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!**

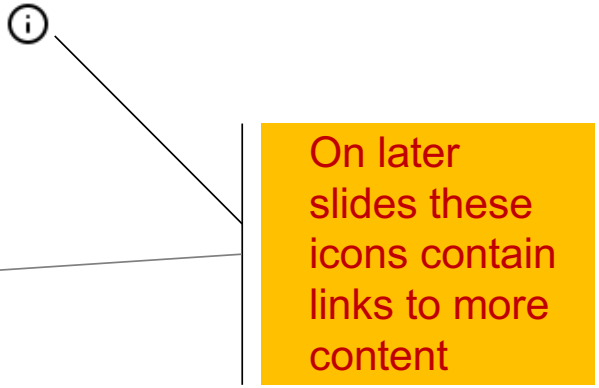
Info in the web

- 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

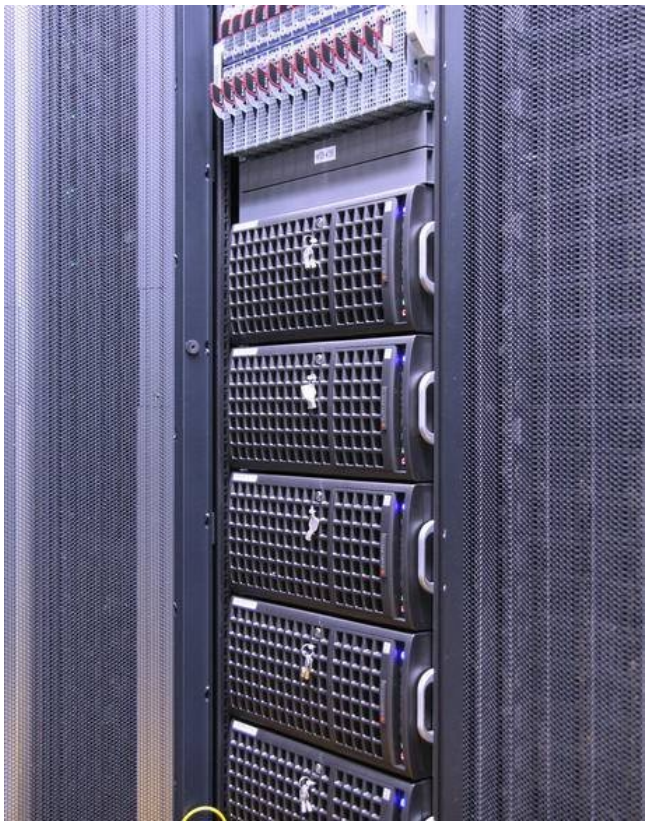
- Intel OmniPath network: Up to 100 Gbit/s
- Price: € 2,5 Mio.

- 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

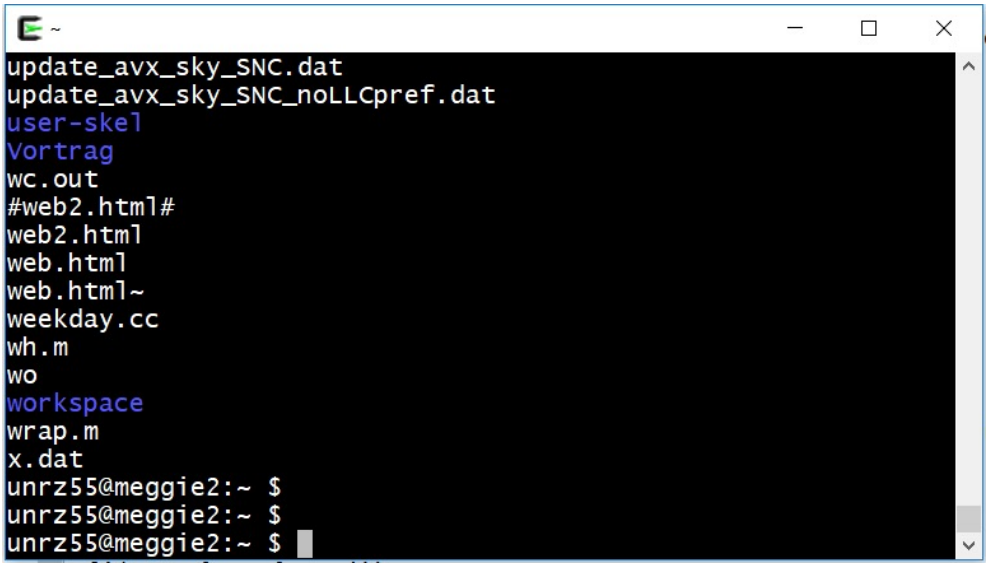
MobaXTerm:
- New session
- Remote host **`cshpc.rrze.uni-erlangen.de`** (or **`meggie.rrze.uni-erlangen.de`**)
- Specify HPC user name **`<hpcuser>`**

