ilifu Online Training – Advanced `slurm`

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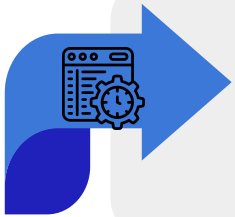
SLURM - Use cases

Login node

Run SLURM & bash commands
cd, mkdir, ls, etc

Jupyter/Dev. node

Development space
New code / workflows / routines
Debugging / testing software

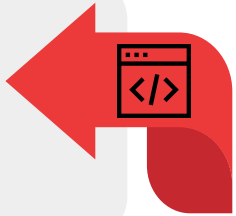


Main partition

Stable, computationally heavy processing

HighMem/GPU

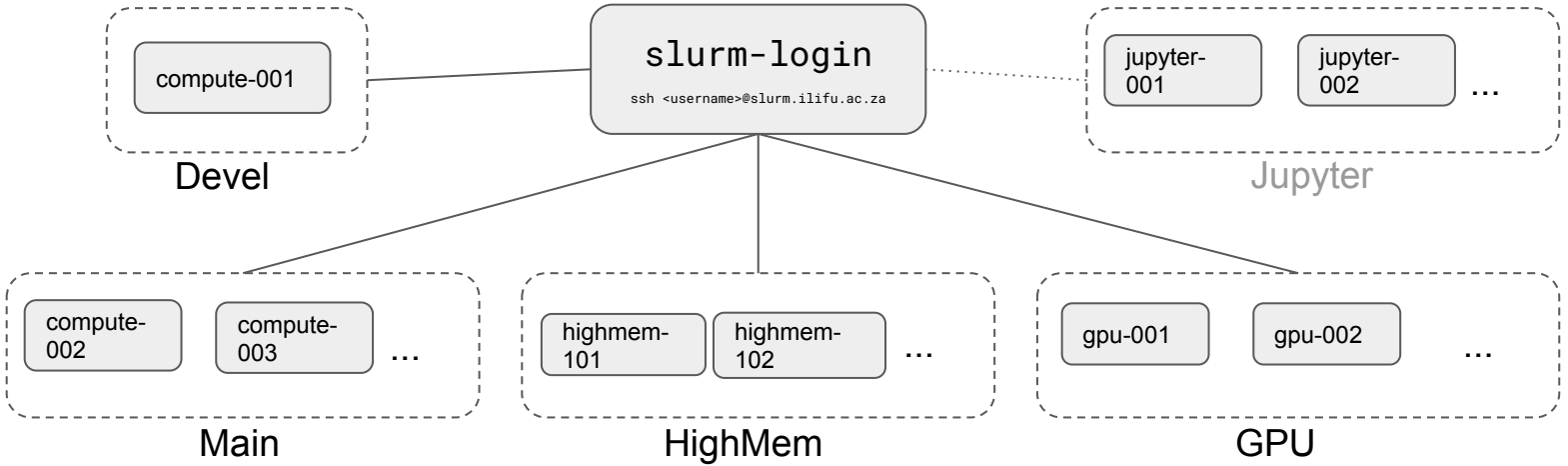
For single-high memory jobs or GPU resources



SLURM

http://docs.ilifu.ac.za/#/tech_docs/running_jobs?id=specifying-resources-when-running-jobs-on-slurm

Main	HighMem	GPU	Devel
~85 nodes	3 nodes	8 nodes	1 node
32 CPUs 232 GB RAM	32 CPUs 500+ GB RAM	32 CPUs, 2 GPUs 232 GB RAM	32 CPUs 237 GB RAM



Interactive Sessions

tmux — terminal multiplexer

```
$ tmux   # start a tmux session

$ tmux attach   # attach to an already running session
```

Keyboard shortcuts

```
Ctrl+b c   # Create new tab
Ctrl+b n   # Next tab
Ctrl+b p   # previous tab
Ctrl+b d   # detach session
```

SLURM - running an interactive job

X11 forwarding support

```
$ ssh -X <username>@slurm.ilifu.ac.za
```

Allocates a Slurm compute node:

```
$ sinteractive --x11   # start interactive job on devel with X11
```

```
$ srun --x11 --pty bash   # start interactive with X11
```

SLURM - advanced user commands

Commands before running jobs

```
$ sinfo  # give information about partitions/queues
$ scontrol  # show information about stuff
$ squeue  # show jobs in the queue
```

Commands starting jobs

```
$ sbatch  # run a traditional batch job
$ sinteractive  # start an interactive Devel job
$ srun  # run a command
```

Commands during jobs

```
$ scontrol  # give information about your job
```

Commands after jobs

```
$ sacct  # give information about partitions/queues
```

SLURM - advanced user commands

- Before running jobs :

List partitions and their specs

```
$ sinfo -O "partition,available,cpus,nodes,memory,statecompact"
```

List your SLURM accounting groups

```
$ sacctmgr show user <username> cluster=ilifu-slurm2021 -s format=account%30
```

- Syntax for `srun`:

Submit to Main under specific account

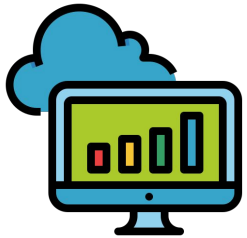
```
$ srun --partition=Main --account=b34-admins-ag
```

