NHR FAU

FRIEDRICH-ALEXANDER
UNIVERSITÄT
ERLANGEN-NÜRNBERG

MuCoSim Introduction

Thomas Gruber and Katrin Nusser (HPC @ Uni Erlangen)

Thomas.Gruber@fau.de

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/

- **Linux intro videos (HPC.NRW): https://www.youtube.com/playlist?list=PLhznUsiowt261tbLSHplkZHcvZAv_hEcT**

On later slides these icons contain links to more content

MuCoSim Introduction

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

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 “Fritz” cluster

for scalable parallel jobs

- 944 Compute nodes (33.984 cores)
  - 2x Intel Xeon Platinum 8360Y (Ice Lake) 2.4 GHz (36 cores)
  - 72 cores/node **No SMT**
  - 256 GB main memory
- No local disks
- Peak Performance:
  R_{peak} = 2.233 PF/s (with 612 nodes)
- Recently, a few SapphireRapids nodes were added to Fritz
- Blocking HDR100 InfiniBand:
  Up to 100 Gbit/s
  Islands with 64 nodes
- Power:
  ≈1MW

NHR@FAU “Alex” cluster

for GPGPU jobs (ML, DataScience, …)

- >50 Compute nodes
  - 2x AMD EPYC 7713 (Milan) 2.4 GHz (64 cores)
  - 128 cores/node No SMT
  - >= 512 GB main memory
- 8 GPUs per node
  - Nvidia A100
  - Nvidia A40
- Local NVMe SSDs
- Peak Performance: R_{peak} = 2.938 PF/s (with parts of the system)

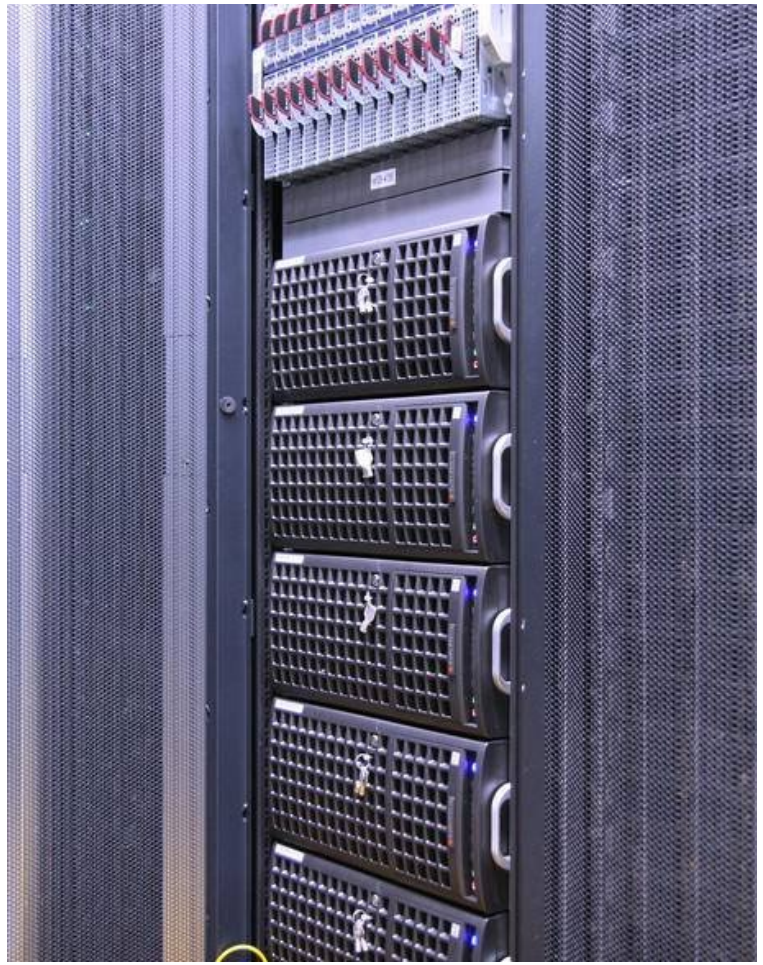
Network:

- 25 GbE
- HDR200 InfiniBand (some)
- Power: <200kW

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!

