NHR FAU

FAU Friedrich-Alexander-Universität Erlangen-Nürnberg

Programming Techniques for Supercomputers Tutorial

Erlangen National High Performance Computing Center (NHR@FAU)

Department of Computer Science

FAU Erlangen-Nürnberg

Sommersemester 2025

Outline

- Course website
- Login to the “Fritz” cluster of NHR@FAU
- Starting cluster jobs
- Some guidelines

Information

- All slides, exercises, and miscellaneous material can be found on the course pages:

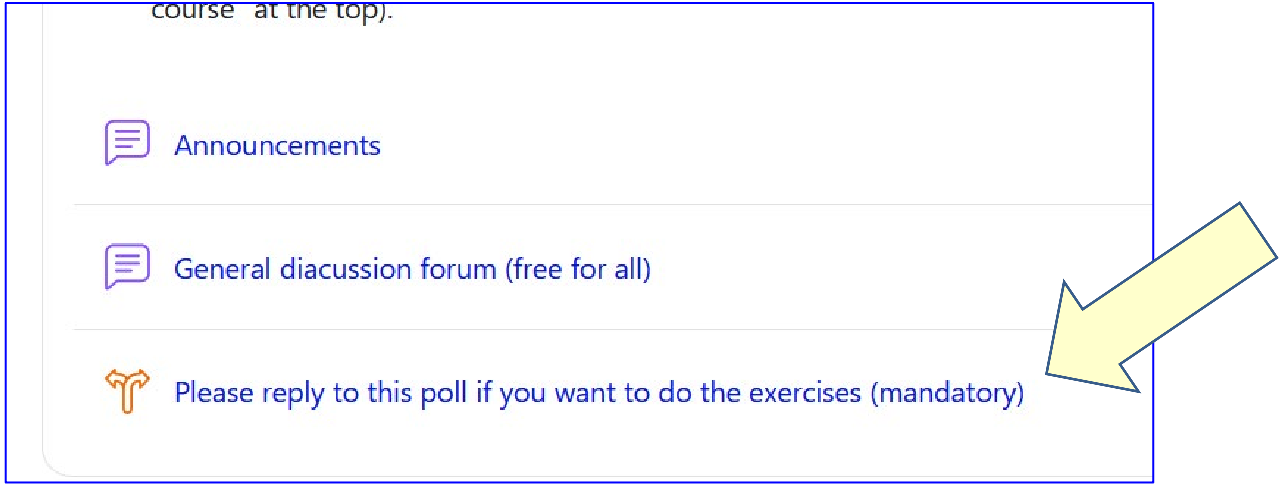
  http://go-nhr.de/PTfS

- Please use the discussion forum there if you have a question that might be of interest to your fellow students

- Please enroll in the course so you get all e-mail announcements

Accounts

- If you haven’t done so already, fill out the poll at: https://moodle.nhr.fau.de/mod/choice/view.php?id=2834
  - You will get an e-mail invitation about your new account (not right away, we are collecting them an will send them out in batches)



course" at the top).

Announcements

General diacussion forum (free for all)

