Numerical Simulation and Scientific Computing I

Exercise 3:
Cluster Setup

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While we discuss

- **Check your email for your cluster credentials**
- **Log in to your Linux machine**
- **Setup the VPN**
- **Download the handout from TUWEL**

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
```

  3. **Enter your initial password**
  4. **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).**
  2. **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_script.sh

```
#!/bin/bash
# Example with 20 cores for OpenMP
# Number of cores
#SBATCH -c 20
# Runtime of this jobs is less then 10 minutes
#                  (hh:mm:ss)
#SBATCH --time=00:10:00
# Clear the environment
module purge > /dev/null 2>&1
# Set OMP_NUM_THREADS to the same value as -c
export OMP_NUM_THREADS=$SLURM_CPUS_PER_TASK
./your_openmp_program_1
./your_openmp_program_2
```

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

HPC Cluster Access Demo Session

1. **Login demo**
2. **Compile and execute demo**