Name	Description
phinally	2x „SandyBridge“ @2.7GHz (8 cores)
ivyep1	2x „IvyBridge“ @3.0GHz (10 cores)
hasep1	2x „Haswell“ @2.3 GHz (14 cores)
broadep2	2x „Broadwell“ @2.3GHz (18 cores)
skylakesp2	2x „Skylake“ @2.4GHz (20 cores)
caslakesp2	2x „Cascade Lake“ @2.5GHz (20 cores)
aurora1	2x (small) „Skylake“ and 2x NEC TSUBASA
medusa	2x „Cascade Lake“ and 4x different NVIDIA GPUs
optane1	2x „Cascade Lake“ and Intel Optane persistent memory
icx32	2x “Icelake“ @2.6GHz (32 cores)
icx36	2x “Icelake“ @2.4GHz (36 cores)
naples	2x „AMD Zen“ (Naples)
rome1	1x „AMD Zen2“ (Rome) (128 cores)
rome2	2x „AMD Zen2“ (Rome) and AMD MI100 GPU
milan1	2x „AMD Zen3“ (Milan) (128 cores)
warmup	2x „Thunder X2“ @2.2GHz (32 cores, ARMv8)
applem1studio	Apple M1 Studio (20 cores, ARMv8)

There are more systems, just no more space

Cluster access

- Primary point of contact: cluster front-ends
  - **`[woody|tinyx|fritz|alex].rrze.uni-erlangen.de`**
  - **`testfront.rrze.uni-erlangen.de`**
  - …
  - For TinyGPU, TinyFat and TinyEth use **`tinyx`** 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
  - Recommendation: Setup SSH config for proxy jump

Secure Shell

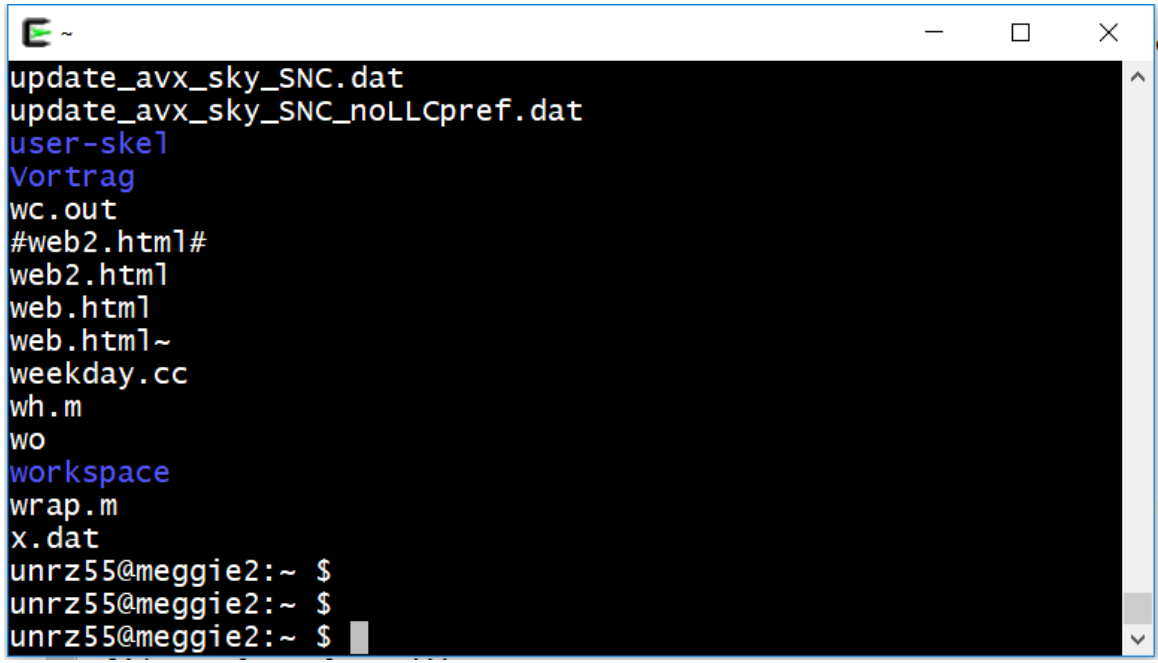
MobaXTerm:
- New session
- Remote host **`cshpc.rrze.fau.de`**
  Specify HPC user name **`<hpcuser>`**