Submit job to GPU partition

```
$ srun --partition=GPU job_script.sh
```

SLURM - advanced user commands

- After / during running jobs :
  - `jobId` is given from sbatch output / squeue



Shows info about job running including working directory

```
$ scontrol show jobID <jobID>
```

Shows info for multi-CPU jobs

```
$ sacct -o JoBID%-15,JobName%-15,Partition,Account,
  Elapsed,NNodes%6,NTASK%6,NCPUS%5,MaxDiskRead,MaxDiskWrite,
 NodeList%20,MaxRSS,CPUTime,State,ExitCode
```

Shows jobs started and completed between these dates

```
$ sacct -S 2021-09-01-09:00 -E 2021-09-14-10:00 -X -o
  Jobid,JobName,Start,End,State
```

SLURM - advanced user commands

- Email parameters

```
$ srun --mail-user=<address> --mail-type=<event_types>
  -   Events : BEGIN,END,FAIL,TIME_LIMIT_80
```

- Exclude nodes
- e.g. problematic nodes (report to ilifu support)

```
$ srun --exclude=compute-[101,101-105]
```

SLURM - running an interactive job

- Specify lower wall-time (default 3 hours) and less memory (default ~7GB) increases chance of job launching immediately
- In steps:

```
$ srun --pty --time=10 --mem=1GB bash
$ singularity shell /idia/software/containers/python-3.6.img
$ python3 job_script.py
```

- In single call:

```
$ srun --pty --time=10 --mem=1GB singularity exec
/idia/software/containers/python-3.6.img python3 job_script.py
```

- Must manually process after this

DEMO TIME!

SLURM - array jobs

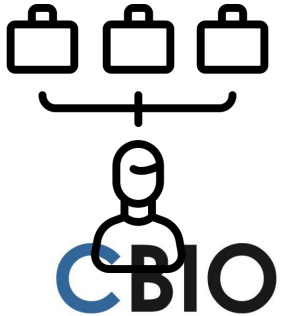
- Array jobs allow quick submission of many similar jobs, each with same resources, without any manual launch

  - Passes array task ID into script, which changes behavior of each job each time i.e different inputs
  - Can be used to run many related steps in a serial process

- Example job array Running, 20 jobs, with 5 run simultaneously

```
#!/bin/bash
#SBATCH --array=1-20%5
#SBATCH --job-name=myarrayjob
#SBATCH --output=logs/%x-%A_%a.out
#SBATCH --error=logs/%x-%A_%a.err

singularity exec python myscript.py --input $SLURM_ARRAY_TASK_ID
```



SLURM - substitutions and environment variables

Parameter	Substitution / filename pattern	Environment Variables
jobID of running job	`%j`	`SLURM_JOB_ID`
Job name	`%x`	`SLURM_JOB_NAME`
Job array's master job allocation number	`%A`	`SLURM_ARRAY_JOB_ID`
Job array task ID (index) number	`%a`	`SLURM_ARRAY_TASK_ID`
CPUs per task		`SLURM_CPUS_PER_TASK`

SLURM - dependencies

- Allow jobs to be scheduled for running, based on the status of a previous job

  - e.g only begin a particular job once previous one successfully completes

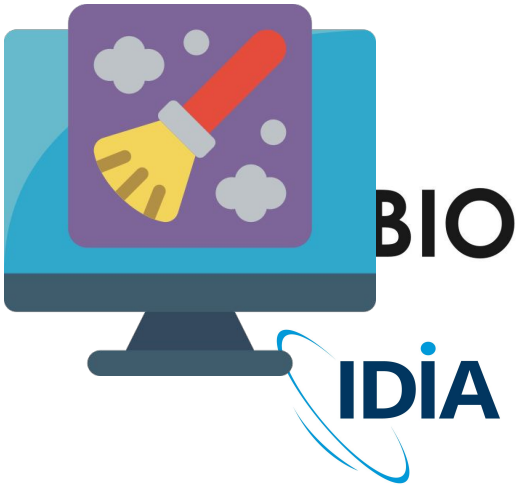
```
Submit another_job.sh to SLURM queue, to begin after jobID 1234 successfully
completes , or cancel the job if jobID 1234 fails
$ sbatch -d afterok:1234 --kill-on-invalid-dep=yes another_job.sh

Submit another_job.sh to SLURM queue, to begin after jobID 1234 & 5678 completes
$ sbatch -d afterany:1234:5678 another_job.sh
```

SLURM - Best practice

Do's :

- Run jobs using sbatch rather than interactive jobs
- Identify job resources requirements:
  - No. of nodes and CPUs, amount of RAM and wall-time.
- Remove files that aren't needed
  - `/scratch3` folder after data processing is complete
  - Old raw data, temporary products , etc.
- Use Singularity (cannot install software on nodes)
- Use **`username@transfer.ilifu.ac.za`** for data transfers



Don't:

- Don't run software/heavy processes on login node
- Don't place large files in your home directory (`/users`)
- Don't transfer using scp/rsync on the login node

Thank you!

Once again to Hope and Jordan for letting me use their slides.

Remember our support channels!

support@ilifu.ac.za
https://docs.ilifu.ac.za