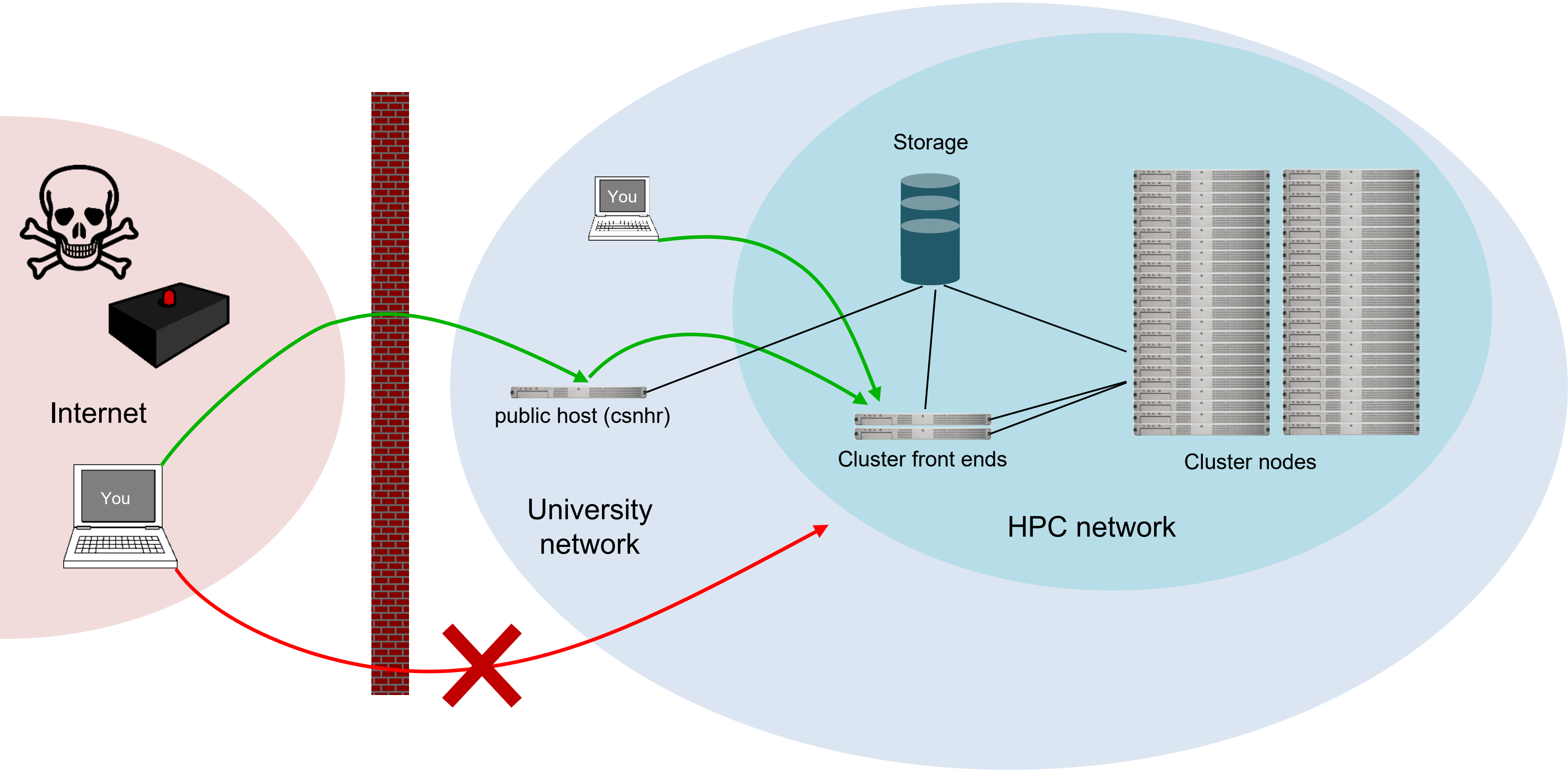
Please reply to this poll if you want to do the exercises (mandatory)

Accounts (for those who will do the homework)

- HPC accounts are different from your IdM accounts
  - No password – login is only possible via SSH public/private key
  - Manage your HPC account on the HPC portal: https://portal.hpc.fau.de
    - Log in with your IdM account
  - Upload an SSH public key to the portal
    - Only an uploaded key will grant access! `~/.ssh/authorized_keys` will be nonfunctional
  - It can take up to one day for your account to become active
  - Video about generating a key pair under Windows, uploading it to the portal, and logging in: https://youtu.be/GQ_yk_P-7Z4

- If you don't know what all this SSH stuff is, learn it. It's a basic skill.

NHR@FAU cluster access



Login to Fritz from inside FAU (or via VPN)

- Login to NHR@FAU cluster front-end machines
  - **`ssh ptfsXXXh@fritz.nhr.fau.de`**
  - Front-end nodes: **`fritz1`**,…,**`fritz4`**

```
$ ssh ptfsXXXh@fritz.nhr.fau.de
===============================================================================
Welcome at "Fritz", FAU's NHR and Tier3 parallel computer
- 944 nodes with 2x Intel Icelake 8360Y
[... BLURB ...]
===============================================================================
Last login: Fri Feb  4 14:54:35 2022 from 2001:638:a000:1001::83bc:397
ptfsXXXh@fritz2:~$
```

- Works only from inside FAU (or w/ VPN)
  https://www.anleitungen.rrze.fau.de/internet-zugang/vpn/
  (German only 🤦)

How to log in if not at the university?

