NHR FAU

FRIEDRICH-ALEXANDER
UNIVERSITÄT
ERLANGEN-NÜRNBERG

MuCoSim Introduction

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HPC High Performance Computing

BEFORE WE START - SSH-SHELL

- https://tinyurl.com/yau5vh2g
- Download „Portable edition“
- Save somewhere (e.g. Desktop)
- No installation required
- **Windows only!**

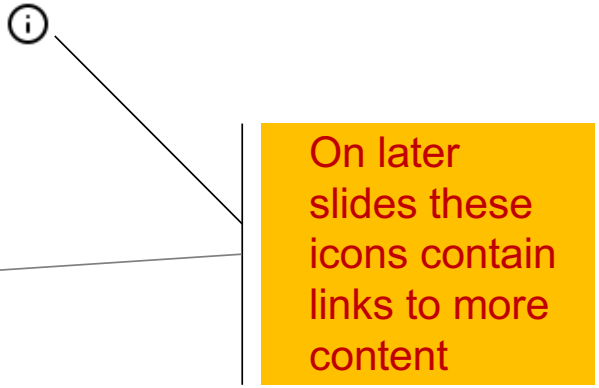
Info in the web

- General info on HPC workflow and tools: HPC Wiki

  https://hpc-wiki.info/hpc/HPC_Wiki

- NHR docs:

  https://hpc.fau.de/systems-services/systems-documentation-instructions/



MuCoSim Introduction

- Introduction to NHR@FAU cluster systems
- How to log into NHR@FAU cluster systems?
- How do I get a job?

NHR@FAU “Woody” cluster + TinyEth

main workhorse for *throughput*

- **Woody:**
  - all nodes with 4 cores and high clock frequency (3.4/3.5 GHz) Intel Xeon E3-12xx v? processors
  - at least 400 GB local HDD
  - and Gbit only
    - 40x Intel Sandybridge, 8 GB
    - 72x Intel Haswell, 8 GB
    - 64x Intel Skylake, 32 GB
    - 112 Kabylake, 32 GB

- **TinyEth:**
  - 20 nodes (480 cores)
    - 12 cores @ 2.66 GHz
    - 48 GB
    - 30/190/420 GB local HDD
  - **Single cores can be requested**
  - **Retires end of 2021**

NHR@FAU “Emmy” cluster

main *parallel* workhorse

- 543 compute nodes (10.880 cores)
  - 2 Intel Xeon E5-2660v2 (Ivy Bridge) 2.2 GHz (10 cores)
  - 20 cores/node + SMT cores
  - 64 GB main memory
  - No local disks
- 16 accelerator nodes same CPUs
  - 6 nodes with 2 x NVIDIA K20 GPGPUs
  - 4 nodes with 1x K20
  - 4 nodes with 1x NVIDIA V100

- Full QDR Infiniband fat tree
  - 40 GBit/s and < 2 µs latency
- Power consumption: ~160 KW (backdoor heat exchanger)
- #210@Top500 (Nov 2013)

R_{max} = 191 TF/s

NHR@FAU “Meggie” cluster

for scalable parallel jobs

- 728 Compute nodes (14.560 cores)
  - 2 Intel Xeon E5-2630 v4 (Broadwell) 2.2 GHz (10 cores)
  - 20 cores/node **No SMT**
  - 64 GB main memory
- No local disks

