ilifu Online Training – Advanced #2

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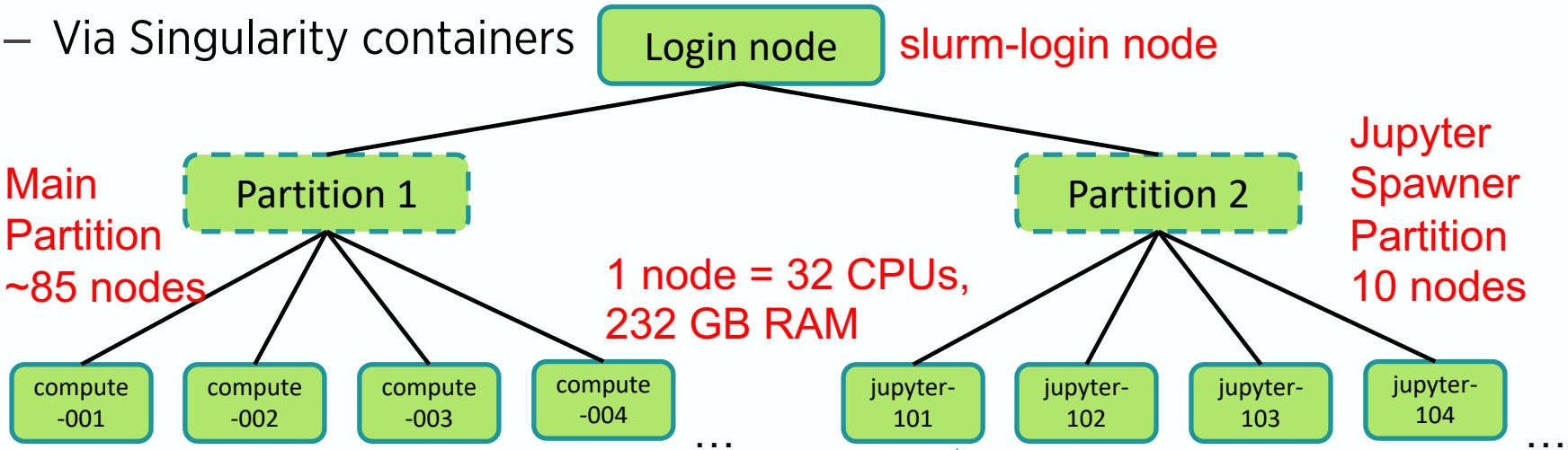
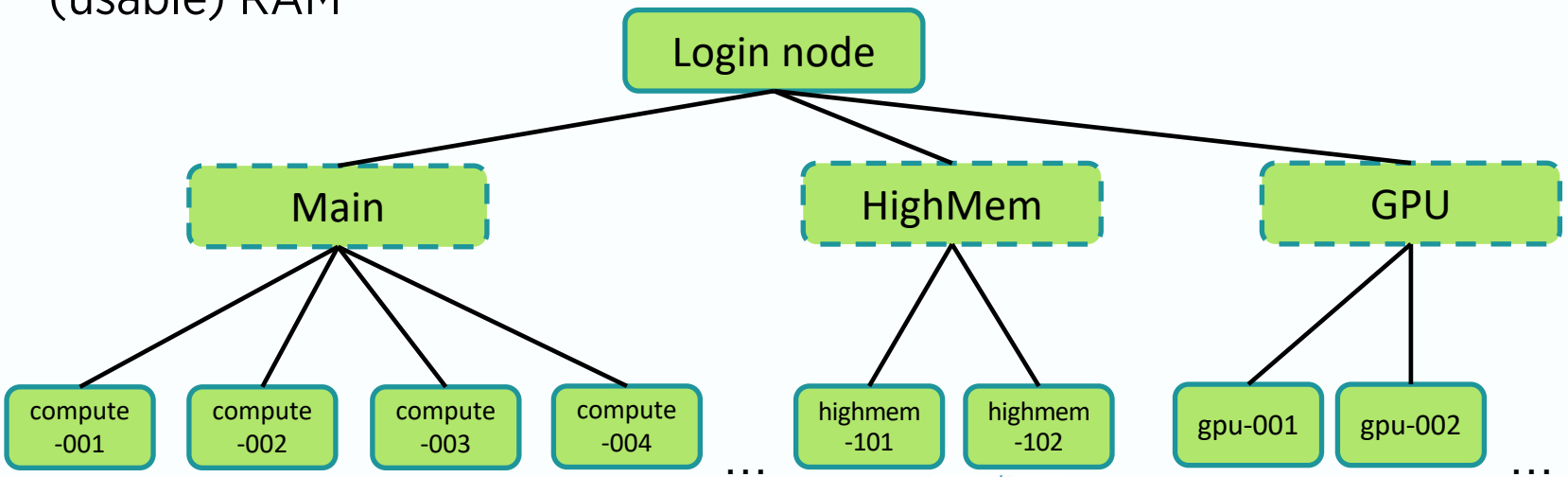
SLURM

- 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: 85 nodes (currently), each w/ 32 CPUs, 232 GB (usable) RAM
  - HighMem: 2 nodes, w/ 32 CPUs, 503 GB (usable) RAM + 96 CPU 1.5 TB RAM
  - GPU: 7 nodes (P100, V100, A40, A100), each w/ 24-48 CPUs, 232-354 GB (usable) RAM



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

What is a program?

