



703309 PS High-Performance Computing A Crash Course in Clusters and Job Submission

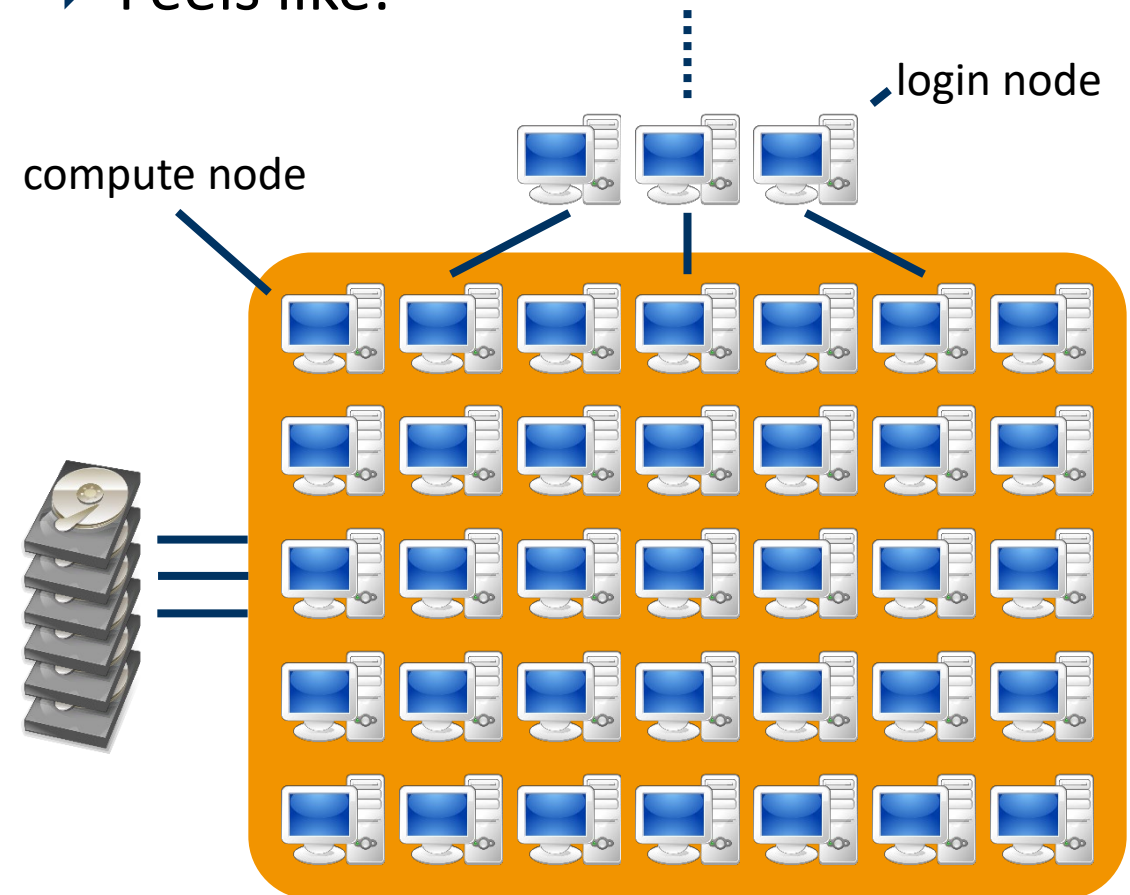
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Clusters and Supercomputers

► Looks like:



► Feels like:



Get User Credentials, Log in and Change Your Password!

- ▶ `ssh cbxxxxxx@login.lcc3.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



Jobs: Submission, Deletion, Status

- ▶ `sbatch name_of_script`
 - ▶ allocates resources
 - ▶ sets up environment
 - ▶ executes application
 - ▶ frees allocation
- ▶ `scancel job_id_list`
 - ▶ terminates application
 - ▶ frees up resources
- ▶ `squ (squeue -u $USER)`
 - ▶ queries for job status
 - ▶ squeue for all users

```
[cb761011@login.lcc3 ~]$ sbatch job.sh
Submitted batch job 184
[cb761011@login.lcc3 ~]$ scancel 184
[cb761011@login.lcc3 ~]$ sbatch job.sh
Submitted batch job 185
[cb761011@login.lcc3 ~]$ squ
```

JOBID	PRIORITY	PARTITION	NAME	USER	STATE	NODES	CPUS	TIME_LIMIT	NODELIST(REASON)
185	504	lva	test	cb761011	RUNNING	1	8	30:00	n002

SLURM Job Scripts

```
#!/bin/bash

# Execute job in the partition "lva" unless you have special requirements.
#SBATCH --partition=lva
# Name your job to be able to identify it later
#SBATCH --job-name test
# Redirect output stream to this file
#SBATCH --output=output.log
# Maximum number of tasks (=processes) to start in total
#SBATCH --ntasks=8
# Maximum number of tasks (=processes) to start per node
#SBATCH --ntasks-per-node=8
# Enforce exclusive node allocation, do not share with other jobs
#SBATCH --exclusive

/bin/hostname
```

Additional Useful SLURM Tools

- ▶ **sinfo**
 - ▶ list information on partitions, nodes, etc.
- ▶ **scontrol**
 - ▶ alter properties of pending jobs
- ▶ **sacct**
 - ▶ show accounting information

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/3.1.6-gcc-12.2.0-d2gmn55`
- ▶ fix the program execution line in the jobscript
 - ▶ `mpirun -n $SLURM_NTASKS /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`

Storage and Compilers on LCC3

- ▶ LCC3 has two main storage mount points
 - ▶ `/home/cb76/<username>` limited to 1 GB
 - ▶ `/scratch/<username>` limited to 16 TB (?)
 - ▶ Both are network-mounted on all login and compute nodes
 - ▶ When using VS Code + Remote SSH, be sure to set
`"remote.SSH.serverInstallPath": { "lcc3": "/scratch/c703429" }`
- ▶ LCC3's system gcc is old (8.5.0)
 - ▶ use modules to find and load newer versions (e.g. 12.2.0)
 - ▶ e.g. `gcc/12.2.0-gcc-8.5.0-p4pe45v`

Further Information on SLURM, Job Scripts and LCC3

- ▶ Refer to ZID's help pages
 - ▶ LCC3 Status: <https://login.lcc3.uibk.ac.at/cgi-bin/slurm.pl>
 - ▶ LCC3: <https://www.uibk.ac.at/zid/systeme/hpc-systeme/leo3/>
 - ▶ SLURM: <https://www.uibk.ac.at/zid/systeme/hpc-systeme/common/tutorials/slurm-tutorial.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