ilifu Online Training

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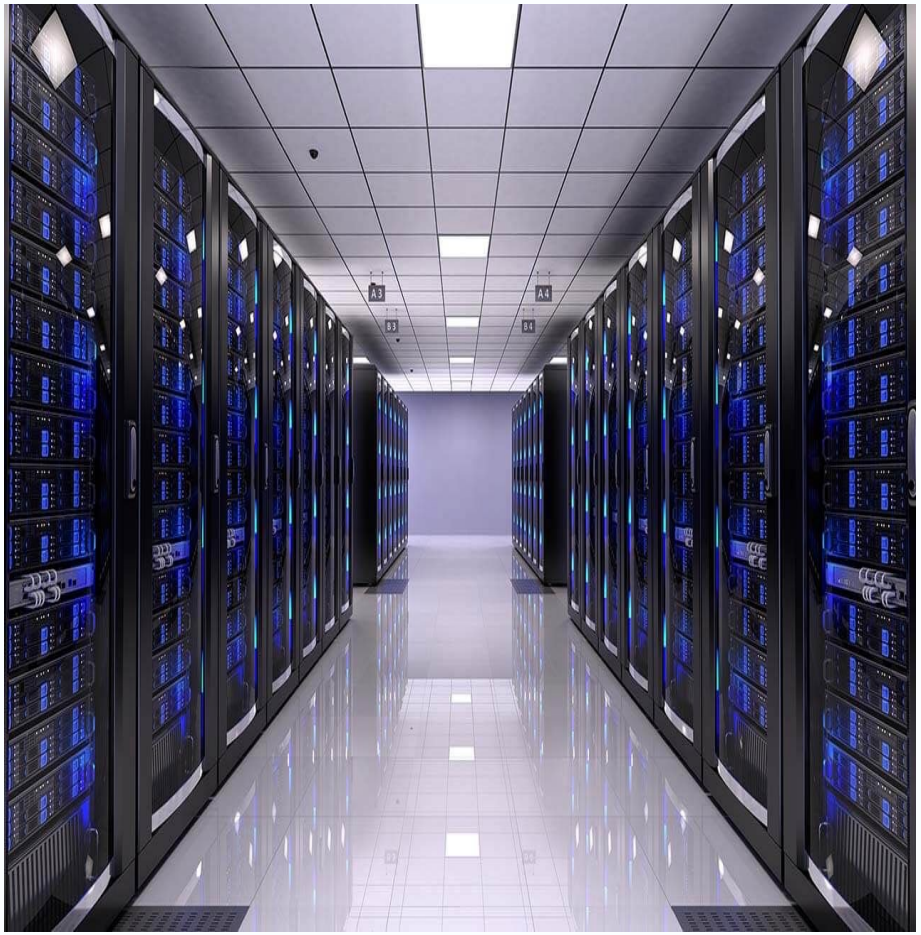
ilifu

