



38th VI-HPS Tuning Workshop

NHR@FAU, Erlangen, Germany, 01-03 March 2021



Where are we?

- Friedrich–Alexander University Erlangen–Nürnberg
 - Established in 1742
 - In Top10 of largest universities in Germany
 - ≈39000 students







Erlangen Regional Computing Center



38TH VI-HPS TUNING WORKSHOP (NHR@FAU, GERMANY, 01-03 MARCH 2021)

Who are we?

NHR & TIER 2 academic HPC computing center



- 2 main and 4 special purpose systems
- In total 1656 nodes and 134 GPGPUs
- 6 people for software and support
- 3 system administrators

Associated computer science research group

- Performance Engineering
- Performance Modeling
- Tool development
- Sparse and stencil solvers





What is NHR?



- A coordinated network of National High Performance Computing (NHR) centres funded by the federal and state governments.
- The NHR network shall also strengthen methodological competence through coordinated training and continuing education
 of users and, in particular, of young scientists.
- Currently 8 NHR Centres
- **Tier 0/1** Gauss Center for Supercomputing (GCS)
- **Tier 2** Centres with a regional supply focus
- Tier 3 Local supply

Official Start 1.1.2021

Application focus

Atomistic simulations using quantum mechanics (QM) and classical molecular dynamics (MD) methods for computational **chemistry**, **life sciences**, and **materials science**.

https://www.atomistic-simlab.hpc.fau.de

HPC methodology

Node-level performance analysis, modelling, and engineering for CPUs and GPUs including effective automatic code generation techniques. https://www.perf-lab.hpc.fau.de

RRZE "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
 - Intel OmniPath network
- No local disks
- Peak Performance:
 - R_{peak} = 0.5 PF/s R_{max} = 0.48 PF/s (#346@Top500 11/2016)
- Power: 120-200 kW (depending on workload)
- Price: € 2,5 Mio







How to access the HPC systems?



Accessing a cluster system



Cluster access

- Primary point of contact: cluster front-ends
 - woody.rrze.fau.de
 - emmy.rrze.fau.de

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- meggie.rrze.fau.de
- Only available from within FAU (private IP addresses)

- Access from outside FAU: dialog server
 - shpc.rrze.fau.de
 - The <u>only</u> machine with a public IP address

Secure Shell

By default: text mode only

- X11 forwarding with option −**x** or −**y**
 - Requires local X server

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 Basic knowledge of file handling, scripting, editing, etc. under Linux is required

Secure Shell Clients

- Linux & Mac: OpenSSH available in any distribution
- Windows
 - Putty (<u>https://putty.org/</u>)
 - OpenSSH under Cygwin (<u>http://cygwin.com/</u>)
 - > Cygwin == GNU/Linux-like environment under Windows
 - WinSCP (data transfer only) (<u>https://winscp.net</u>)
 - MobaXterm (https://mobaxterm.mobatek.net/)
 - includes an embedded X server

Overview ssh

- User is authenticated to the system, system is authenticated to the user
- All transmitted data is encrypted
- ssh [<username>@]<Remote-Host> [<command>]
 - -1 <name> use <name> as username for login
 - -f fork to background
 - -p <port> connect to <port>
- Data transfer
 - scp [-r] <source(s)> <target>
 - -r recursive copying into subfolders
 - Remote source or target: <username>@<Remote-Host>:<path>
 - -P <port> connect to <port>

me@AtHome \$ cat ~/.ssh/config
Host meggie
HostName meggie.rrze.fau.de
ProxyJump cshpc.rrze.fau.de
User <username>
me@AtHome \$ ssh meggie

Windows GUI for SSH: MobaXterm

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UNREGISTERED VERSION - Please support MobaXterm by subscribing to the professional edition here: https://mobaxterm.mobatek.net

Windows GUI for scp: WinSCP

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NoMachine NX

- Similar to Windows Terminal Server
- User can attach/detach to/from running GUI session (Linux desktop) via network
- Local client installation required (available for Win/Linux/Mac) <u>https://www.nomachine.com/download-enterprise#NoMachine-Enterprise-Client</u>
- Uses SSH connection "under the hood"
- NX server running on cshpc

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

Config: Use the system login, Authentication by Password