- Set of discrete instructions
- Carried out sequentially
- Example: print average grade of a class

1. total = 0
2. for grade in grades:
   total = total + grade
3. average = total / number_of_grades
4. print(average)

Parallelism

- Executing portions of program simultaneously
- Possible when we have many processors (cores/CPUs)
- Capacity dependent on structure of both hardware AND software
- Requires overall control/coordination mechanism
  - i.e. message passing

Parallelism on the cluster

- A cluster includes many connected nodes
- Each node has RAM and multiple cores
- Work of job is partitioned into smaller jobs
- Sometimes with a partition of the data

Parallel execution of a program

- Partition grades into 2:

1. total = 0
2. for grade in 1/2 grades:

   total = total + grade

3. average1 = total / number_of_grades

1. total = 0
2. for grade in 1/2 grades:

   total = total + grade

3. average2 = total / number_of_grades

- Combine results

average = (average1 + average2) / number_of_partitions

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 5)
    - Version of wrapper outside and inside container / venv must match

- 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` (not inherited from #SBATCH)
    - 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`
    - Best to wrap singularity in MPI call
- Cannot exceed 32 CPUs (or tasks) per node

SLURM – serial and multi-CPU jobs

- If code is serial, i.e. doesn't use OpenMP or MPI, increasing CPUs or nodes will not decrease execution time

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

- Using multiple CPUs within a node with OpenMP, where N is an optional number of CPUs (utilised by myscript.py)

```
#SBATCH --nodes=1
#SBATCH --ntasks-per-node=1
#SBATCH --cpus-per-task=N
#SBATCH --mem-per-cpu=XGB
srun --cpus-per-task=N singularity exec /path/to/container.simg python myscript.py
```

- *Note: The maximum number of CPUs per node (32) will not always give the maximum speedup*

SLURM – multi-task and multi-node jobs

- Can also specify tasks or tasks per node

```
#SBATCH --ntasks=N
#SBATCH --cpus-per-task=1
#SBATCH --mem=XGB
/path/to/mpirun singularity exec /path/to/container.simg python myscript.py
```

- Above example doesn't require knowledge of number of node's CPUs; below one does

```
#SBATCH --nodes=1
#SBATCH --ntasks-per-node=N
#SBATCH --cpus-per-task=1
#SBATCH --mem=XGB
/path/to/mpirun singularity exec /path/to/container.simg python myscript.py
```

SLURM – multi-task and multi-CPU jobs

- Using multiple nodes with MPI

```
#SBATCH --nodes=N
#SBATCH --ntasks-per-node=n
#SBATCH --cpus-per-task=1
#SBATCH --mem=XGB
/path/to/mpirun singularity exec /path/to/container.simg python myscript.py
```

- *Note: Need to consider that internode communication is slower than intranode communication*
- --mem is memory per node, so N times XGB allocated overall (usable by some software)
- Using multiple nodes with MPI as well as multiple cores within node with OpenMP (utilised by myscript.py)

```
#SBATCH --ntasks=N
#SBATCH --cpus-per-task=n
/path/to/mpirun singularity exec /path/to/container.simg python myscript.py
```

IDIA MeerKAT Pipeline – A Good Framework

- Parallelised package for HPC processing (SLURM + cluster)
- HPC-friendly – dynamically uses resources & submits to queue to give calibrated data with the push of a button
- Each job/script is a logical step that does / doesn't use MPI, and optionally uses a different container
  - Managed by wrapper software sourced by user so that it's in their path
  - This could also be venv and is updated more regularly
    - Design: wrapper software manages the jobs you submit to SLURM
- User can insert their scripts at start, middle or end
  - Design: jobs run within containers that include software dependencies
- https://idia-pipelines.github.io/docs/processMeerKAT
- Demo time!

ilifu: a shared resource-limited cluster

- ilifu
  1. Supports a diverse range of projects
     - Astronomy and Bioinformatics
     - Varying resource requirements
  2. Shared environment
  3. Resource-limited

- Efficient use of resources essential
  - Practices laid out in allocation guide
  - Additional:
    - Select lowest Jupyter resource possible
    - Shut down Jupyter server after use
    - Use sbatch with non-default parameters

Services and partitions

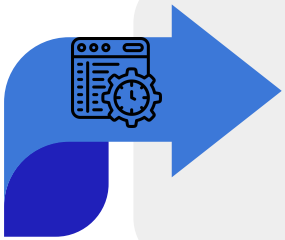
- http://docs.ilifu.ac.za/#/getting_started/access_ilifu

