intro/data/03.txt: 0c40e2d2
```

Takes ~15-20s per file!

The Fletcher 32 Checksum - Objective

- Our objective is to compute the checksums of all 8 files in parallel
- We will use the compute nodes available to us and the 40 available cores per node
- We will start by using a ***Slurm batch script*** as opposed to running ***interactively*** which we have been doing so far

The Fletcher 32 Checksum – Creating the Batch Script

- Copy from `/nvme/scratch/edu27/Intro/02/fletcher.sh`

```
#!/bin/bash
#SBATCH -J fletcher32
#SBATCH -o f32.txt
#SBATCH -e f32.err
#SBATCH -p cpu
#SBATCH -A edu19
#SBATCH --reservation=edu27
#SBATCH -t 00:02:00
#SBATCH -n 1
#SBATCH -N 1
#SBATCH --ntasks-per-node=1

module load Python

date +"%T.%6N"
srun python fletcher32.py
/nvme/scratch/edu27/Intro/data/03.txt
date +"%T.%6N"
```

- `date +"%T.%6N"` prints the current time, including milliseconds (you can try this on the command line interactively)
- The lines starting with `#SBATCH` are parsed by Slurm, even though they are ignored as comments by bash.
- The options are the same as you would pass to `srun`. Notice that `srun` now takes no options

The Fletcher 32 Checksum – Running on the Compute Node

- Submit the script via `sbatch`:

```
[cstyl@front02 02]$ sbatch fletcher.sh
Submitted batch job 397847
```

- Check the status via `squeue`:

```
[cstyl@front02 02]$ squeue -u $USER
JOBID     PARTITION NAME     USER  ST TIME NODES NODELIST(REASON)
397850    cpu       fletcher cstyl R  0:01 1     cn04
```

  `R` means "Running". You may see `PD` for "Pending" (not yet running) or `CG` for "Completing"
- When the job has finished, `squeue -u $USER` should not show any jobs
- The output is now in `f32.txt`. Any errors will be in `f32.err`
- This is the output that would be shown on the terminal had you run the program interactively. Slurm redirects the output and error to those two files
- Check the Output:

```
[cstyl@front02 02]$ cat f32.txt
22:19:41.134499
/nvme/scratch/edu27/data/session1/03.txt: 0c40e2d2
22:19:55.669549
```

Now let's loop over the 8 files

- Could just copy-paste the line to have 8 `srun` lines
- But here we will go with something a little more elegant:

```
date +"%T.%6N"
for((i=0; i<8; i++)); do
    filename=$(printf "%02.0f.txt" $i)
    srun python fletcher32.py /nvme/scratch/edu27/Intro/data/$filename
done
date +"%T.%6N"
```

- The `#SBATCH` lines not shown are unchanged compared to before.

- Submit and check output once completed (will overwrite previous output). Note that the 8 iterations need about 2 minutes:

```
[cstyl@front02 02]$ cat f32.txt
22:36:50.344613
/nvme/scratch/edu27/Intro/data/00.txt: 04d70552
/nvme/scratch/edu27/Intro/data/01.txt: 19708cd4
/nvme/scratch/edu27/Intro/data/02.txt: ed737a1c
/nvme/scratch/edu27/Intro/data/03.txt: 0c40e2d2
/nvme/scratch/edu27/Intro/data/04.txt: f7bde74d
/nvme/scratch/edu27/Intro/data/05.txt: 562ddd6c
/nvme/scratch/edu27/Intro/data/06.txt: 6f2cd2f1
/nvme/scratch/edu27/Intro/data/07.txt: 016db6c6
22:38:46.696467
```

The Fletcher 32 Checksum – Batch Script for Running in Parallel (1)

- Now we will modify the script to run the 8 iterations ***in parallel***

```
#!/bin/bash
#SBATCH -J fletcher32
#SBATCH -o f32.txt
#SBATCH -e f32.err
#SBATCH -p cpu
#SBATCH -A edu27
#SBATCH --reservation=edu27
#SBATCH -t 00:02:00
#SBATCH -n 8
#SBATCH -N 2
#SBATCH --ntasks-per-node=4
module load Python
date +"%T.%6N"
for((i=0; i<8; i++)); do
    filename=$(printf "%02.0f.txt" $i)
    srun --exclusive -n 1 -N 1 python fletcher32.py /nvme/scratch/edu27/Intro/data/$filename &
done
wait
date +"%T.%6N"
```

The Fletcher 32 Checksum – Batch Script for Running in Parallel (2)

- 8 processes in total, 2 nodes, 4 processes per node
  - `-n 8`
  - `-N 2`
  - `--ntasks-per-node=4`
- Each instance of `srun` will run on one node and a single process
  - `srun -n 1 -N 1`)
- `--exclusive` means that each process will be dedicated a processor
  - i.e., a "CPU core"
- The ampersand "&" at the end of the `srun` line indicates that the command in this line should be ***sent to the background***
  - i.e. the loop will go to the next iteration without waiting for the current iteration to complete
- `wait` means wait for all background processes to finish before moving to the next line

The Fletcher 32 Checksum –Running in Parallel

- Submit and check the output once completed!

```
[cstyl@front02 02]$ cat f32.txt
22:31:47.057209
/nvme/scratch/edu27/Intro/data/05.txt: 562ddd6c
/nvme/scratch/edu27/Intro/data/03.txt: 0c40e2d2
/nvme/scratch/edu27/Intro/data/07.txt: 016db6c6
/nvme/scratch/edu27/Intro/data/00.txt: 04d70552
/nvme/scratch/edu27/Intro/data/04.txt: f7bde74d
/nvme/scratch/edu27/Intro/data/01.txt: 19708cd4
/nvme/scratch/edu27/Intro/data/06.txt: 6f2cd2f1
/nvme/scratch/edu27/Intro/data/02.txt: ed737a1c
22:32:03.237708
```

- The 8 checksums should be identical to before
- The order is random. Which checksum completes first is undetermined. The only guarantee is that the last line in the script (the second `date +"%T.%6N`) is run after all 8 are complete (because of the preceding wait)
- All 8 checksums complete within ~15 seconds

Outline of major points covered

- Job scheduling system for reserving and running on compute nodes
- Interactive versus batch jobs
- Modules system for selecting build environment
- Running programs concurrently on multiple cores and multiple nodes

Important points *not* covered

- Here we parallelized the execution of otherwise ***scalar*** programs
- We have not covered implementing parallelism and concurrency ***within*** the programs, which is the standard approach in parallel computing
- Examples:
  - Multi-threading, using a shared memory paradigm. For example using OpenMP
  - Distributed memory parallelization, e.g. using MPI

Up next: Distributed Memory Parallelisation in Python

Thank you for your attention!

More information:

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