ilifu Online Training – Advanced

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IDIA Inter-University Institute for Data Intensive Astronomy

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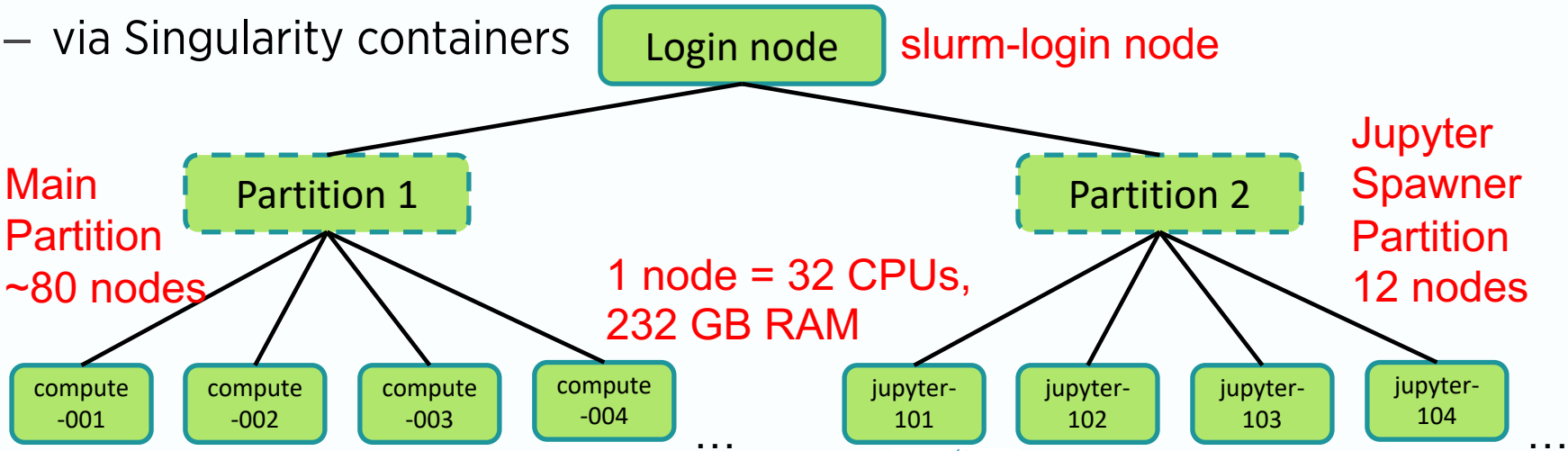
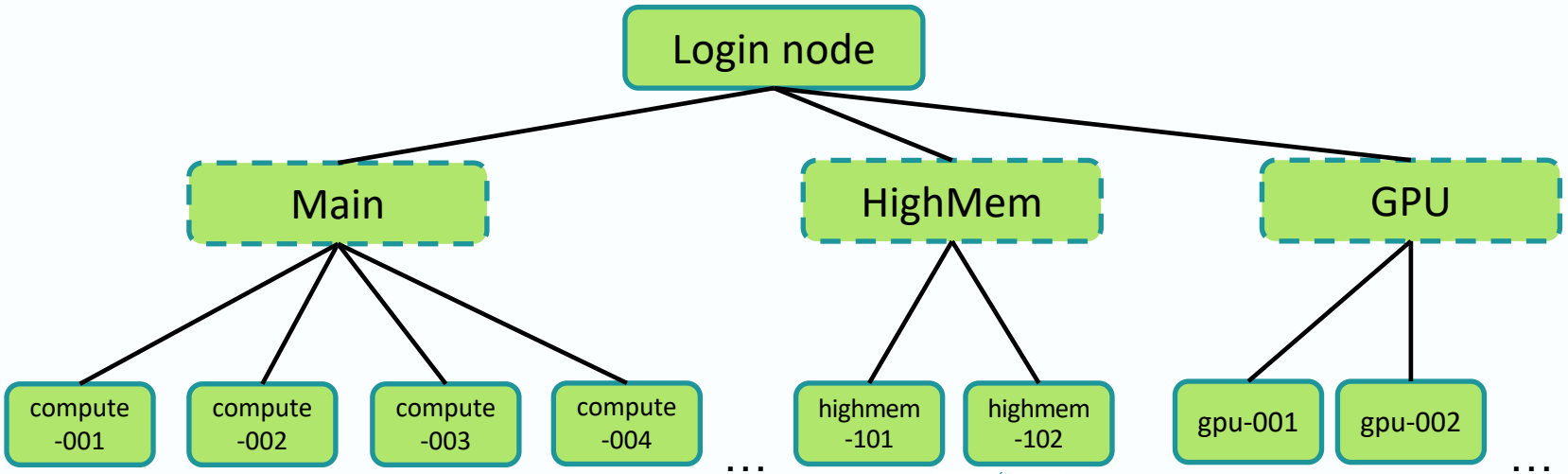
SLURM

