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CRUK cluster practical sessions (SLURM)

Part I – processes & scripts

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login

Log in to the head node, clust1-headnode, using **ssh** and your usual user name & password.

```
SSH Secure Shell 3.2.9 (Build 283)
Copyright (c) 2000-2003 SSH Communications Security Corp - http://www.ssh.com/

This copy of SSH Secure Shell is a non-commercial version.
This version does not include PKI and PKCS #11 functionality.


Last login: Mon Sep 19 10:44:07 2016 from bp7r25j.cri.camres.org
[user@cluster ~]$
```

You're ready to start.

navigate

Find out where you are using **pwd**.

Make a directory (**mkdir**) and move into it (**cd**)

```
[user@cluster ~]$ pwd
/home/user
[user@cluster ~]$ mkdir training
[user@cluster ~]$ cd training/
[user@cluster training]$
```

processes

You can see your current processes using **ps**.

```
[user@cluster training]$ ps
  PID TTY          TIME CMD
14859 pts/22   00:00:00 bash
18511 pts/22   00:00:00 ps
```

You can see what else *this* computer is doing using **top**

```
[user@cluster training]$ top
```

top output

top uses the whole screen. Type ‘q’ to get your screen back.

```
top - 16:26:38 up 58 days, 22:33, 36 users,  load average: 0.12, 0.14,
0.12
Tasks: 618 total,   1 running, 617 sleeping,   0 stopped,   0 zombie
Cpu(s):  0.1%us,  0.2%sy,  0.0%ni, 99.5%id,  0.2%wa,  0.0%hi,  0.0%si,
0.0%st
Mem:  16437908k total, 10473016k used,  5964892k free,  2611564k buffers
Swap: 16779852k total,   162896k used, 16616956k free,  2158536k cached

  PID USER      PR  NI  VIRT  RES  SHR S %CPU %MEM    TIME+  COMMAND
  975 root       0 -20 22712 3832 2196 S    1  0.0  28:44.67 lim
 4686 root      15   0     0    0    0 S    0  0.0   3:11.36 nfsd
19175 user      15   0 11048 1592  864 R    0  0.0   0:00.14 top
    1 root      15   0 10364  600  564 S    0  0.0   0:12.04 init
```

The ‘sleep’ command

The **sleep** command doesn’t do much – but you can control how many seconds it does it for, and it doesn’t use much CPU or I/O

```
[user@cluster training]$ sleep 10
[user@cluster training]$
```

Stop and suspend

If we get bored, change our mind, or think something is wrong we can interrupt jobs.
To stop a job, type '^C' at the command line (that's [Ctrl]+[C] together).

```
[user@cluster training]$ sleep 100
[user@cluster training]$
```

If you don't want to stop the job, you can suspend it. Type '^Z' (that's [Ctrl]+[Z]).
Type 'fg' to bring the job back to the foreground.

```
[user@cluster training]$ sleep 100
[1]+  Stopped                 sleep 100
[user@cluster training]$ fg
```

backgrounding

When we have suspended a job (which will never finish). To get it to carry on, we can put it in the 'background' using **bg**

```
[user@cluster training]$ sleep 100
[1]+  Stopped                 sleep 100
[user@cluster training]$ bg
[1]+ sleep 100 &
[user@cluster training]$ ps
  PID TTY          TIME CMD
14859 pts/22   00:00:00 bash
24799 pts/22   00:00:00 sleep
25377 pts/22   00:00:00 ps
```

You can put a job in the background deliberately using the '&' character at the end of the command.

```
[user@cluster training]$ sleep 100 &
[1] 787
[user@cluster training]$ ps
  PID TTY          TIME CMD
  787 pts/22   00:00:00 sleep
  804 pts/22   00:00:00 ps
14859 pts/22   00:00:00 bash
```

Killing processes

If you don't want to wait for it to finish, or think it is broken in some way, you can terminate it using the **kill** command.

Kill has a variety of gentle options to allow the process to exit gracefully. If these fail one – signal **-9**, or **–KILL** will normally remove the process.

```
[user@cluster training]$ sleep 100 &
[1] 787
[user@cluster training]$ ps
  PID TTY          TIME CMD
  787 pts/22   00:00:00 sleep
  804 pts/22   00:00:00 ps
14859 pts/22   00:00:00 bash
[user@cluster training]$ kill -KILL 787
[user@cluster training]$
[1]+  Killed                  sleep 100
[user@cluster training]$
```

A simple example

Sleep is a good example, but it doesn't produce any output. We want to wrap it up with messages – in unix you use **echo** to do this.

The colon here allows us to put multiple commands on a single line.