Login node

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

Jupyter/Dev. node

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



Main partition

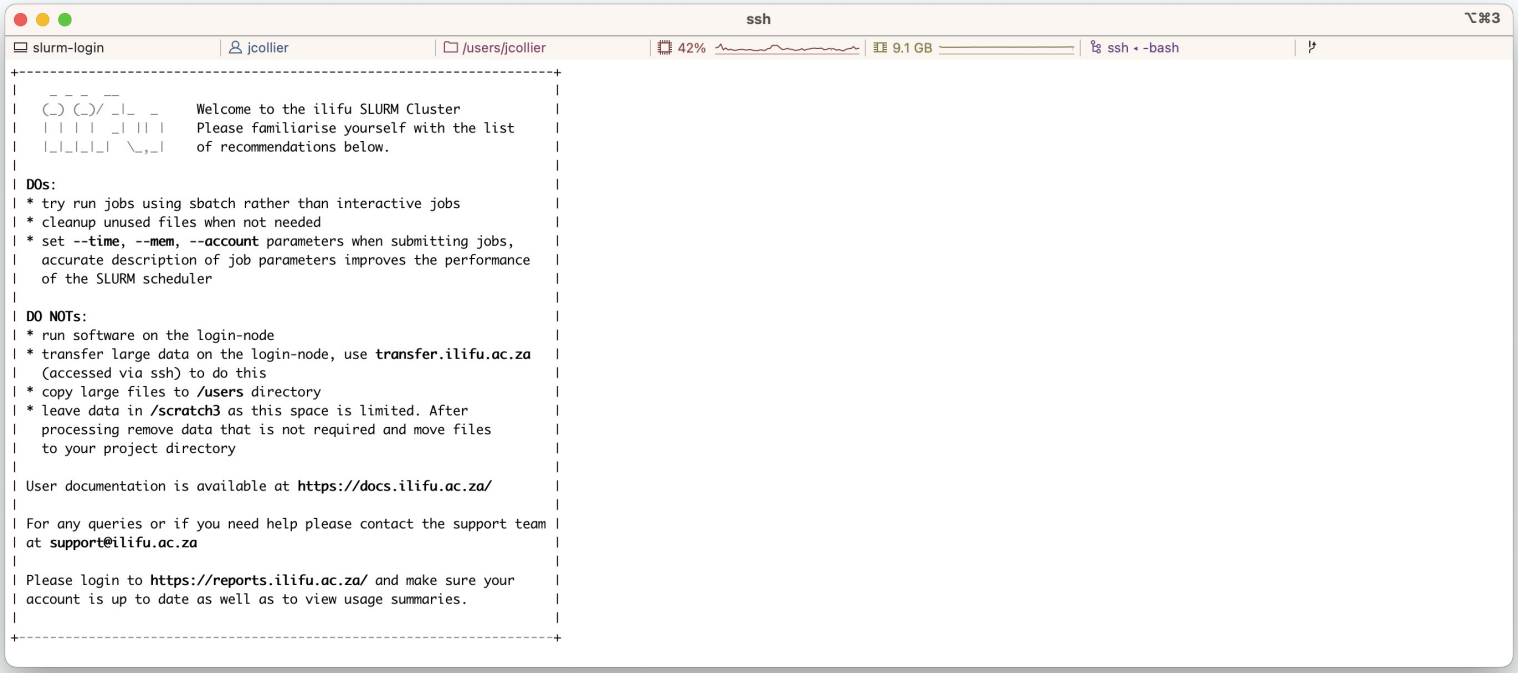
Stable, computationally heavy processing

HighMem/GPU

For single-high memory jobs or GPU resources

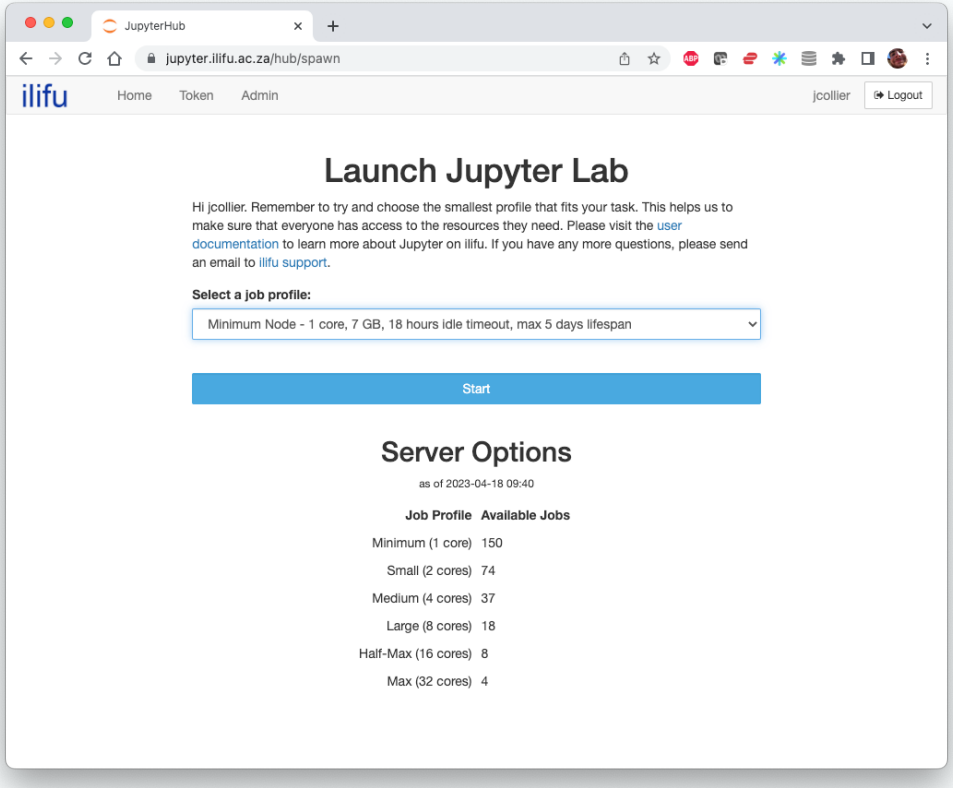
Services and partitions

- Login node
  - Where you land when logging in on ilifu Slurm cluster (slurm.ilifu.ac.za)
  - For running basic bash commands (cd, mkdir, ls, etc)
  - For running Slurm commands (srun, sbatch, scancel, squeue, sacct, etc)