- 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/#/tech_docs/running_jobs?id=_4-specifying-resources-when-running-jobs-on-slurm
- Partitions (other than Jupyter) – see with ‘sinfo’:
  - Main: 70 nodes (currently), each w/ 32 CPUs, 232 GB (usable) RAM
  - HighMem: 2 nodes, each w/ 32 CPUs, 480 GB (usable) RAM
  - GPU: 4 nodes, each w/ 2 GPUs, 32 CPUs, 232 GB (usable) RAM



Compute Workflow

- Login node
  - Run SLURM commands and basic bash commands (cd, mkdir, ls, etc)
- Jupyter / development node
  - Development space – new code / workflows / routines
  - Debugging or testing software
- Main partition
  - Generally for stable, computationally-heavy processing
- HighMem partition
  - For single high-memory jobs that can't be split into multiple jobs by MPI
- Transfer node
  - Internal or external copying (see later slide)

SLURM – advanced user commands

- https://slurm.schedmd.com/ (shows long and short form)
- See basic training for basic SLURM user commands
- Before running jobs:

```
$ sinfo -O "partition,available,cpus,nodes,memory,
statecompact" #list partitions and their specs

$ sacctmgr show user $USER -s #list your SLURM
format=account%30,cluster%15 accounting groups
```

- Syntax for srun and sbatch (after #SBATCH) params:

```
$ srun --partition=Main --account=b05-pipelines-ag
script.sh #submit to Main under specific account

$ srun --partition=GPU script.sh
#submit job to GPU partition
```

SLURM – advanced user commands

- https://slurm.schedmd.com/
- After / during running jobs
  - jobID given from sbatch output (to screen) or from squeue

```
$ scontrol show jobID 129916 #shows extensive info about job running (including working directory)

$ sacct -o JobID%-15,JobName%-15,Partition,Account,Elapsed,NNodes%6,NTasks%6,NCPUS%5,MaxDiskRead,MaxDiskWrite,NodeList%20,MaxRSS,CPUTime,State,ExitCode #shows useful information for multi-CPU jobs

$ sacct -S 2021-04-10-09:00 -E 2021-04-12-12:00 -X -o JobID,JobName,Start,End,State #shows jobs started and completed between these dates

$ sacct -j 882242 --cluster=ilifu-slurm #shows job on old cluster
```

SLURM – advanced user commands

- https://slurm.schedmd.com/
- http://docs.ilifu.ac.za/#/tech_docs/running_jobs?id=_4-specifying-resources-when-running-jobs-on-slurm
- Email parameters:

```
$ srun --mail-user=<address> --mail-type=<event_types>
```

  - May want (comma-separated) events: BEGIN,END,FAIL,TIME_LIMIT

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

```
$ srun --exclude=compute-[101,102-105]
```