- Solution 1: Use a VPN (see previous slide)

- Solution 2: Use our “dialog server” `csnhr.nhr.fau.de`
  - All necessary tools installed (Ubuntu 22.04)
  - Access to all HPC systems and most file systems
  - Linux Desktop from Windows: XRDP (think „Windows terminal server“ but with Linux) https://doc.nhr.fau.de/access/xrdp/
  - csnhr is not for compiling your code! (see later)

```
$ ssh ptfsXXXh@csnhr.nhr.fau.de
[...BLURB...]
ptfsXXXh@csnhr:~$ ssh ptfsXXXh@fritz.nhr.fau.de
[...BLURB...]
ptfsXXXh@fritz2:~$
```

Login via proxy jump

- If you need csnhr only as a “jump host,” there is a faster way to log in
- Add this to your **`~/.ssh/config`**:

```
Host fritz
      HostName fritz.nhr.fau.de
      User ptfsXXXh                        # adapt this
      IdentityFile /home/pi/.ssh/id_rsa    # adapt this
      ProxyJump csnhr
Host csnhr
      HostName csnhr.nhr.fau.de
      User ptfsXXXh                        # adapt this
      IdentityFile /home/pi/.ssh/id_rsa    # adapt this
```

- … and then, just:

```
$ ssh fritz
```

Work from the Computer Science CIP pools

- CIP Account registration: https://account.cip.cs.fau.de/

- Start any kind of shell, e.g. **`konsole`**
  (All workstations in the tutorial room should run linux)

- Login to NHR@FAU cluster front-end machines as usual:
  - **`ssh ptfsXXXh@fritz.nhr.fau.de`**

Compiling on Fritz (only on the frontends `fritz*`)

- Make compiler available for use:
  - `module load intel`
  - `icx` → Intel C compiler
  - `icpx` → Intel C++ compiler
  - `ifx` → Intel Fortran compiler
- Recommended Intel compiler options
  - `-O3` high optimization level
  - `-xHost` optimize for CPU the compiler is running on
  - `-fno-alias` assume no overlap between any arrays or elements
  - Other options (`-c`, `-o`, `-S`, `-L`, `-I`, `-l`,…) are the same as for GCC
- Additional software
  - `module available` → overview over all available software
  - `module list` → currently loaded modules
  - `module unload <modulename>` → unload module

Acquiring a cluster node

- Issue an interactive job (1 node) on Fritz:
  - `salloc --nodes=1 --time=01:00:00`
  - Requests one full node for one hour
  - Gives you an interactive login shell on the compute node
  - For short jobs (< 1h), a node should usually be available right away

- The node is yours alone for the allocated time

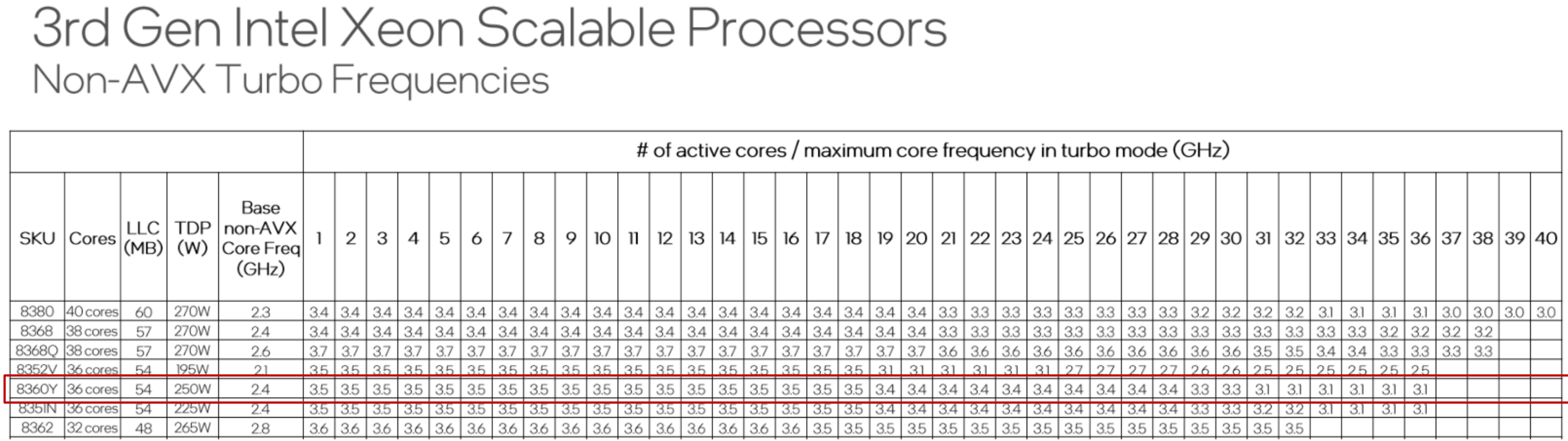
```
ptfsXXXh@fritz2:~$ salloc --nodes=1 --time=01:00:00
salloc: Pending job allocation 56425
salloc: job 56425 queued and waiting for resources
salloc: job 56425 has been allocated resources
salloc: Granted job allocation 56425
[... BLURB ...]
ptfsXXXh@f0772:~$ ./a.out   # this is your program
```

