703651 PS Parallel Systems
A Crash Course in Clusters and Job Submission

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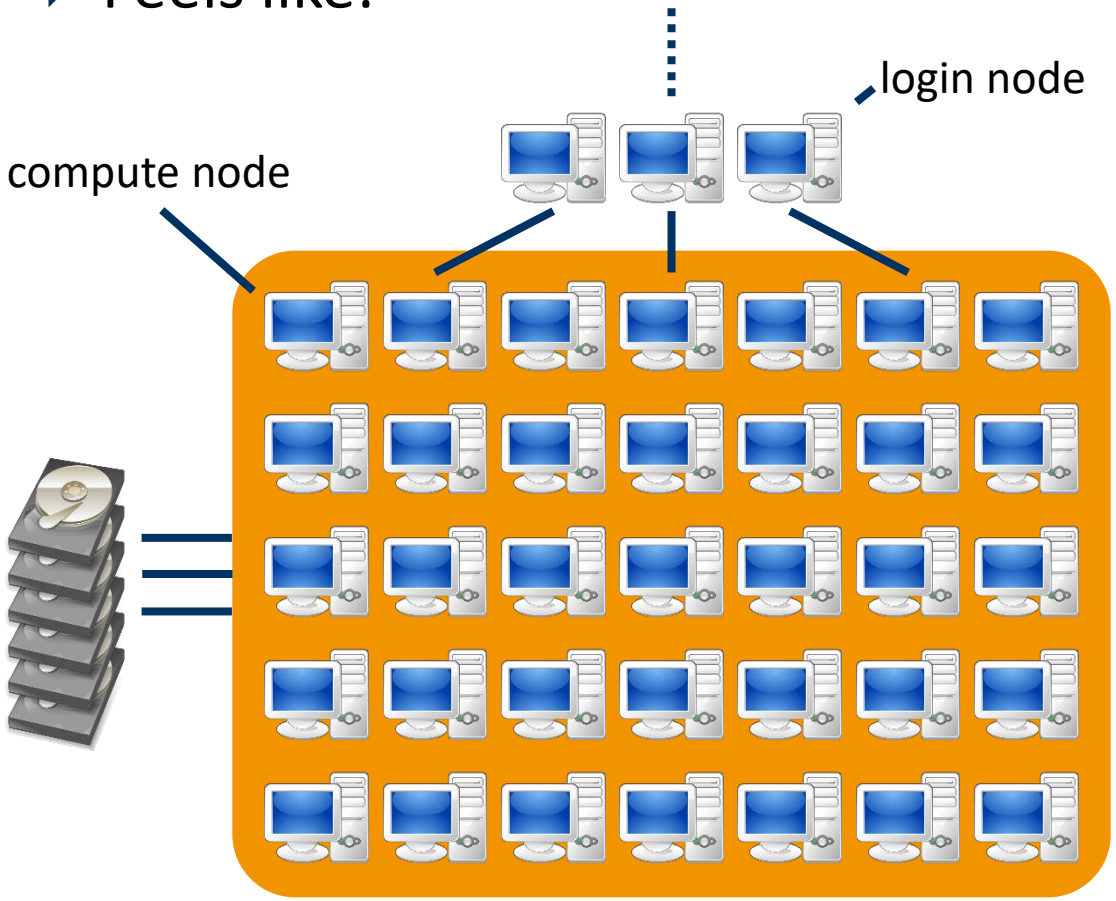
Clusters and Supercomputers

- Looks like:

- Feels like:



Get User Credentials, Log in and Change Your Password!

- `ssh cbxxxxxx@lcc2.uibk.ac.at`
- Change password with `passwd`
- don’t use these credentials for anything other than this course
  - coin mining isn’t worth it anyways…

Submission Systems

- Responsible for resource management and job orchestration
  - used to submit or cancel “jobs”, query their status, get information about cluster, …
- Very popular: SLURM
  - modern, complex but very capable
  - de-facto standard on most systems these days

- On LCC2: Sun Grid Engine (SGE)
  - older and deprecated ☹
  - switch to SLURM currently in progress

Jobs: Submission, Deletion, Status

- `qsub name_of_script`
  - allocates resources
  - sets up environment
  - executes application
  - frees allocation
- `qdel job_id_list`
  - terminates application
  - frees up resources
- `qstat`
  - queries for job status
  - `qstat -u '*'` for all users (mind the quotes!)

```
[cb761011@login.lcc2 ~]$ qsub job.script
Your job 30369 ("my_test_job") has been submitted
[cb761011@login.lcc2 ~]$ qdel 30369
cb761011 has deleted job 30369
[cb761011@login.lcc2 ~]$ qsub job.script
Your job 30370 ("my_test_job") has been submitted
[cb761011@login.lcc2 ~]$ qstat
job-ID  prior   name       user       state submit/start at     queue  slots ja-task-ID
-----------------------------------------------------------------------------------------
  30370 0.00000 my_test_jo cb761011   qw    09/30/2019 15:02:01           8
```

SGE Job Scripts

```
#!/bin/bash

# Execute job in the queue "std.q" unless you have special requirements.
#$ -q std.q
# The batch system should use the current directory as working directory.
#$ -cwd
# Name your job. Unless you use the -o and -e options, output will
# go to a unique file name.o<job_id> for each job.
#$ -N my_test_job
# Redirect output stream to this file.
#$ -o output.dat
# Join the error stream to the output stream.
#$ -j yes
# Specify parallel environment (list available ones with qconf -spl)
#$ -pe openmpi-2perhost 8

/bin/hostname
```

Parallel Environments

- Specifies number of CPU/core slots to allocate per node and in total
  - `openmpi-Xperhost Y` …… X slots per node, Y slots in total

- List available environments with `qconf -spl`
  - `openmpi-1perhost`
  - `openmpi-2perhost`
  - `openmpi-4perhost`
  - `openmpi-8perhost`

- Be careful with non-exclusive allocations!

Action!

- Submit the job, wait for it to finish, check the output
  - What happened and what did you expect?

Modules System

- Used to modify the user environment
  (environment variables, most notably PATH & LD_LIBRARY_PATH)

- `module avail`
- `module load`
- `module list`
- `module unload`

Fix Job Script

- add a line to load the required MPI module (e.g. just before program execution)
  - `module load openmpi/4.0.1`
- fix the program execution line in the jobscript
  - `mpiexec –n 8 /bin/hostname`
- Re-submit and check the output
- Happy now?

Compiling and Running MPI programs

- MPI is an inter-process communication library
  - provides a header + library files (*.so/*.a)
  - more information in the lecture

- compiler wrappers for C/C++ (set all required flags and directories)
  - `mpicc`
  - `mpic++`

- execution wrapper for MPI programs
  - `mpiexec -n [num_processes] /path/to/application`

Further Information on SGE, Job Scripts and LCC2

- Refer to ZID's help pages
  - LCC2 Status: http://login.lcc2.uibk.ac.at/cgi-bin/state.pl
  - LCC2: https://www.uibk.ac.at/zid/systeme/hpc-systeme/lcc2/
  - SGE: https://www.uibk.ac.at/zid/systeme/hpc-systeme/common/tutorials/sge-howto.html
- Consult manpages or "The Internet"
- Ask me

Image Sources

- Cluster Photo: https://forschungsinfrastruktur.bmbwf.gv.at/de/fi/hpc-compute-cluster-leo3-leo3e_513
- SLURM: https://justjimsthoughts.blogspot.com/2017/07/trivia_24.html