SLURM – array jobs

- Array jobs allow quick submission many similar jobs, each with same resources, without need to manually launch each
  - Ideally passes array task ID into script, which changes the behaviour of the job each time – i.e. different input selection
  - Can also be used to run several related steps in a serial process
- Example job array, running 20 jobs, with 5 run concurrently

```
#!/bin/bash

#SBATCH --array=1-20%5

#SBATCH --output=logs/%x-%A_%a.out

#SBATCH --error=logs/%x-%A_%a.err

#SBATCH --mail-user=jordan@idia.ac.za

#SBATCH --mail-type=FAIL,ARRAY_TASKS

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

SLURM substitutions & environment variables

- https://slurm.schedmd.com/sbatch.html

Parameter	Substitution / filename pattern	Environment Variable
jobID of the 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

- Useful for multi-CPU jobs:
  `export OMP_NUM_THREADS=$SLURM_CPUS_PER_TASK`

SLURM – running an interactive job

- http://docs.ilifu.ac.za/#/tech_docs/running_jobs?id=_3-interactive-sessions
- Specifying lower wall-time (default 3 hours) and less memory (default ~7 GB) increases chance of job launching immediately
- In steps:

```
$ srun --pty --time=10 --mem=1GB bash
$ singularity shell /idia/software/containers/casa-stable.img
$ casa --nologger --log2term
```

- In single call:

```
$ srun --pty --time=00:10:00 --mem=1GB singularity exec
/idia/software/containers/casa-stable.img casa --nologger --log2term
```

- Must manually process after this

SLURM – running a job

- In previous srun example, job run in your bash session, output printed on screen, and process is volatile (srun / screen / tmux / mosh), subject to restarting SLURM login node
- Best to write sbatch job, which runs in the background and writes to log files. An sbatch file of the previous example:

```
#!/bin/bash

#SBATCH --job-name=casa_job

#SBATCH --time=01:00:00

#SBATCH --mem=1GB

#SBATCH --output=logs/%x-%j.out

#SBATCH --error=logs/%x-%j.err

singularity exec /idia/software/containers/casa-stable.img casa --nologger --nogui
--logfile logs/${SLURM_JOB_NAME}-${SLURM_JOB_ID}.casa -c myscript.py

$ sbatch casa_job.sh
```

SLURM – dependencies

- Allows 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

```
$ sbatch -d afterok:882242 --kill-on-invalid-dep=yes another_job.sh #submit another_job.sh to SLURM queue, to begin after jobID 882242 successfully completes (exit code 0), or cancel the job if jobID 882242 fails

$ sbatch -d afterany:882242:882243 another_job.sh #submit another_job.sh to SLURM queue, to begin after jobIDs 882242 & 882243 complete (any exit code)
```

Parallelism

- Oxford definition for parallel processing
  - *a mode of operation in which a process is split into parts, which are executed simultaneously on different processors attached to the same computer [or different computers attached to the same cluster].*
  - A cluster includes many connected nodes, each with its own RAM & CPUs
  - A node = single computer / server / VM / machine / box
- The work is partitioned into smaller jobs, sometimes with a partition of the dataset

Parallelism

- Can be achieved on a single machine / node
  - Distributes work over many CPUs
  - Typically implemented using OpenMP

- Or over multiple machines / nodes
  - Distributes work over many tasks, over 1+ nodes
  - Each given amount of memory to use
  - Generally requires a cluster
  - Typically implemented using OpenMPI
  - Requires a message passing interface (MPI) wrapper
    - mpirun, aprun, srun (SLURM), mpicasa (CASA)

- Managed on ilifu by SLURM

Parallelism

- Implementing a normal job in SLURM
  - Will only use 1 CPU, 1 task, and 1 node
  - Default for many processes
- Implementing an OpenMP job in SLURM
  - Need to use >1 CPU, while nodes & tasks must be 1 (unless also using MPI)
    - `cpus-per-task`
    - May need to export `OMP_NUM_THREADS`
- Implementing an MPI job in SLURM
  - Need to use >1 task, while nodes and CPUs can be 1
    - `nodes, ntasks-per-node, cpus-per-task`
    - Need to wrap singularity in MPI call
- Cannot exceed 32 CPUs (or tasks) per node

SLURM – multi-CPU and multi-task jobs

- Example sbatch job using many CPUs within 1 node