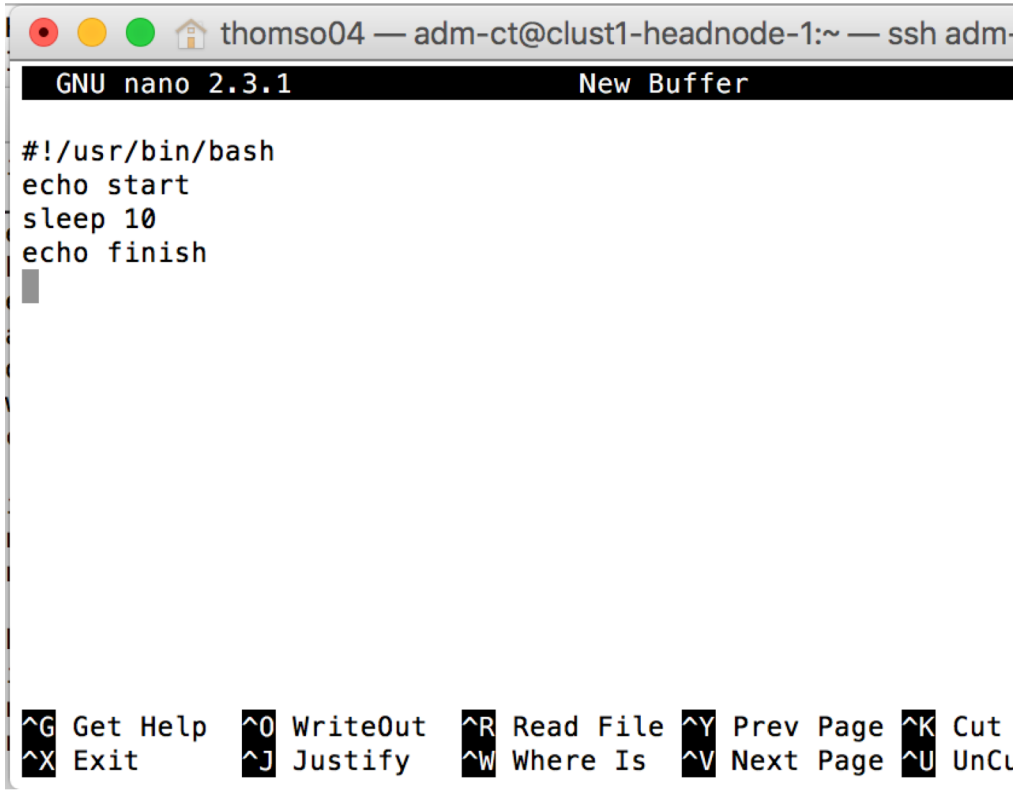
```
[user@cluster training]$ echo start; sleep 1; echo finish
start
finish
[user@cluster training]$
```

Creating a script

Cluster programming makes use of scripts, so we'll turn this list of commands into a script.

Use the nano text editor to enter the following script:

```
[user@cluster training]$ nano script.sh
```



You can run a script by executing **bash <scriptname>** or by making it directly executable with **chmod**. The './' is important – the shell only looks for executables in certain places – the '**PATH**'.

```
[user@cluster training]$ chmod u+x script.sh
[user@cluster training]$ ./script.sh
start
finish
```

Running the script

Now we are ready to start running our script, or sending it as a cluster job.

```
[user@cluster training]$ ./script.sh > script.out &
[1] 7594
[user@cluster training]$ ps
  PID TTY          TIME CMD
 7594 pts/22   00:00:00 bash
 7595 pts/22   00:00:00 sleep
 7598 pts/22   00:00:00 ps
14859 pts/22   00:00:00 bash
[user@cluster training]$
[1]+  Done                    ./script.sh > script.out
```

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Cluster practical sessions

Part II – cluster job submission

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Submitting a job

Now we know enough to run our script on the cluster.

Simply submit the job using **sbatch**.

- the output file is written to a **Lustre file system** directory
- Create directory with username if it doesn't exist – e.g. mkdir /scratcha/stlab/garret01
- **/home** is writeable from cluster nodes, but won't perform as well.

```
[user@cluster training]$ sbatch --time=10 --output=/scratcha/stlab/garret01/%N-%j.out script.sh
Submitted batch job 200875
```

- All read and write operations from within jobs running on nodes should use either /scratchb or /scratcha directories.

SLURM time formats

Acceptable time formats include "minutes", "minutes:seconds", "hours:minutes:seconds", "days-hours", "days-hours:minutes" and "days-hours:minutes:seconds".

Look at running jobs

While the job is running, you can see it with **squeue**.

```
[user@cluster training]$ squeue
             JOBID PARTITION     NAME     USER ST       TIME  NODES NODELIST(REASON)
            200876   general script.s     user  R       0:02      1 clust1-node-3
            200867   general     bash  sawle01  R    4:01:05      1 clust1-node-2
            175393   general MB99.6.v eldrid01  R 9-00:28:46      1 clust1-node-30
            175330   general vardict_ eldrid01  R 9-01:40:03      1 clust1-node-1
```

Once it's finished, you can see the output.

```
[user@cluster training]$ squeue
             JOBID PARTITION     NAME     USER ST       TIME  NODES NODELIST(REASON)
            200867   general     bash  sawle01  R    4:01:33      1 clust1-node-2
            175393   general MB99.6.v eldrid01  R 9-00:29:14      1 clust1-node-30
            175330   general vardict_ eldrid01  R 9-01:40:31      1 clust1-node-1
[user@cluster training]$ ls /scratcha/group/user/
clust1-node-3-200877.out
```

What happened?

