

Bioinformatics Support, ilifu University of Cape Town, 12 September 2023



UNIVERSITY OF CAPE TOWN



IDIA Inter-University Institute for Data Intensive Astronomy







Job scheduling & cluster management tool

- Framework : Login node & Compute nodes

Login node

- Accessed via ssh (\$ ssh <username>@slurm.ilifu.ac.za)
- Submit jobs and manage work directories

Compute nodes

- Where processes/code runs
- via singularity containers or modules

Partitions / Queues

Main, Jupyter, Devel 32 core, ~232GiB RAM	GPU 32 core, ~232GiB RAM, Nvidia GPUs	HighMem 32 core, 503GiB RAM 96 core, 1.5TiB RAM
85 + 12 Nodes	7 nodes	3 nodes







SLURM - Use cases





Login node

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



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





Main partition

Stable, computationally heavy processing

HighMem/GPU

For single-high memory jobs that can't be split into multiple jobs for MPI

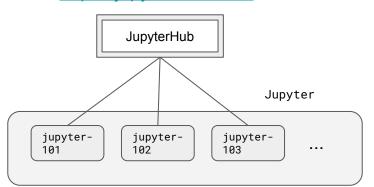


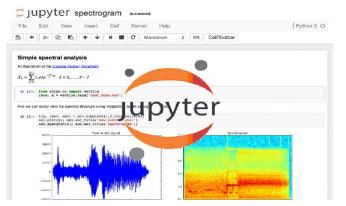


http://docs.ilifu.ac.za/#/getting_started/submit_job_slurm

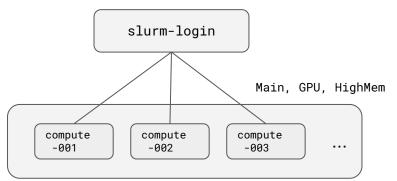


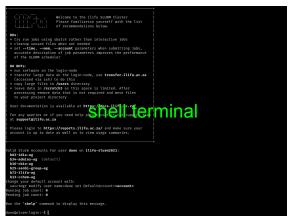
https://jupyter.ilifu.ac.za





\$ ssh <username>@slurm.ilifu.ac.za











SLURM - user commands



- \Rightarrow sinfo \rightarrow shows partitions and resources
- \Rightarrow squeue \rightarrow shows all jobs in SLURM queue/partition
- \$ squeue -u \$USER \rightarrow shows your jobs
- \$ sbatch slurm_job_script.sh \rightarrow submitjob to SLURM
- \Rightarrow sbatch --help \rightarrow info. on job submission parameters
- \$ scancel <jobid> → cancel running/pending job







SLURM - running a job



#!/bin/bash
module add python/3.11.2
python hello_world.py







SLURM - running a job



https://github.com/ilifu/ilifu_user_training/tree/main/introduction/tutorial2

```
#!/bin/bash
#SBATCH --job-name=tutorial2_R_container
#SBATCH --time=00-00:01:00
#SBATCH --mem=4G
#SBATCH --mem=4G
#SBATCH --output=R_container-%j.stdout
#SBATCH --error=R_container-%j.stderr
#SBATCH --mail-user=YOUR_EMAIL_ADDRESS
#SBATCH --mail-type=BEGIN, END, FAIL, TIME_LIMIT_80
#SBATCH --account=ACCOUNTING_GROUP

singularity exec /software/common/containers/RStudio2023.06.1-524-R4.3.1.sif Rscript hello_world.R

container

Describe job parameters / resources

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```





DEMO TIME!







SLURM - Best practices



Do's:

- Run jobs using sbatch rather than interactive jobs
- Identify job resources requirements:
 - o 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 for coming and for your time.

And special thanks to Hope and Jordan for letting me copy their slides.

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

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support@ilifu.ac.za