```
#!/bin/bash
#SBATCH --nodes=1
#SBATCH --ntasks-per-node=1
#SBATCH --cpus-per-task=8
#SBATCH --mem-per-cpu=1GB
singularity exec /path/to/container.simg python myscript.py
```

- Example sbatch job using many tasks within 1 node

```
#!/bin/bash
#SBATCH --nodes=1
#SBATCH --ntasks-per-node=16
#SBATCH --cpus-per-task=1
/path/to/mpirun singularity exec /path/to/container.simg python myscript.py
```

SLURM – multi-task jobs

- Example sbatch job using many tasks over multiple nodes

```
#!/bin/bash

#SBATCH --nodes=2

#SBATCH --ntasks-per-node=8

#SBATCH --cpus-per-task=1

#SBATCH --mem=10GB #memory per node, so 20GB allocated overall (usable by some software)

/path/to/mpirun singularity exec /path/to/container.simg python myscript.py
```

- Example sbatch job using many tasks and CPUs within 1 node

```
#!/bin/bash

#SBATCH --nodes=1

#SBATCH --ntasks-per-node=4

#SBATCH --cpus-per-task=8

/idia/software/pipelines/casa-prerelease-5.3.0-115.el7/bin/mpicasa singularity exec
/idia/software/containers/casa-stable-5.6.2-2.simg casa –c tclean_script.py
```

IDIA MeerKAT Pipeline – A Good Framework

- Parallelised package for HPC processing (SLURM + cluster)
  - Uses multi-measurement sets (MMS) to parallelise across a cluster
- Outputs calibrated data (push of button!)
- HPC-friendly – dynamically uses resources & submits to queue
- Each job/script is a logical step that does / doesn't use MPI, and optionally uses a different container
- User can insert your scripts at start, middle or end
- https://idia-pipelines.github.io/docs/processMeerKAT
- Demo time!

Data Transfers

- http://docs.ilifu.ac.za/#/data/data_transfer
- Do not use login node!
- Don’t write large files to /users, only scripts/config files
- transfer.ilifu.ac.za
  - For cp, scp and rsync (internal ilifu transfers, or external transfers)
    - e.g. `$ scp /path/to/file/<filename> <username>@transfer.ilifu.ac.za:/idia/users/<username>/scripts/`
- Globus
  - Faster than scp and rsync
  - Uses dedicated data transfer node (DTN)

Data Transfers: Globus

- GridFTP transfer service setup between SARAO and IDIA
  - Used by collaborators in UK, Netherlands, Italy, India, etc
- User-friendly globus connect built on top of gridFTP
  - GUI/web app or CLI
- Can connect any arbitrary end points
  - Server (DTN), desktop, etc for Mac OS X, Windows & Linux
  - Offers user-friendly but computationally efficient transfer service

CARTA

- Cube Analysis and Rendering Tool for Astronomy
  - IDIA (South Africa) – NRAO (US) – ASIAA (Taiwan)
  - Cloud-based Visual analytic of remote large image cubes
  - Supports many image formats: FITS, CASA, Miriad, and HDF5
- CARTA on ilifu
  - http://docs.ilifu.ac.za/#/astronomy/astronomy_software?id=carta
  - https://carta.idia.ac.za – login with same credentials as Jupyter
  - The only visible files are in /carta_share/
  - User should write IDIA HDF5 file to this filesystem
  - Even for continuum (single channel) image
    - `srun /carta_share/hdf_convert/run_hdf_converter -o /carta_share/users/$USER/image.hdf5 image.fits`
- 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 / mosh 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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