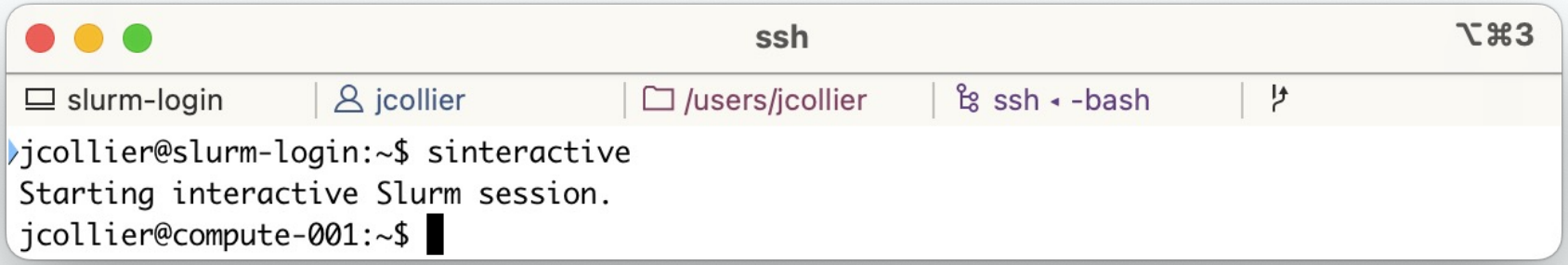
Services and partitions

- Jupyter (Jupyter.ilifu.ac.za)
  - Development space for writing, testing and debugging
  - New code, software, workflows or routines
  - Highly interactive Jupyter notebook environment
    - tab-completion, viewing doc strings, running subroutines within cells
  - May be primary interface for stable workflows that shouldn't use Slurm
    - short analysis routines or other highly interactive workflows



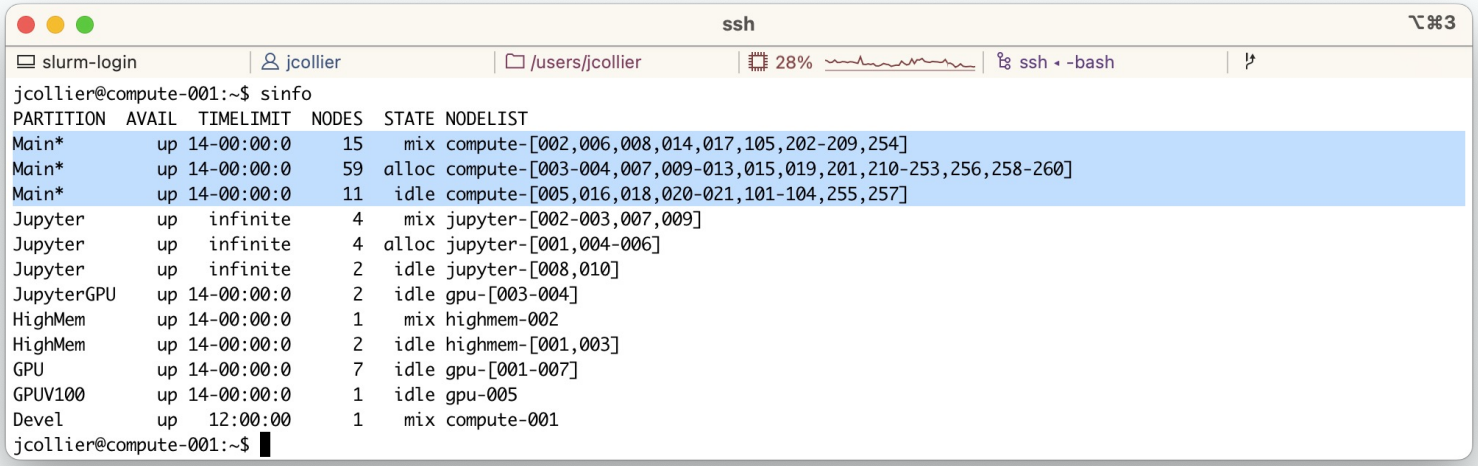
Services and partitions

- Devel (--partition=Devel)
  - Development of routines within shared resource environment
    - Submit jobs instantly / quickly
    - Resources shared, not solely allocated to your jobs
  - Interactivity via a shell
  - Generally for testing higher level workflows and pipelines
  - Access simply using the sinteractive command