The output went into the file as expected:

```
[user@cluster training]$ cat /scratcha/group/user/clust1-node-3-200877.out
start
finish
```

Other information is stored, and available via sacct:

```
[user@cluster training]$ sacct -j 200877
       JobID    JobName  Partition    Account  AllocCPUS      State ExitCode
------------ ---------- ---------- ---------- ---------- ---------- --------
200877        script.sh    general      group          1  COMPLETED      0:0
200877.batch      batch                 group          1  COMPLETED      0:0


[user@cluster training]$ sacct -j 200877 --format JobID,MaxRSS,State,AllocCPUS
       JobID     MaxRSS      State  AllocCPUS
------------ ---------- ---------- ----------
200877                   COMPLETED          1
200877.batch      2012K  COMPLETED          1
```

An alternative way to submit

You can submit a job directly to SLURM with **srun**. This still requires resources – it's more commonly used as part of an existing job.

```
[user@cluster training]$ srun --time=1-12:30:59 /usr/bin/bash script.sh
start
finish
```

You can also generate an interactive session:

```
[user@cluster training]$ sintr
[user@clust1-node-3 training]$
```

sintr is a local implementation of a script written by Pär Andersson (National Supercomputer Centre, Sweden) which will sort out X Forwarding, launch screen on a node, and connect you to the session.

Killing a job

Just as for processes, but using **scancel**

```
[user@cluster training]$ sbatch --output=/scratcha/group/user/%N-%j.out script.sh
Submitted batch job 200889
[user@cluster training]$ squeue
             JOBID PARTITION     NAME     USER ST       TIME  NODES NODELIST(REASON)
            200889   general script.s     user  R       0:02      1 clust1-node-3
            200867   general     bash  sawle01  R    4:28:21      1 clust1-node-2
            175393   general MB99.6.v eldrid01  R 9-00:56:02      1 clust1-node-30
            175330   general vardict_ eldrid01  R 9-02:07:19      1 clust1-node-1

[user@cluster training]$ scancel 200889
[user@cluster training]$ squeue
             JOBID PARTITION     NAME     USER ST       TIME  NODES NODELIST(REASON)
            200867   general     bash  sawle01  R    4:28:21      1 clust1-node-2
            175393   general MB99.6.v eldrid01  R 9-00:56:02      1 clust1-node-30
            175330   general vardict_ eldrid01  R 9-02:07:19      1 clust1-node-1
```

NOTE: Do not use **skill** it is **NOT** a SLURM command!

Killing isn't bad…

The scheduler manages the shutdown and still records details of the job.

```
[user@cluster training]$ sacct -j 200889
       JobID    JobName  Partition    Account  AllocCPUS      State ExitCode
------------ ---------- ---------- ---------- ---------- ---------- --------
200889        script.sh    general      group          1 CANCELLED+      0:0
200889.batch      batch                 group          1  CANCELLED     0:15
```

Basic parallelism

Now we're ready to use the cluster at full power!

One way to do this is with a job array. You can create one of these using the

--array=1-N syntax in **sbatch**

```
[user@cluster training]$ sbatch --time=10 --array=1-10 --output=/scratcha/group/user/%N-
%j.out script.sh
Submitted batch job 200900
[user@cluster training]$ ls /scratcha/group/user
clust1-node-10-200908.out  clust1-node-12-200900.out  clust1-node-4-200902.out
clust1-node-10-200904.out   clust1-node-12-200906.out   clust1-node-11-200909.out
clust1-node-3-200901.out   clust1-node-5-200903.out   clust1-node-7-200905.out
clust1-node-9-200907.out
```

Or using the **srun** with the **–n** or **–N** parameters.

```
[user@cluster training]$ srun --time=10 -n hostname
clust1-node-9.cri.camres.org
…
clust1-node-13.cri.camres.org
[user@cluster training]$
[user@cluster training]$ srun --time=10 -N 3 hostname
clust1-node-19.cri.camres.org
clust1-node-25.cri.camres.org
clust1-node-8.cri.camres.org
[user@cluster training]$
```

The final example maps specific names to their file position in a reference file list. The map is written to names-list.out

```
#!/bin/bash

for i in Matthew Luca Mohammed Lochlan Leighton Keegan Dawid Magnie Zygmunt Zen
do
   srun --time=10 -e /<YOUR SCRATCH DIR/%j-names-list.err -o /<YOUR SCRATCH DIR/names-list.out grep -n $i
/scratchb/training/refdata/names-list.txt 2>&1 &
done
```

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