IDIA Inter-University Institute for Data Intensive Astronomy

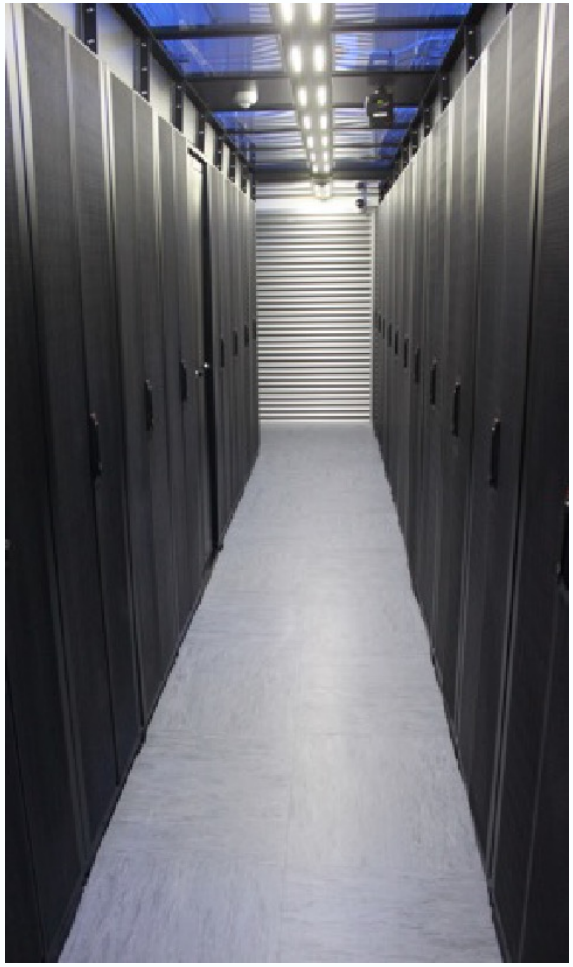
WESTERN SYDNEY UNIVERSITY

ilifu: from laptop to VM to cluster



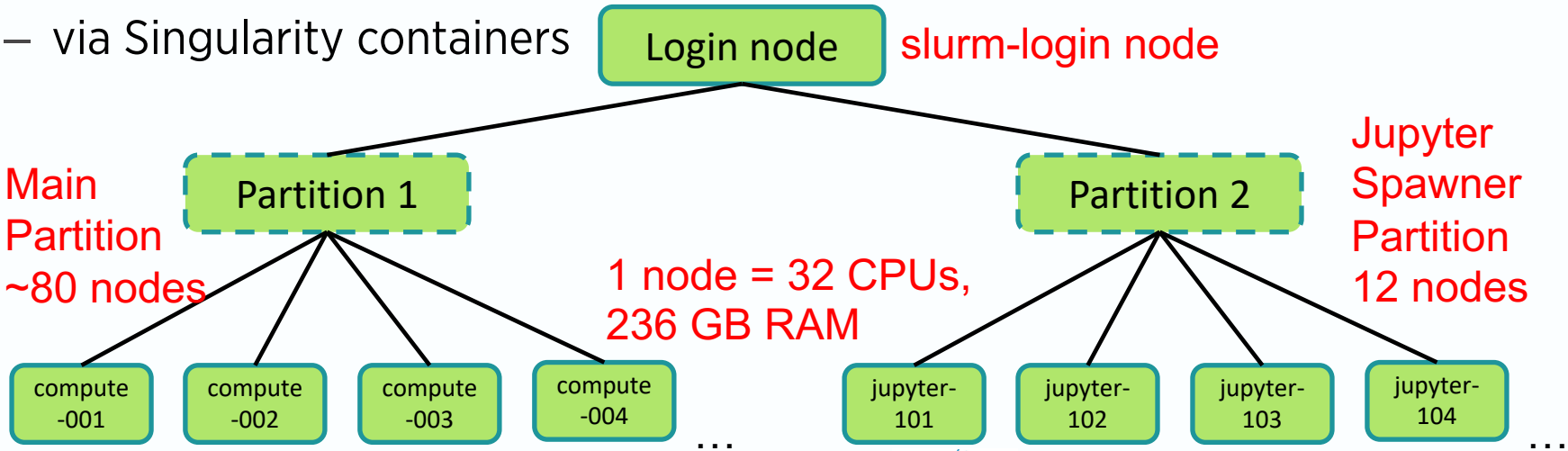
ilifu

- ilifu (http://ilifu.ac.za)
  - Tier 2 Data Intensive Research Facility
  - Joint Cloud Platform for Astronomy and Bioinformatics
  - Cluster w/ ~85 nodes (32 CPUs, 256/512 GB)
  - ~6 PB usable storage (BeeGFS & CephFS)
  - 10 Gb/s network to South African National Research Network (SANReN)



SLURM

- http://docs.ilifu.ac.za/#/getting_started/submit_job_slurm
- Login node (job submission & management)
  - where you land when you log in (also known as “head node”)
  - **run SLURM commands/submit jobs, but not software/heavy processes**
- Compute nodes
  - Where your processes run (also known as “worker nodes”)
  - via Singularity containers

