Our HPC Cluster



Compute nodes (12x)

- 2x INTEL Xeon Gold 6248, 2.5GHz, 20C/40T
- 192/768GB RDIMM, 2933MT/s
- 480GB SSD
- Broadcom 10Gbit/s Base-T
- INTEL Omni-Path Host Fabric Adapter

Login node

- 2x INTEL Xeon Gold 5217, 3.0GHz, 8C/16T
- 128GB RDIMM, 2666MT/s
- 24X 2TB SAS
- PERC H730P+ RAID Controller
- Broadcom 10Gbit/s Base-T
- INTEL Omni-Path Host Fabric Adapter

Network switches

- S4148T-ON 48x 10GBase-T, 10Gbit/s
- H1024-OPF 24x Omni-Path, 100Gbit/s

HPC Cluster Access: Login

- You will receive your access credentials via email: username (nssc_lastname) and password
- Every user is linked to the TISS user: You are identifiable.
- To access the cluster:
 - 1. Establish a TU Wien VPN connection (also when already on TU Wien network)
 - 2. Use ssh and your credentials to access the cluster's login node
 - \$ ssh nssc_doe@tcad30.iue.tuwien.ac.at
 - → Enter your initial password
 - →You will be asked to change your password upon first login →
 - →Provide again your initial password → afterwards the new password
 → needs to be repeated.

HPC Cluster Access: File Transfer

File transfer via scp

- Transfer file (some file) to your home directory on the cluster:
- \$ scp some_file nssc_doe@tcad30.iue.tuwien.ac.at:
- Transfer folder (some_folder) to your home directory on the cluster:
- \$ scp -r some_folder nssc_doe@tcad30.iue.tuwien.ac.at:
- Transfer file (some_file) from your home directory on the cluster to a specific directory (/path/) on your machine:
- \$ scp nssc_doe@tcad30.iue.tuwien.ac.at:some_file /path/
- Transfer folder (some_folder) from your home directory on the cluster to a specific directory (/path/) on your machine:
- \$ scp -r nssc_doe@tcad30.iue.tuwien.ac.at:some_folder
 /path/

HPC Cluster Access: Job Submission

- The login server is used for compilation, job submission, and data exchange platform.
 - Shared file system with compute nodes
 - Same software environment as compute nodes
- The login server must not be used for job execution: Every exercise submission must include a functioning SLURM script
- To schedule the execution of your program:
 - 1. Compile as usual (preferably with a build tool, e.g., Makefile).
 - Setup a job submission script (which tells the job submission manager which executable is to be executed and how).
 - 3. Submit the job submission script and wait for completion.

HPC Cluster Access: Job Submission Script

Submit the job with:

```
$ sbatch submit_script.sh
```

Note that terminal output will be written continuously into the file slurm-JOBID.out file. Read it with, e.g., less, vim. For realtime file update read access use:

- \$ tail -f slurm-JOBID.out
- Show current job queue for your user:
 - \$ squeue -u nssc_username
- Cancel a specific job from your queue (JOBID number from squeue output):
 - \$ scancel JOBID
- Cancel of your jobs
 - \$ scancel -u nssc_username

HPC Cluster Access: Job Submission Script

Hints:

- You can submit several jobs at once one script and submission per job. For instance, submit 4 jobs to execute 4 different benchmarks (e.g. different thread numbers).
- Alternatively, you can also execute several programs (one after the other) in a single job submission script (.e.g. two executions where you provide different resolutions as input parameters) – see example submit_script.sh in handouts.
- If your job takes longer than specified (see –time parameter), then the job is being automatically aborted: Make sure you estimate reasonably!

HPC Cluster Development

Best practices

- Develop code on your local machine
- Test with small thread sizes on your local machine
- When ready, move to cluster:
 - Transfer source code and build file to cluster
 - Compile on the cluster (g++ 8.2.1 is the default compiler)
 - Setup job submission script
 - Submit job (aka execute application on cluster)
 - Collect data (e.g. output files) and transfer to your local machine for analysis

Topology

Login Node

User:

tcad30.iue.tuwien.ac.at

ssh / scp Slurm Workload Manager requires active TUW-VPN



Shared Filesystem

Compute Nodes









