

Erlangen Regional
Computing Center

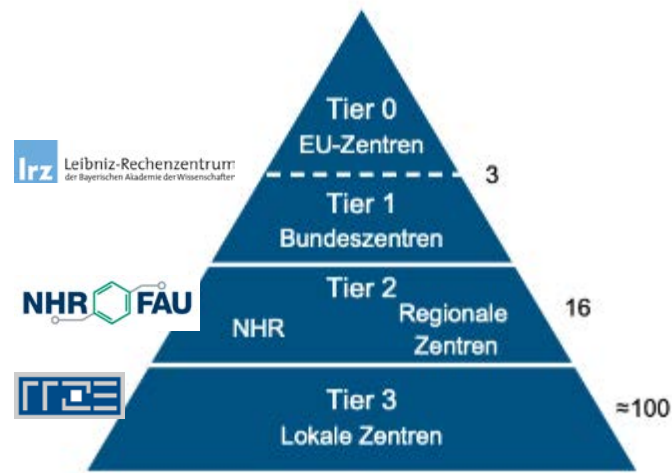
NHR@FAU

Dr. Jan Eitzinger, Dr. Georg Hager, **Prof. Gerhard Wellein**, Dr. Thomas Zeiser



What is NHR?

HPC Supply Pyramide



Tier 0/1 – 3 Centres in the Gauss Center for Supercomputing (GCS)

Tier 2 – Centres with a regional supply focus

Tier 3 – Local supply

- 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.
- Total funding **625M Euro** (2021-2030)
- Currently **8 NHR Centres**
- **Official Start 1.1.2021**

NHR Network members

- Berlin University Alliance (Zuse-Institut Berlin; ZIB)
 - Universität Göttingen (GWDG)
 - Technische Hochschule Aachen (IT Center)
 - Technische Universität Darmstadt (Hochschulrechenzentrum)
 - Technische Universität Dresden (ZIH)
 - **Universität Erlangen-Nürnberg (RRZE)**
 - Karlsruher Institut für Technologie (KIT; Steinbuch Centre for Computing)
 - Universität Paderborn (Paderborn Center for Parallel Computing)
- } „HLRN“

Application areas: Support / hardware (selection)

Atomic Structure Simulations

(Chemistry, Life Sciences, Materials Science)

- **RRZE / FAU**
- Paderborn Center for Parallel Computing
- Zuse-Institut Berlin / HLRN

Physics

- KIT
- Paderborn Center for Parallel Computing

Engineering applications

- RWTH Aachen
- TU Darmstadt
- KIT

Earth System Sciences

- ZIH
- KIT
- ZIB / HLRN



Total funding:

70M Euro for hardware,
operating costs, and personnel

Principal Investigators

- Prof. Dr. Erik Bitzek, Dept. Materials Science and Engineering
- Prof. Dr. Rainer Böckmann, Dept. of Biology
- Prof. Dr. Andreas Görling, Dept. of Chemistry and Pharmacy
- Prof. Dr. Petra Imhof, Computer Chemie Center (CCC)
- Prof. Dr. Ulrich Rüde, Dept. of Computer Science
- Prof. Dr. Heinrich Sticht, Institute of Biochemistry
- Prof. Dr. Gerhard Wellein, Dept. of Computer Science

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>

NHR@FAU Governance and Structure

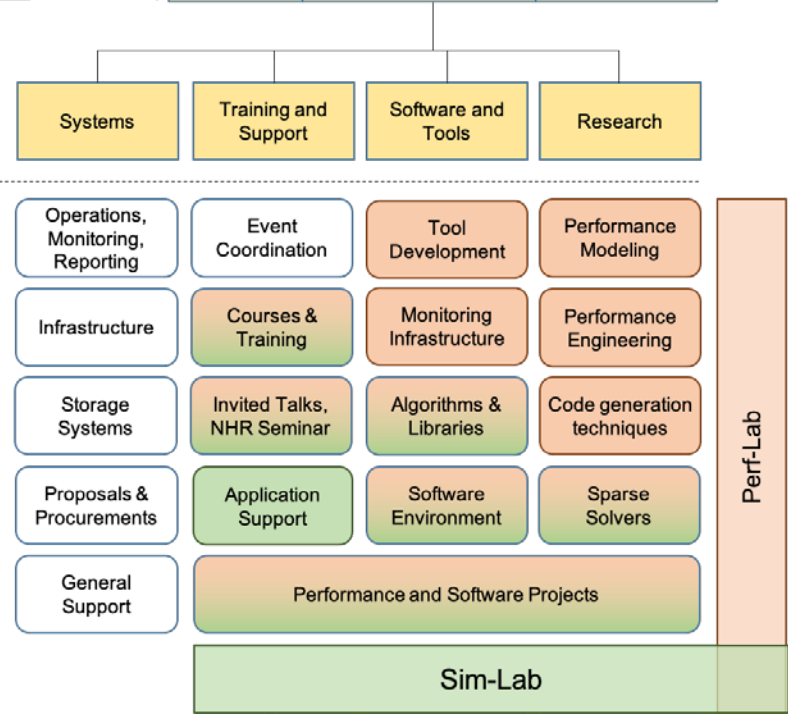
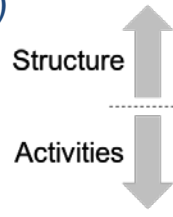


