

Bioinformatics Support, ilifu University of Cape Town, 3 September 2024



# 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





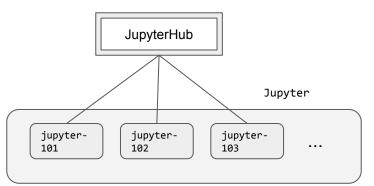


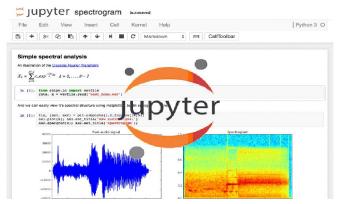


#### http://docs.ilifu.ac.za/#/getting\_started/submit\_job\_slurm

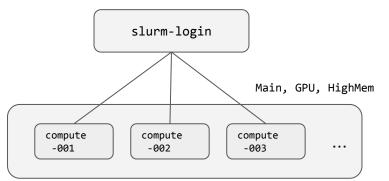


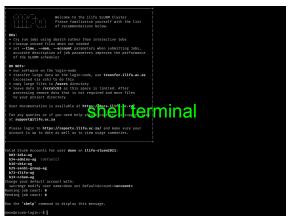
#### https://jupyter.ilifu.ac.za





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











## SLURM - user commands



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







# SLURM - running a job



https://github.com/ilifu/ilifu\_user\_training/tree/main/introduction/tutorial2

#!/bin/bash

module add python/3.11.2

python hello\_world.py







## SLURM - defaults



https://docs.ilifu.ac.za/#/tech\_docs/running\_jobs?id=customising-your-job-using-sbatchsrun-parameters

-time=0-03:00:00 # 3 hours

-mem=3G # 3 GiB

-ntasks=1 # one task

-nodes=1 # one node

-partition=Main

-account=<your default>







# 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 --partition=Main
#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

software
```







# SLURM - defaults and maximums per partition



#### https://docs.ilifu.ac.za/#/tech\_docs/resource\_allocation?id=maximum-allocation

Partition	Node names	Default CPUs	Max CPUs	Default Memory (GiB)	Max Memory (GiB)	Default wall-time	Max wall- time
Main	compute- [002-021]	1	32	3	232	3 hours	14 days
Main	compute- [101-105]	1	48	3	232	3 hours	14 days
Main	compute- [201-260]	1	32	3	251	3 hours	14 days
HighMem	highmem- [001-002]	1	32	15	503	3 hours	14 days
HighMem	highmem- 003	1	96	15	1508	3 hours	14 days
GPU	gpu-[001- 004]	1	32	7	232	3 hours	14 days
GPU	gpu-005	1	24	7	232	3 hours	14 days
GPU	gpu-006	1	48	7	354	3 hours	14 days
GPU	gpu-007	1	48	7	354	3 hours	14 days
Devel	compute-001	1	32	-	-	3 hours	12 hours









## **DEMO TIME!**

https://github.com/ilifu/ilifu\_user\_training/tree/main/introduction/tutorial2







# **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.

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

support@ilifu.ac.za