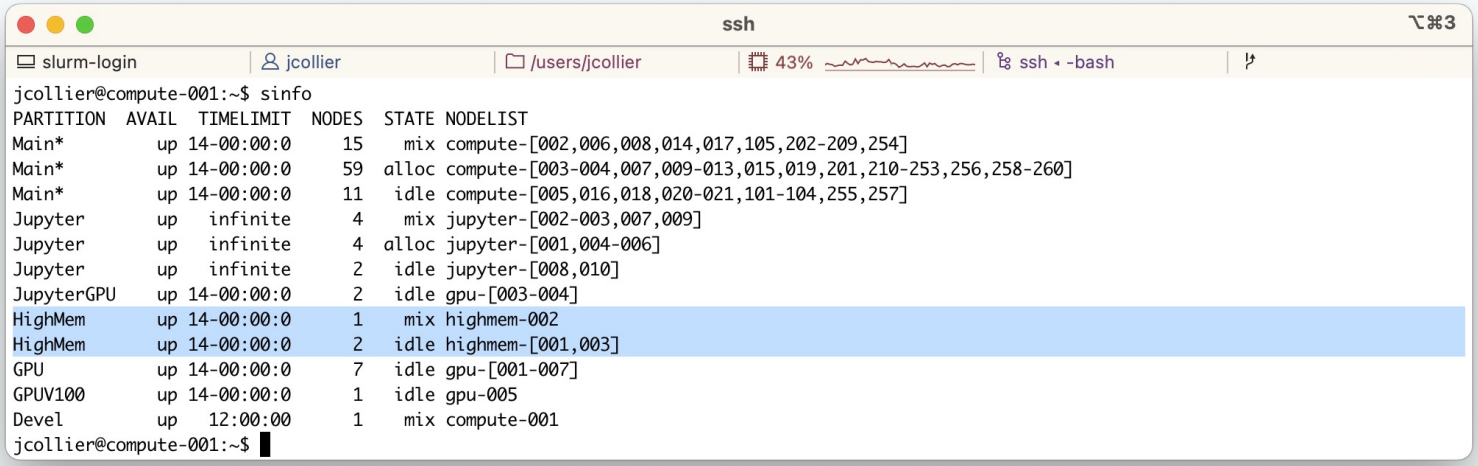
Services and partitions

- Main partition
  - Default Slurm partition
  - Generally for stable, computationally-heavy workflows and pipelines
    - Many small jobs allocated few resources or
    - A few large jobs allocated many resources
  - Have first been tested on one of the previous services (where applicable)



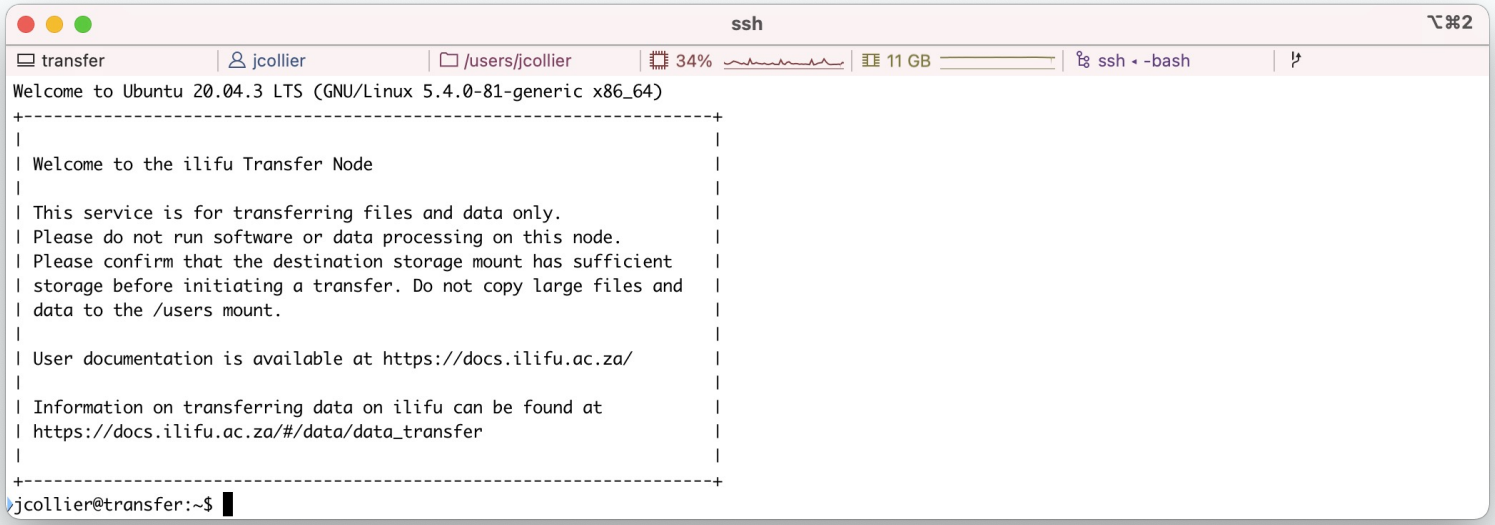
Services and partitions

- HighMem partition
  - Single high-memory jobs that can't be split into multiple jobs using MPI
- GPU partition
  - Jobs making use of GPUs
  - Not for jobs that only require CPUs (rather use Devel)



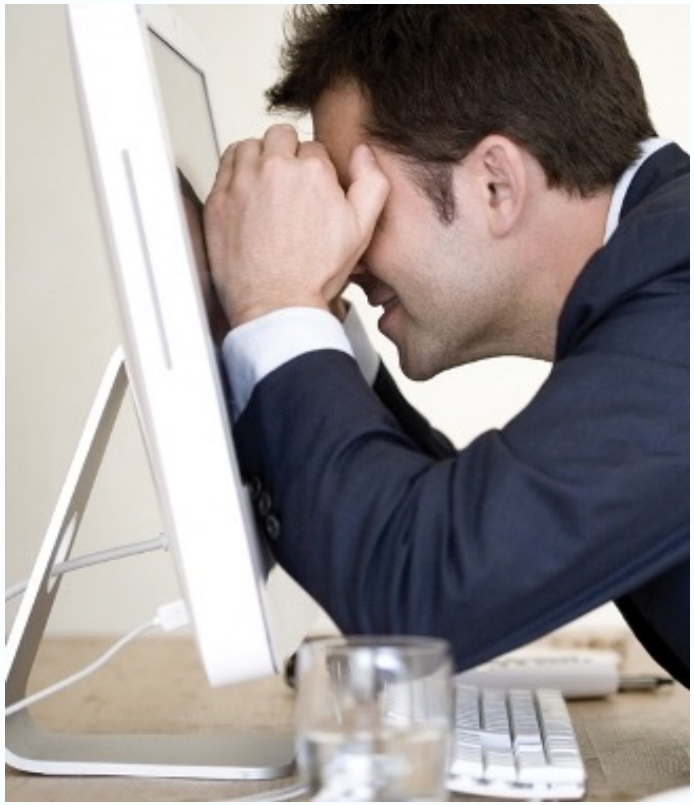
Services and partitions

- Transfer node (transfer.ilifu.ac.za)
  - Internal and external copying of data (cp, scp, rsync, etc)
  - Smaller or less frequent transfers (i.e. not requiring Globus)
  - Other basic bash commands inappropriate for login node (wget, rm)
    - Also possible on Slurm compute node (e.g. 1 CPU, 1 GB RAM)