Fixing the clock frequency

- Modern CPUs can adjust their own clock speed depending on some conditions (“Turbo Mode” etc.)
  - # of active cores
  - Temperature
  - ???
- Accurate and reproducible benchmarking requires a constant clock speed
- Fritz allows you to set the clock speed when running your binary
  - Use `srun` with the `--cpu-freq=<MIN>-<MAX>:<governor>` option as a wrapper to your binary
  - Clock frequency is specified in kHz here (god knows why…)

```
ptfsXXXh@f0772:~$ srun --cpu-freq=2000000-2000000:performance ./a.out
```

A glance at clock speeds on Intel server CPUs



3rd Gen Intel Xeon Scalable Processors

Non-AVX Turbo Frequencies

					# of active cores / maximum core frequency in turbo mode (GHz)																																							
SKU	Cores	LLC (MB)	TDP (W)	Base non-AVX Core Freq (GHz)	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18	19	20	21	22	23	24	25	26	27	28	29	30	31	32	33	34	35	36	37	38	39	40
8380	40 cores	60	270W	2.3	3.4	3.4	3.4	3.4	3.4	3.4	3.4	3.4	3.4	3.4	3.4	3.4	3.4	3.4	3.4	3.4	3.4	3.4	3.4	3.4	3.3	3.3	3.3	3.3	3.3	3.3	3.3	3.3	3.2	3.2	3.2	3.2	3.1	3.1	3.1	3.1	3.0	3.0	3.0	3.0
8368	38 cores	57	270W	2.4	3.4	3.4	3.4	3.4	3.4	3.4	3.4	3.4	3.4	3.4	3.4	3.4	3.4	3.4	3.4	3.4	3.4	3.4	3.4	3.4	3.3	3.3	3.3	3.3	3.3	3.3	3.3	3.3	3.3	3.3	3.3	3.3	3.3	3.3	3.2	3.2	3.2	3.2		
8368Q	38 cores	57	270W	2.6	3.7	3.7	3.7	3.7	3.7	3.7	3.7	3.7	3.7	3.7	3.7	3.7	3.7	3.7	3.7	3.7	3.7	3.7	3.7	3.7	3.6	3.6	3.6	3.6	3.6	3.6	3.6	3.6	3.6	3.6	3.5	3.5	3.4	3.4	3.3	3.3	3.3	3.3		
8352V	36 cores	54	195W	2.1	3.5	3.5	3.5	3.5	3.5	3.5	3.5	3.5	3.5	3.5	3.5	3.5	3.5	3.5	3.5	3.5	3.5	3.5	3.1	3.1	3.1	3.1	3.1	3.1	2.7	2.7	2.7	2.7	2.6	2.6	2.5	2.5	2.5	2.5	2.5	2.5				
8360Y	36 cores	54	250W	2.4	3.5	3.5	3.5	3.5	3.5	3.5	3.5	3.5	3.5	3.5	3.5	3.5	3.5	3.5	3.5	3.5	3.5	3.5	3.4	3.4	3.4	3.4	3.4	3.4	3.4	3.4	3.4	3.4	3.3	3.3	3.1	3.1	3.1	3.1	3.1	3.1				
8351N	36 cores	54	225W	2.4	3.5	3.5	3.5	3.5	3.5	3.5	3.5	3.5	3.5	3.5	3.5	3.5	3.5	3.5	3.5	3.5	3.5	3.5	3.4	3.4	3.4	3.4	3.4	3.4	3.4	3.4	3.4	3.4	3.3	3.3	3.2	3.2	3.1	3.1	3.1	3.1				
8362	32 cores	48	265W	2.8	3.6	3.6	3.6	3.6	3.6	3.6	3.6	3.6	3.6	3.6	3.6	3.6	3.6	3.6	3.6	3.6	3.5	3.5	3.5	3.5	3.5	3.5	3.5	3.5	3.5	3.5	3.5	3.5	3.5	3.5	3.5	3.5								