- By default: text mode only

```
$ ssh <hpcuser>@cshpc.rrze.fau.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



Secure Shell – SSH Keypairs

- There are no passwords anymore for accounts at NHR@FAU

- Your key is ”at home”
- Connect to **`cshpc`** works with your key
- If you do “**`ssh X`**” at **`cshpc`**, no key is available
  - Use **`ProxyJump`** over **`cshpc`** from home (home key is used)
  - Generate a separate key at **`cshpc`** for NHR@FAU internal SSH

Recommendation:
Use a passphrase for the SSH key. This increases security for you and the HPC systems

Log into frontend meggie.rrze.fau.de

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

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

From external: Connect to cshpc first!

For PTfS Students: use fritz.rrze.fau.de instead

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 task will be killed
  - MPI jobs are not allowed on front ends at NHR@FAU
- 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`):

Always use `bash -l`

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

- Submission:

Resource specification

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

Job Identifier

`sbatch`: queue job and run it “in the background“
`salloc`: queue job and run it “in the foreground“
`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$ salloc --nodes=2 --ntasks-per-node=20 \
                        --time=01:00:00
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
- Attach to a running job:

```
$ srun --pty --jobid YOUR-JOBID bash -l
```

SLURM pitfalls

- Setting CPU frequency on Fritz/Alex can only be done via **`srun`**:

```
$ salloc …
$ srun --cpu-freq=<min>-<max>:performance …
```

- Access to hardware performance counters needs to be requested

```
$ salloc --constraint hwperf
$ srun -C hwperf
```

SLURM user commands (non-exhaustive)

Command	Purpose	Options

`sbatch [<options>] <script>`
`salloc [<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

PTfS Students: Similar on fritz

NHR FAU

FRIEDRICH-ALEXANDER
UNIVERSITÄT
ERLANGEN-NÜRNBERG

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 constraints
  - 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
  - Module availability can be different each system

- 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/compiler ------------------------
gcc/9.4.0  gcc/10.3.0  gcc/11.2.0  gcc/12.1.0  intel/2021.4.0  intel/2022.1.0

----------------------- /apps/modules/data/development -----------------------
intelmpi/2021.6.0  openmpi/4.1.2-gcc11.2.0
intelmpi/2021.7.0  openmpi/4.1.2-intel2021.4.0

$
```

The `module` command

Load a module: `module load <modulename>`

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

```
$ module load intel
$ icc --version
icc (ICC) 2021.6.0 20220226
Copyright (C) 1985-2022 Intel Corporation.  All rights reserved.
```

Display loaded modules: `module list`

```
$ module list
Currently Loaded Modulefiles:
 1) intel/2022.1.0          3) intelmpi/2021.7.0
 2) python/3.9-anaconda     4) mkl/2022.1.0
```

Older systems (e.g. meggie):

- Intel compilers are named intel64/<version>
- Modules commonly load other modules (mkl or intelmpi module when loading intel64)

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 the default **`java`** module?

Preparation:

Copy **`~unrz139/mucosim`** to your home

(WARNING: may overwrite existing files!)

Let‘s start with some recap:

Go to **`mucosim/stream`** and compile the code with latest **Intel** suite

Run code with **`OMP_NUM_THREADS=4`** a few times and determine min. and max. bandwidth for the **`copy`** kernel.