- Peak Performance: R_{peak} = 0.5 PF/s

- #346@Top500 (Nov. 2016) R_{max} = 0.48 PF/s

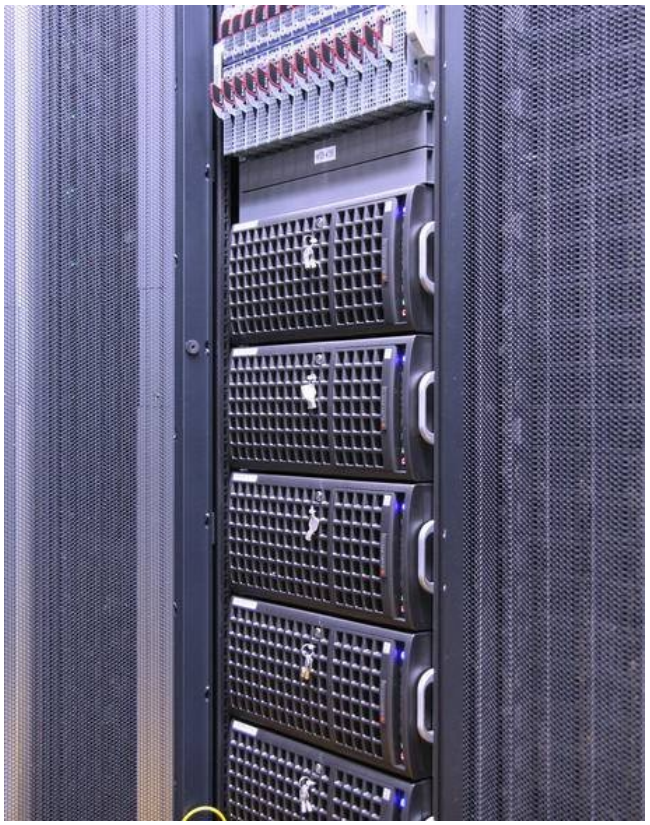
- Intel OmniPath network: Up to 100 Gbit/s
- Price: € 2,5 Mio.

- Power: 120-200 kW (depending on workload)

NHR@FAU “TinyGPU” cluster

most nodes paid by individual user groups

- 7 nodes with 2x “Nehalem” @2.66 GHz, 24 GB, HDD, 2x GTX980
- 7 nodes with 2x “Broadwell” @2.2 GHz, 64 GB, 980 GB SSD, 4x GTX1080
- 10 nodes with 2x “Broadwell” @2.2 GHz, 64 GB, 980 GB SSD, 4x GTX1080Ti
- 4 nodes with 2x “Skylake” @ 3.2 GHz, 96 GB, 2.9 TB SSD, 4x Tesla V100
- 12 nodes with 2x “Skylake” @ 3.2 GHz, 96 GB, 1.8 TB SSD, 4x RTX2080Ti
- 8 nodes with 2x ”Cascadelake” @ 2.9 GHz, 384 GB, 3.8 TB SSD, 8x RTX3080
- 8 nodes with AMD Rome @ 2.0 GHz, 512 GB, 5.8 NVMe SSD, 4x A100



NHR@FAU „Test“ cluster

Playground with different systems

Accessible only after request!

- 1 node with 2x „SandyBridge“ @2.7GHz (8 cores)
- 1 node with 2x „IvyBridge“ @3.0GHz (10 cores)
- 1 node with 2x „Haswell“ @2.3 GHz (14 cores)
- 1 node with 2x „Broadwell“ @2.3GHz (18 cores)
- 1 node with 2x „Skylake“ @2.4GHz (20 cores)
- 2 nodes with „AMD Zen“ (Ryzen+Naples)
- 1 node with small „Skylake“ and 2x NEC TSUBASA
- 1 node with 2x „ARMv8“ @2.2GHz (32 cores)
- 1 node with 1x „AMD Zen2“ (Rome) (128 cores)
- 1 node with 2x „Cascade Lake“ and 4x NVIDIA GPUs
- 1 node with 2x „AMD Zen3“ (Milan) (128 cores)

- phinally
- ivyep1
- hasep1
- broadep2
- skylakesp2
- naples
- aurora1
- warmup
- rome1
- medusa
- milan1

Cluster access

- Primary point of contact: cluster front-ends
  - `[woody|emmy|meggie].rrze.uni-erlangen.de`
  - `testfront.rrze.uni-erlangen.de`
  - …
  - For TinyGPU, TinyFat and TinyEth use `woody` frontend
  - Only available from within FAU (private IP addresses)

- Access from outside FAU: dialog server
  - `cshpc.rrze.uni-erlangen.de`
  - The only machine with a public IP address