Allocating Resources

- http://docs.ilifu.ac.za/#/tech_docs/resource_allocation
- Primary resources
  1. CPU
  2. Memory
  3. Wall-time
- Notes
  - Nodes have 2 CPUs (sockets), each with 16 cores, all of which Slurm calls “CPUs”
  - Wall-time (elapsed time) is total run-time of job according to a clock on the wall
    - When > 1 CPU, differs from CPU time, measured in CPU hours



Allocating Resources

- How to allocate resources
  - Accurately determine your resource requirements
  - Use what you require
- Effect
  - Avoid wasting resources (allocated but not used)
  - Increase resource availability
  - Allow other (users') jobs to run
  - Improves efficiency of Slurm scheduler
  - Increase your fairshare priority
  - Potentially decrease your job wait times

Allocating Resources

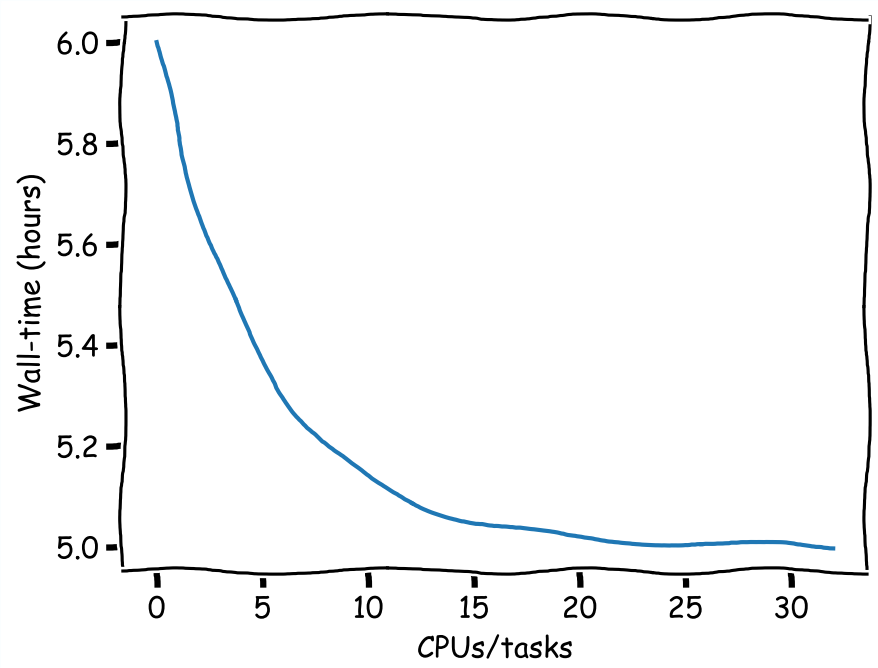
- Determine your resource requirements
  1. Determining parallelism of software
  2. Profiling previous similar jobs
  3. Scaling up test jobs

Allocating Resources

- Determining parallelism of software
  - See previous slides
    - CPU-level vs. task-level parallelism
    - Many software packages only use 1 CPU

Allocating Resources

- Determining parallelism of software
  - Most parallel processing software doesn't scale linearly
  - Maximum performance often least efficient
    - i.e. shortest wall-time but large allocation necessary
  - Need to find middle ground
  - MPI jobs may perform worse for larger allocations (scatter/gather)
  - Most efficient generally to break into many small independent jobs
    - High-throughput approach

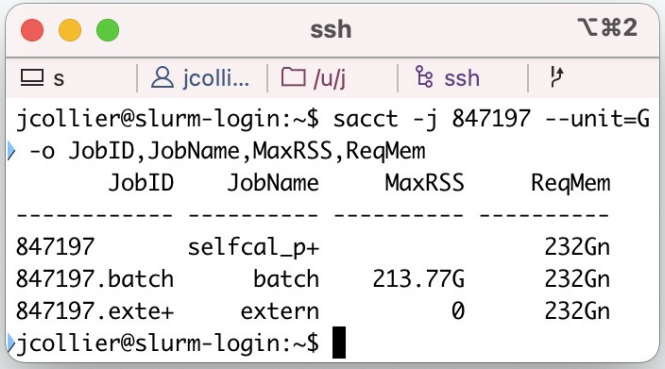


Profiling previous similar jobs

- Find job ID
  - Output when job submitted
  - Can search for historical jobs
  - Display jobs named ‘my-job’ submitted during particular time range:
  - `sacct -X --name=my-job --starttime=YYYY-MM-DD --endtime=YYYY-MM-DD`
  - Omit job name (or end time) to show all jobs
  - Add following to query (very) old Slurm databases (before upgrades)
  - `--cluster=ilifu-slurm20` or `--cluster=ilifu-slurm`
- Once you have job ID, you can search for specific information about resource usage