NHR FAU

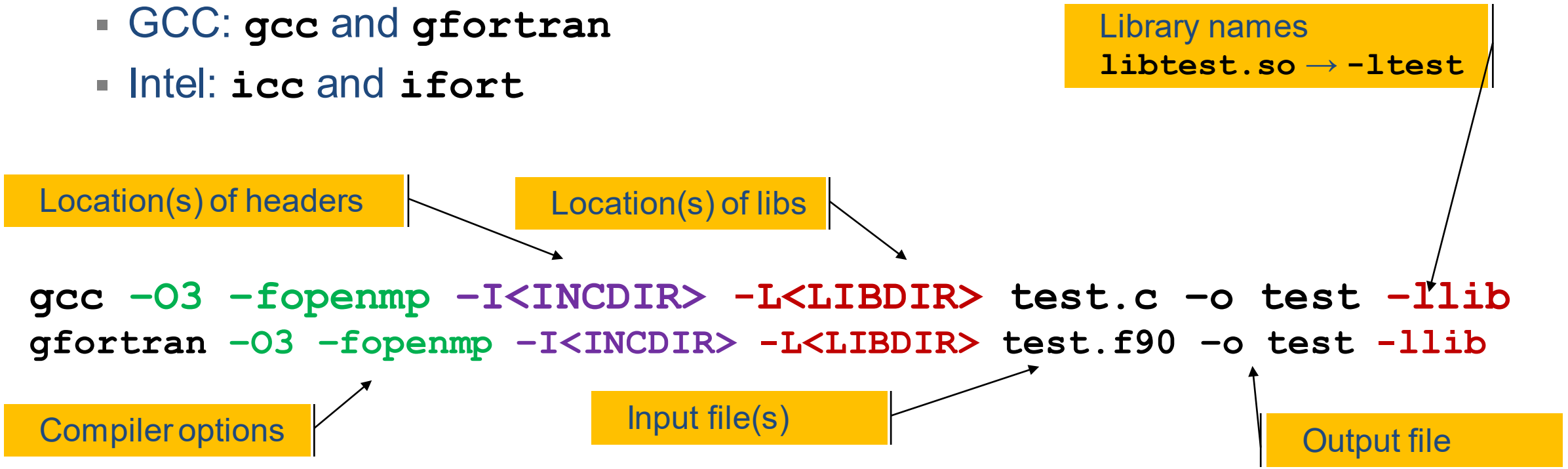
FRIEDRICH-ALEXANDER
UNIVERSITÄT
ERLANGEN-NÜRNBERG

MuCoSim Introduction

COMPILERS

Compilers @ RRZE

- We provide GCC, Intel C/C++ Compiler (and PGI and others)
- On warmup also arm-clang (/opt/arm/… license up-on-request)
- Provided through **`module`** system
- Common compiler names:
  - GCC: **`gcc`** and **`gfortran`**
  - Intel: **`icc`** and **`ifort`**



Compilers @ RRZE

- Common compiler switches:

Meaning	GCC	Intel compilers
General optimization level	`-O1`, `-O2`, `-O3` (some vendor specific options like `-Ofast`)	
Hardware feature flags	`-m` like `-mavx2`	`-x` like `-xCORE-AVX2`
Compiler feature flag	`-f` like `-fopenmp`	`-q` like `-qopenmp`

- In many cases, the Intel compiler
  - produces „better“ code and often better performing
  - provides fallbacks for GCC flags (`-fopenmp` accepted by ICC)

- CUDA compilers only available at nodes with GPUs

Compile **`compile/get_cpuflags.c`** with GCC and run it

What is the widest SIMD the system supports?

(MMX → SSE → SSE2 → SSE3 → SSE4 → AVX → AVX2 → AVX512)

128 bit vectors (2 doubles, 4 floats)

256 bit vectors (4 doubles, 8 floats)

512 bit vectors (8 doubles, 16 floats)

Compile **`compile/triad.c`** with recent GCC and ICC and …

What's the minimum runtime you can achieve on the compute node?

Single hardware thread? Do optimization flags help?

All hardware threads?

Remember: Copy folder to your home/workdir/…

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