Secure Shell

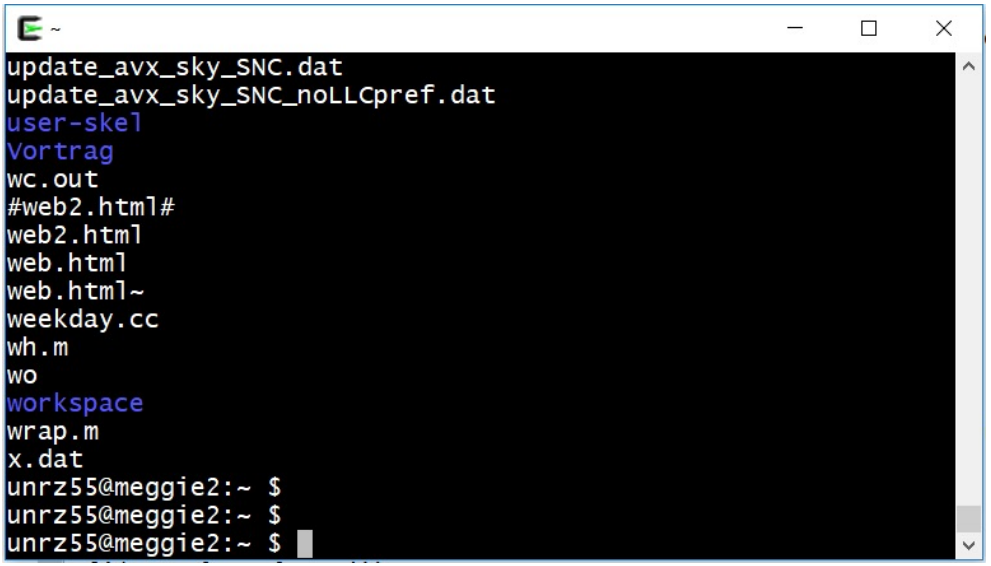
MobaXTerm:
- New session
- Remote host **`cshpc.rrze.uni-erlangen.de`** (or **`meggie.rrze.uni-erlangen.de`**)
- Specify HPC user name **`<hpcuser>`**

- By default: text mode only

```
$ ssh <hpcuser>@meggie.rrze.uni-erlangen.de
```

- Basic knowledge of file handling, scripting, editing, etc. under Linux is required
- X11 forwarding with option **`-X`**/**`-Y`**
  - Requires local X server

Included in MobaXterm



Log into frontend meggie.rrze.uni-erlangen.de

- Use your <hpcuser> account!
- Copy folder **~unrz139/mucosim** to your home

```
cp -r ~unrz139/mucosim $HOME
```

From external: Connect to cshpc first!

Interactive runs on the front-ends

- The cluster front-ends are for interactive work
  - Editing, compiling, preparing input,…
  - Amount of compute time per binary is limited by system limits
    - E.g., after 1 hour of CPU time your run will be killed
  - MPI jobs are not allowed on front ends at RRZE
- Front-ends are shared among all users, so be considerate!

```
iww042@meggie1$ emacs Makefile
iww042@meggie1$ make all
iww042@meggie1$ ./scripts/preprocess.py < inputfile
iww042@meggie1$ ./bin/a.out arg1 arg2 arg3
```

Batch jobs

- All clusters have resource manager software
  - “Batch system”
  - Users can request resources for their jobs
    - Number of nodes (optionally: type of nodes, memory, …)
    - Job runtime
    - What to run (normally a shell script)
  - Popular batch systems: PBS Pro, Torque, SLURM, LSF, GridEngine
  - Some setups (e.g., at RRZE) allow interactive batch jobs
- What you do with your node allocation is entirely up to you
- Most queues at RRZE have a 24 hour wall time limit

Example: Simple SLURM batch script (Meggie, …)

- Most simple batch script (**job1.sh**):

```
#!/bin/bash -l
~/bin/a.out arg1 arg2 arg3
```