- 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

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MuCoSim Introduction

Software Environment

Pre-installed software packages

- Linux standard distro packages
- “Full” installation available on cluster front-ends
  - Easy to add additional packages
- Node installation: usually stripped down
  - Not easy to add new software due to space contraints
  - On some nodes you cannot even compile your code (no headers)
    → Compile on front-ends

The module system

- Software provided locally by RRZE
  - Compilers, libraries, commercial and open software
  - Installed on central server and available on all cluster nodes

- Software has to be loaded in the user's environment to become usable
  - Command: **`module`**
  - All module commands affect the current shell only!

The `module` command

Show available modules: `module avail`

```
$ module avail
--------------------- /apps/modules/data/applications ----------------------------------------------
amber-gpu/14p13-at15p06-gnu-intelmpi5.1-cuda7.5 gromacs/4.6.6-mkl-IVB
amber-gpu/16p04-at16p10-gnu-intelmpi5.1-cuda7.5 gromacs/5.0.4-mkl-IVB
amber/12p21-at12p38-intel16.0-intelmpi5.1       gromacs/5.1.1-mkl-IVB_d
---------------------- /apps/modules/data/development ----------------------------------------------
cuda/7.5                            intel64/16.0up04                  intelmpi/5.1up03-intel
cuda/8.0                            intel64/17.0up05(default)         llvm-clang/3.8.1
cuda/9.0                            intel64/18.0up02                  opencl/intel-cpuonly-5.2.0.10002
cuda/9.1                            intel64/18.0up03                  openmpi/1.08.8-gcc
$
```

The `module` command

Load a module: `module load <modulename>`

At RRZE, the Intel compilers are named intel64/<version>
Without <version>, the default is loaded

```
$ module load intel64
$ icc -V
Intel(R) C Intel(R) 64 Compiler for applications running on Intel(R) 64, Version 17.0.5.239 Build
20170817
Copyright (C) 1985-2017 Intel Corporation.  All rights reserved.
```

Display loaded modules: `module list`

```
$ module list
Currently Loaded Modulefiles:
 1) python/3.5-anaconda      2) intelmpi/2017up04-intel  3) mkl/2017up05       4) intel64/17.0up05
```

Module command summary

Command	What it does
`module avail`	List available modules
`module whatis`	Shows over-verbose listing of all modules
`module list`	Shows which modules are currently loaded
`module load <pkg>`	Loads module *pkg (default)*, i.e., adjusts environment
`module load <pkg>/<version>`	Loads specific version of *pkg* instead of default
`module unload <pkg>`	Undoes what the load command did
`module help <pkg>`	Shows a detailed description of *pkg*
`module show <pkg>`	Shows what environment variables pkg modifies and how

How many Intel MPI modules are available?

What is the latest installed GCC version?

Is it possible to load IntelMPI and OpenMPI at the same time? Why?

What‘s the **`JAVA_ROOT`** for java module?