Source: Intel

Job scripts

- Use job scripts for “production runs”
  - Parameter studies
  - Long runs
- Job scripts can be submitted to be executed later when resources are available

```
#!/bin/bash
#SBATCH --nodes=1 --time=06:00:00
#SBATCH --job-name=TEST01
#SBATCH --export=NONE

unset SLURM_EXPORT_ENV

# the script runs where you submitted it
# do your thing
module load intel
cd ~/PTfS/assignment4
srun ./a.out
```

Block user env from tainting job env

Use srun to fix clock frequency to the value specified with –cpu-freq

- Options can be specified in the script or on the command line at submission
- Example script: `~ptfs100h/GettingStarted/job.sh`

Job scripts

- Submit via **sbatch** command, view via **squeue**:

```
ptfsXXXh@fritz2:~$ sbatch job.sh
Submitted batch job 56430
ptfsXXXh@fritz2:~$ squeue
             JOBID PARTITION     NAME     USER ST       TIME  NODES NODELIST(REASON)
             56430 singlenod   TEST01 ptfsXXXh  R       0:01      1 f0767
```

- After job termination, the stdout and stderr of your job can be found (by default) in a file **<JOBNAME>.o<JOBID>**:

```
ptfsXXXh@fritz2:~$ ls TEST01*
TEST01.o56430
```

Measuring elapsed time

- Remember: Performance $P = \frac{W}{T_{wall}}$

  W = work

  T_{wall} = “wallclock time,” elapsed time
- Accurate time measurement is important!
  - Very short periods are difficult to measure
  - Measure at least for 100 ms

```
#include “timing.h”
int main(int argc, char *argv[])
{
  double wcTime,wcTimeStart,wcTimeEnd;
  wcTimeStart = getTimeStamp();

  /* PUT YOUR CODE HERE */

  wcTimeEnd = getTimeStamp();
  wcTime = wcTimeEnd-wcTimeStart;
  printf("Walltime: %.3lf s\n",wcTime);

  return 0;
}
```

- Example code in `~ptfs100h/GettingStarted/timing.*`

General guidelines

- Do not run benchmarks on the frontend nodes, as multiple programs and users interact there

- You may do test runs, e.g., compilation tests and verification, on frontends

- For obtaining lots of results, write your own scripts and execute them via the batch system

- Check your results for plausibility (Cool! My code runs @ petaflop/s!)

Some links

- Linux tutorial for n00bs:
  - https://ryanstutorials.net/linuxtutorial/
- MobaXterm SSH client & X server for Windows (choose free version):
  - https://mobaxterm.mobatek.net/
- Intel processor details (here for the one used in “Fritz”):
  - https://en.wikipedia.org/wiki/Ice_Lake_(microprocessor)
- Confused about all those CPU code names?
  - https://en.wikipedia.org/wiki/Xeon
  - https://en.wikipedia.org/wiki/Epyc

- Fritz cluster official docs:
  - https://doc.nhr.fau.de/clusters/fritz/

Assignments

- New homework assignments are released Wednesday around 10:00 a.m.
- Report submission
    - Deadline: eight days later, i.e., Thursday 10:00 a.m. No extensions!
    - Deadline for Assignment 0: Thursday, May 8 at 10:00 a.m.
    - Upload a single file in Moodle
        - (searchable) PDF report (no screenshots!) or
        - compressed archive including a (searchable) PDF report and supporting material
    - Grading will be done based on PDF report
    - If coding was required, submit the code as well!
- Submission allowed in groups of up to 3 students
    - Everyone still needs to submit on their own
    - Clearly indicate the partners in your group

Tutorial Sessions

- Presentation of solution to previous assignment

- Presentation of current (new) assignment

- Opportunity to ask questions

Report Guidelines

- Report must include
  - Specific answers to questions/tasks mentioned in assignments
  - Explanation on how you arrived at your answer
  - Description of the steps you took to measure performance/timings/etc.
  - Documentation of compiler switches, frequencies and anything necessary to reproduce your results by someone else (including code, if applicable)
- Write complete sentences
  - A part of becoming a scientist is being able to produce intelligible prose
- Never forget units!
  - The unit of time is “seconds” or “cycles”
- When using plots: Label your axes!
  - A graph without proper units and scales on the axes will be ignored in grading