- Submission:

```
unrz139@meggie1$ sbatch --nodes=1 --ntasks=1 \
                        --cpus-per-task=20 --time 01:00:00 \
                        job1.sh
Submitted batch job 966578
```

Resource specification

Job Identifier

sbatch: queue job and run it “in the background“
srun: run job directly and wait for results

Example: SLURM batch script (Meggie, Testcl.)

```
#!/bin/bash -l
#SBATCH --nodes=4 --ntasks-per-node=20 --time=06:00:00
#SBATCH --job-name=Sparsejob_33
#SBATCH --export=NONE
unset SLURM_EXPORT_ENV              # avoid evil login shell settings

# jobs always start in $HOME: change to a temporary job dir on $WOODYHOME
mkdir ${WOODYHOME}/$SLURM_JOB_ID
cd ${WOODYHOME}/$SLURM_JOB_ID
# copy input file from location where job was submitted, and run
cp ${SLURM_SUBMIT_DIR}/inputfile .
srun --mpi=pmi2 --ntasks=80 --ntasks-per-node=20 ${HOME}/bin/a.out \
                                        -i inputfile -o outputfile

# save output
mkdir -p ${WOODYHOME}/output/$SLURM_JOB_ID
cp outputfile ${WOODYHOME}/output/$SLURM_JOB_ID
cd
# get rid of the temporary job dir
rm -rf ${WOODYHOME}/$SLURM_JOB_ID
```

Job option sentinel

Job submission options: Nodes, cores p/ node,…

`$SLURM_*` variables contain job-relevant data

For MPI jobs!

Actual run of your binary

SLURM batch job submission (Meggie, Testcluster)

```
iww042@meggie1$ sbatch job3.sh
Submitted batch job 357074
iww042@meggie1:~ $ squeue -l
Mon Jan 28 17:38:52 2019
             JOBID PARTITION     NAME     USER    STATE       TIME TIME_LIMI  NODES NODELIST(REASON)
            357074      work Sparsejo   iww042  RUNNING       0:35   1:00:00      4 m[0101-0104]
iww042@meggie1:~ $
```

- Request additional resources (like GPUs)
  - **`--gres=gpu:X`** for any **`X`** GPUs
  - **`--gres=gpu:a100:X`** for **`X`** Nvidia A100 GPUs
  - (maybe) you have to select a different partition: **`--partiton=a100`**
- The amount of GPUs correspond to the amount of CPU hardware threads and available memory

Interactive batch job with SLURM (Meggie, Testcluster)

- srun command can queue/run a job directly

```
unrz139@meggie1$ srun --nodes=2 --ntasks-per-node=20 \
                      --time=01:00:00  --pty /bin/bash -l
unrz139@m0101$ echo $SLURM_SUBMIT_DIR
/home/hpc/iww0/iww042
unrz139@m0101$
```

- X11 forwarding currently not supported
  - Workaround
    - submit job with sleep command in batch script
    - use **`ssh -X`** to log in to node

SLURM user commands (non-exhaustive)

Command	Purpose	Options

`sbatch [<options>] <script>`
`srun [<options>] <script>`
	Submit batch job	`--time=HH:MM:SS`
		`--nodes=#`
		`--ntasks-per-node=#`
		`--error=<stderr_filename>`
		`--output=<stdout_filename>`
		`--mail-user=<address>`
		`--mail-type=ALL|BEGIN|END|...`

`squeue [<options>]`	Check job status	`-j <JobID>` show job `-t RUNNING` show only running jobs `-u <USER>` this user only
`scancel <JobID>`	Delete batch job	–
`srun <options>`	Run program	Many options; see man page

Submit **`jobs/job1.sh`** to batch system on meggie

(more complex **`jobs/job2.sh`**, can be used as reference)

Start an interactive job on a single node with 2 hours time limit and **`-C hwperf`** option

Which host are you on?

(You can use the interactive session for the following hands-on, so don‘t close it!)

Open a separate shell to meggie for compilation