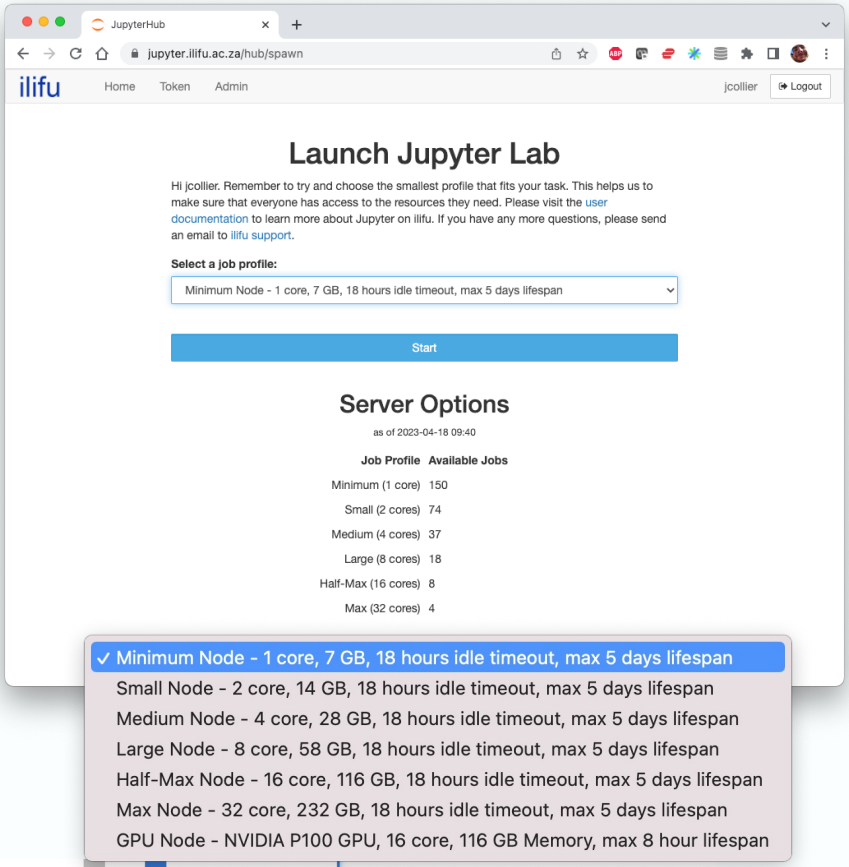
Profiling previous similar jobs

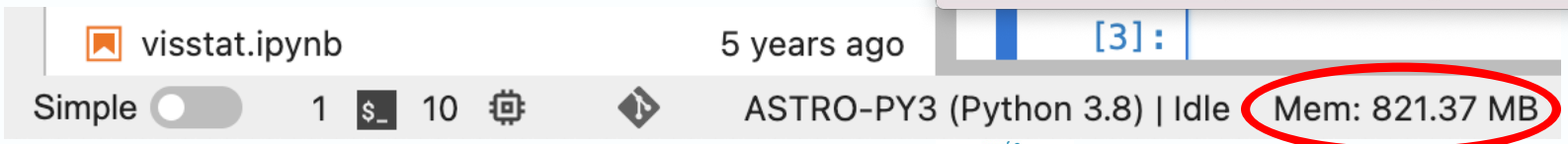
- Memory usage
  - Find MaxRSS statistic
    - Maximum memory usage of a job (sampled every 20 seconds)
    - Display MaxRSS for job ID 123456 compared to requested memory
    - `sacct -j 123456 --unit=G -o JobID,JobName,MaxRSS,ReqMem`
    - Can run this from Jupyter terminal (to determine resource selection)
    - *Notes: 232 Gn = 232 GB per node; 7.25c = 7.25 GB per CPU*
  - Once memory requirement determined
    - Schedule future jobs with ~10-20% buffer
      - Avoids out-of-memory (OOM) error
    - Avoid excessive usage of memory
      - e.g. minimum node in Jupyter



An aside for Jupyter

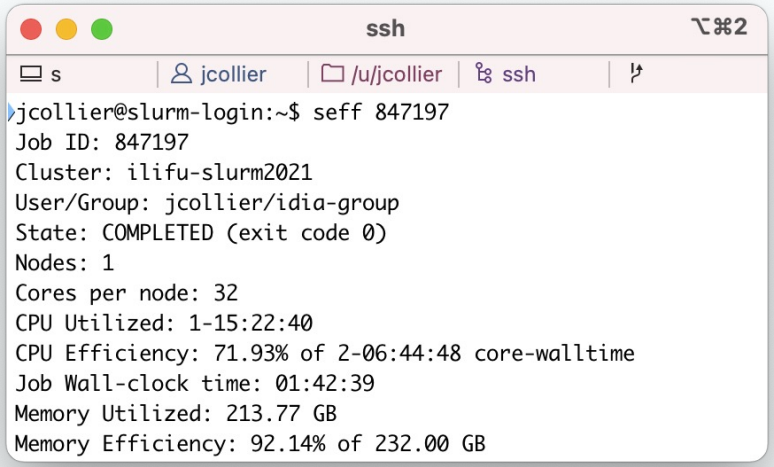
- Select job profile to match your requirements (avoid excess)
- Jupyter shows you maximum memory usage down the bottom of your session
- You will be emailed usage stats after a job has completed that selected a high job profile and used very low CPU & memory
- Shut down your session