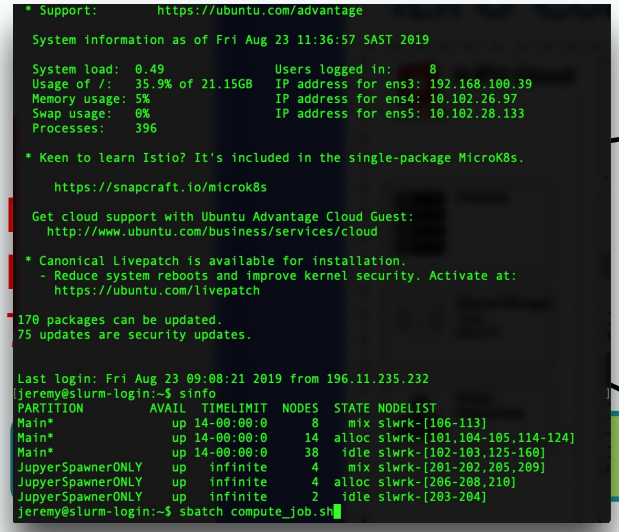


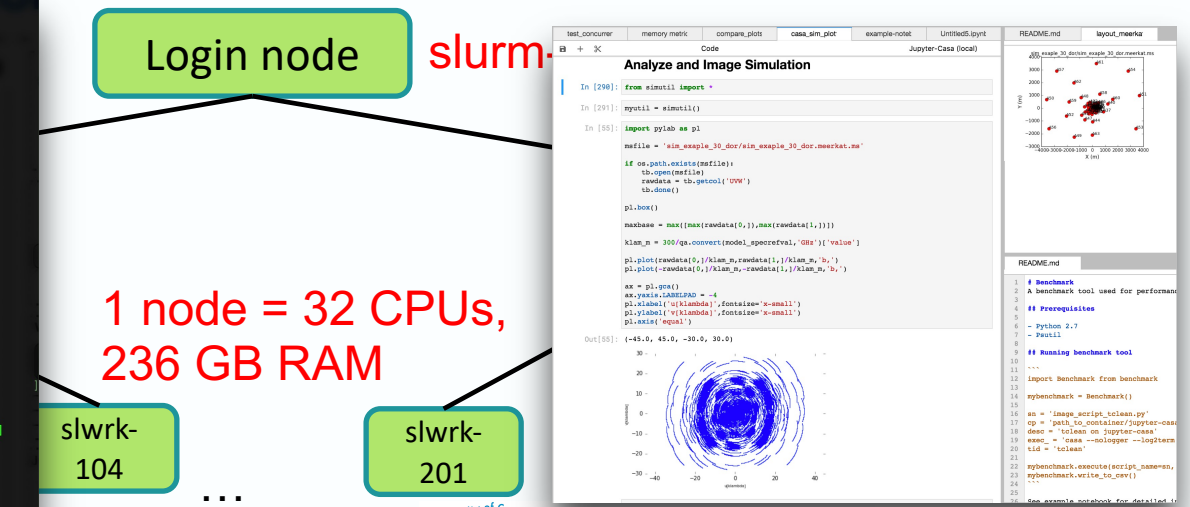
SLURM

- http://docs.ilifu.ac.za/#/getting_started/submit_job_slurm
- `ssh <username>@slurm.ilifu.ac.za`
- https://jupyter.ilifu.ac.za
- Partitions: Main (~80 nodes), HighMem (2), GPU (4), Jupyter (12)

ssh – shell terminal

JupyterHub





SLURM – user commands

- https://slurm.schedmd.com/

```
$ sinfo #shows partitions and resources
$ squeue #shows all jobs in SLURM queue
$ squeue –u <username> #shows your jobs
$ sbatch slurm_job_script.sh #submit job to SLURM queue
$ sbatch --help #describes input parameters
$ scancel <jobid> #cancels job
$ sacct #shows status of recent jobs that have run, or are running
```

SLURM – running a job

```
$ cat slurm_job_script.sh
#!/bin/bash
#SBATCH --job-name=demo_job
#SBATCH --time=00:01:00
#SBATCH --mem=4GB
#SBATCH --output=demo-job-%j.out
#SBATCH --error=demo-job-%j.err
#SBATCH --account=b03-idia-ag

module load python/3.7.7
python myscript.py

$ sbatch slurm_job_script.sh #submit job to SLURM queue
```

SLURM – running a job

```
$ cat slurm_job_script.sh
#!/bin/bash
#SBATCH --job-name=demo_casa
#SBATCH --time=01:00:00
#SBATCH --mem=4GB
#SBATCH --output=demo-job-%j.out
#SBATCH --error=demo-job-%j.err
#SBATCH --account=b03-idia-ag

echo "Submitting demo SLURM job"
singularity exec /idia/software/containers/casa-stable-5.7.0.simg casa -c myscript.py

$ sbatch slurm_job_script.sh #submit job to SLURM queue
```

Describe job parameters/resources

container software script

what's being executed with above parameters

SLURM – running a job

```
$ cat slurm_job_script.sh

#!/bin/bash

#SBATCH --job-name=demo_casa

#SBATCH --time=01:00:00

#SBATCH --mem=4GB

#SBATCH --output=demo-job-%j.out

#SBATCH --error=demo-job-%j.err

#SBATCH --account=b03-idia-ag


module load casa/5.7.0

casapy -c myscript.py


$ sbatch slurm_job_script.sh #submit job to SLURM queue
```

SLURM – running an interactive job

- http://docs.ilifu.ac.za/#/getting_started/submit_job_slurm?id=interactive-slurm-session

```
$ srun --pty bash #opens bash shell session on compute
                  #node with default 3 hours and ~7GB RAM


$ srun --pty --time=01:00:00 --mem=64GB singularity exec
/idia/software/containers/casa-stable.img casa

        #opens interactive CASA session on compute node,
        #with 1 hour walltime, 64GB RAM,
        #using Singularity CASA container


$ srun --help

        #view srun help docs for input parameters
```

SLURM – running an interactive job

- With X11 support for viewing GUI

```
$ ssh –Y <username>@slurm.ilifu.ac.za

#important to include the –Y parameters when
logging into the SLURM login node, for X-forwarding


$ srun --x11 --pty bash

#opens bash shell session on compute node
#with X11 support; default 3 hours, ~7GB RAM


$ srun --x11 --pty --time=00:10:00 --mem=1GB ––qos qos-interactive bash
```

Demo Time!

Best practices

- Don't run software / heavy processes / scp on the login node
  - Only submit jobs and run SLURM commands (sbatch, srun, squeue, etc)
  - Use transfer.ilifu.ac.za to transfer data (external/internal), not login node
- Before running a large job, identify the available resources
  - Use sinfo. Don't hog the cluster. Reduce your allocation if possible
  - Increase likelihood of jobs running with less memory and less walltime
- Use sbatch (srun / screen / tmux are volatile)
- Cleanup files that aren't needed
  - Old raw data, temporary products, scratch data, etc
- Don't place large files in your home directory (/users)
- Use Singularity (you cannot install software on the nodes)

THANK YOU

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