NHR@FAU will be a **standalone organisational unit** within FAU (but closely connected to RRZE)

Close collaboration of **Sim-Lab** and **Perf-Lab** with **CSC** (Competence Unit for Scientific Computing)

Scientific Review Board:
Reviews Compute projects and reports to Advisory Board: 12 – 14 members from different application areas.

There are plans to build a **new modern HPC computing centre** building in 2025+ (40+M Euro investment).



What does this mean for me?

- **FAU will maintain investments in Tier-3 systems but at lower budgets**
- **FAU Tier 3 users** with moderate compute requirements will always have **low barrier access** to a modern **HPC system**
- **No application required**
- **Tier 3 system architecture will be „coherent“ with NHR system**

What does this mean for me?

- **NEW** There will be a state of the art **Tier 2 HPC system** aimed at **atomistic simulation** codes with special capabilities for machine learning
- **NHR investments of 6-7 M€ for Tier-2 system every approx 3 years**
- The NHR systems will be **open** for **all application areas** and users from all **German academic institutions**
- **NHR will strengthen** all areas of **HPC services at FAU**
 - Support and collaborative performance projects
 - Training events
 - HPC Systems and Software environment

What does this mean for me?

- **NEW:** You need to **apply for compute time at FAU NHR system or any other NHR system**
- **Scientific quality of your project can be demonstrated by a DFG reviewed project**
- **2021/2:** There will be a central application platform for all NHR funded systems
- **FAU will accept applications from Q2/2021 for allocations in 2/2021 on our new system**

Next steps for 2021 (lets forget about 2020)

- **Establish governance and structure**



- **Build up personnel (We are hiring!)**



- **Start with training program and organize NHR Seminar**



- **You can already apply** for a NHR account in 03/2021

- We hope the **new system** will be available starting 08/2021



Ausbau der HPC-Ressourcen am RRZE

- **April 2020:** Bewilligung des Forschungsgroßgeräteantrags „Hochleistungscompute-Cluster“ über 4,5 Mio EUR durch die DFG
- **November 2020:** NHR-Förderbescheid durch die GWK
- ➔ 8 Mio EUR für die gemeinsame Beschaffung von Tier3 und NHR-System im Zuge eines „wettbewerblichen Dialogs“
- ➔ Veröffentlichung des Teilnahmewettbewerbs noch vor Weihnachten; ca. 5 Bewerber erwartet
- ➔ (teilweise) Unterbringung in der neuen NatFak-Kältezentrale, da im RRZE-Bestand der Strom (und Platz) nicht ausreicht

(künftiger) Zugang zu HPC-Systemen am RRZE

- **Tier3 (1/4 der neuen Ressourcen)**
 - wie bisher unbürokratisch für FAU & Region
- **NHR (3/4 der neuen Ressourcen)**
 - ausschließlich über einen wissenschaftlichen Antrag
 - bundesweite Nutzer
 - thematischer Schwerpunkt: „atomistische Simulationen“ und „Performance Engineering“
 - FAU & Region sind aber nicht an den thematischen Schwerpunkt gebunden

Geplante/erwartete Hardware

- **„Parallelrechner“ (2/3 des Budgets)**
 - Ca. 600 Dual-Socket Knoten mit 256 GB Hauptspeicher, schnellem Interconnect und parallelem Dateisystem; insges. über 35k Cores
- **GPGPU-Cluster (1/3 des Budgets)**
 - 32 GPGU-Knoten für Machine Learning (mi jeweils 4x Nvidia A100, lokaler NVMe Storage)
 - Ca. 64 preisoptimierte GPGPU-Knoten (Nvidia Quadro RTX?) für Molekulardynamik-Simulationen und Machine Learning Durchsatz

Inbetriebnahme für Q3/Q4 2021 geplant