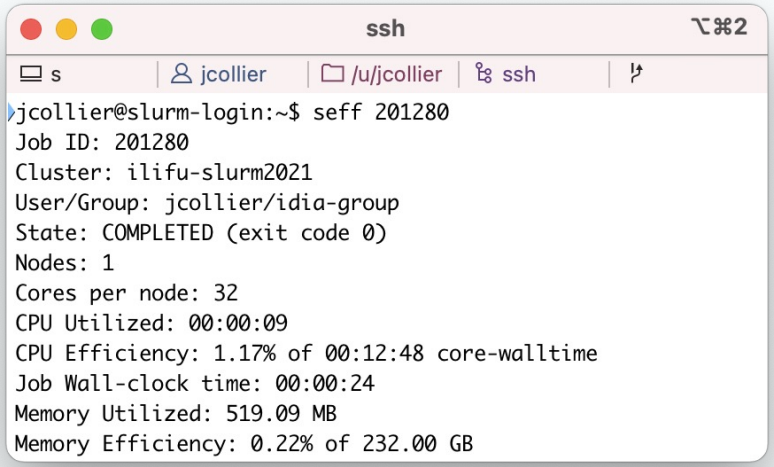




Profiling previous similar jobs

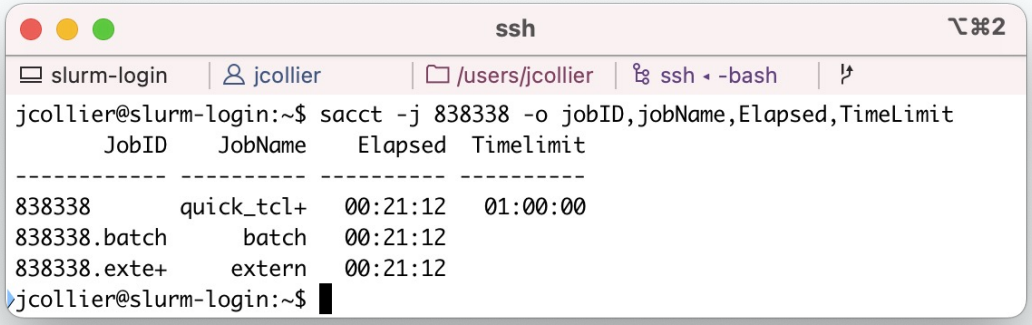
- CPU (and memory) usage
  - Determine used vs. allocated/requested
  - Show Slurm resource efficiency (seff) for job ID 123456
  - Shows % used vs. allocated (for memory, uses MaxRSS stat)
  - `seff 123456`
  - Can run this from Jupyter terminal (to determine resource selection)





Profiling previous similar jobs

- Wall-time usage
  - Accurate estimation improves Slurm scheduler efficiency and may reduce your job wait time
  - Show used vs. requested wall-time for job ID 123456 (also in Jupyter)
  - `sacct -o jobID,jobName,Elapsed,TimeLimit`
  - Once wall-time requirement determined
    - Schedule future jobs with ~20-30% buffer (avoids job timing out)
    - Avoid excessive wall-time
    - Contact support@ilifu.ac.za to see if we may increase your time limit



Scaling tests

- Accurately estimating wall-time difficult to do
- Profile previous similar jobs, or
- Run test / scaling jobs
  - Start small test job (e.g. small allocation on small subset of data)
  - Test the wall-time, run again with increased resources
    - Reasonable to over-allocate when running scaling test
      - Briefly inefficient, until get an idea of requirements
    - Or if under-estimate, and test small enough, doesn't matter if crashes
  - Repeat process to see how resource usage scales
    - as a function of input (e.g. data volume)
    - as a function of CPUs / tasks (if doing parallel processing)
  - By the end, should have good idea of scaling and efficient choice
    - Allow for buffer for future jobs

Usage of running jobs

- e.g. during scaling tests
- Get MaxRSS for running job
  - `sstat -j 123456 -o MaxRSS`
  - Given in kB units. Divide by 1024^2 for GB
- Display real time stats on dashboard (top / htop)
  - ssh compute-001 or open Jupyter terminal
    - Requires job running on node and authentication forwarding
    - e.g. first run `ssh -A <username>@slurm.ilifu.ac.za`
  - `htop -u $USER`
- Shows different (e.g. master and spawned) running processes
- Can monitor real-time usage

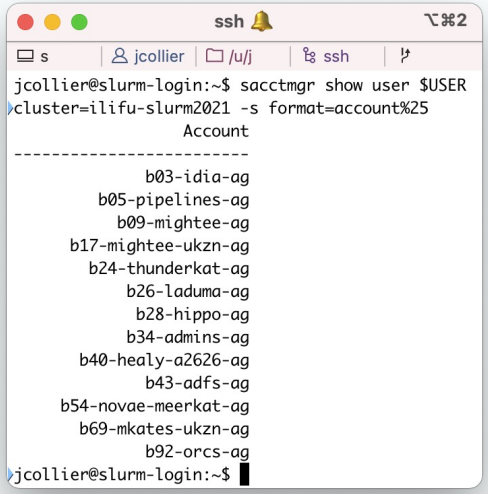
Maximum Resources

- If using **all** CPUs or memory, node becomes fully allocated
  - Any remaining CPUs / memory unavailable to other jobs (incl. your own)
- *Note: Jobs on Devel node cannot allocate memory*

Partition	Node names	Default CPUs	Max CPUs	Default Memory (GB)	Max Memory (GB)	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
Devel	compute-001	1	32	-	-	3 hours	12 hours

Account allocation

- Each ilifu project has a Slurm account
- Resource usage charged against account (affects fairshare)
- View your accounts
  - `sacctmgr show user $USER cluster=ilifu-slurm2021 -s format=account%25`
- View your default account
  - `sacctmgr show user $USER`
- Change default
  - `sacctmgr modify user name=${USER} set DefaultAccount=<account>`
- Set account (after #SBATCH for sbatch jobs)
  - `--account=b05-pipelines-ag`



Resource Allocation Guide

- Demo

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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