Erlangen Regional Computing Center

FRIEDRICH-ALEXANDER UNIVERSITÄT ERLANGEN-NÜRNBERG

# NHR@FAU @ HPC-Café

13. Juli 2021

NHR FAU

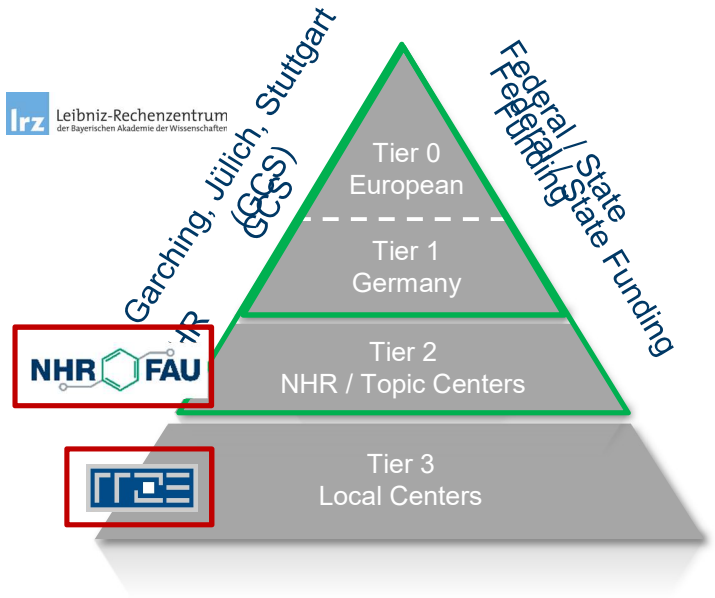
High Performance Computing

# Agenda

- Begrüßung
- Status NHR-Verbund (Gerhard Wellein)
- NHR@FAU
  - Beschaffung MEGWARE (Thomas Zeiser)
  - Antragsverfahren/Zugang zu NHR-Systemen (Gerhard Wellein)
  - Fachberater und Liaison Scientists (Harald Lanig)
- KONWIHR
  - Vorstellung der Förderlinie (Katrin Nusser)
  - Kommende Ausschreibung (Katrin Nusser)

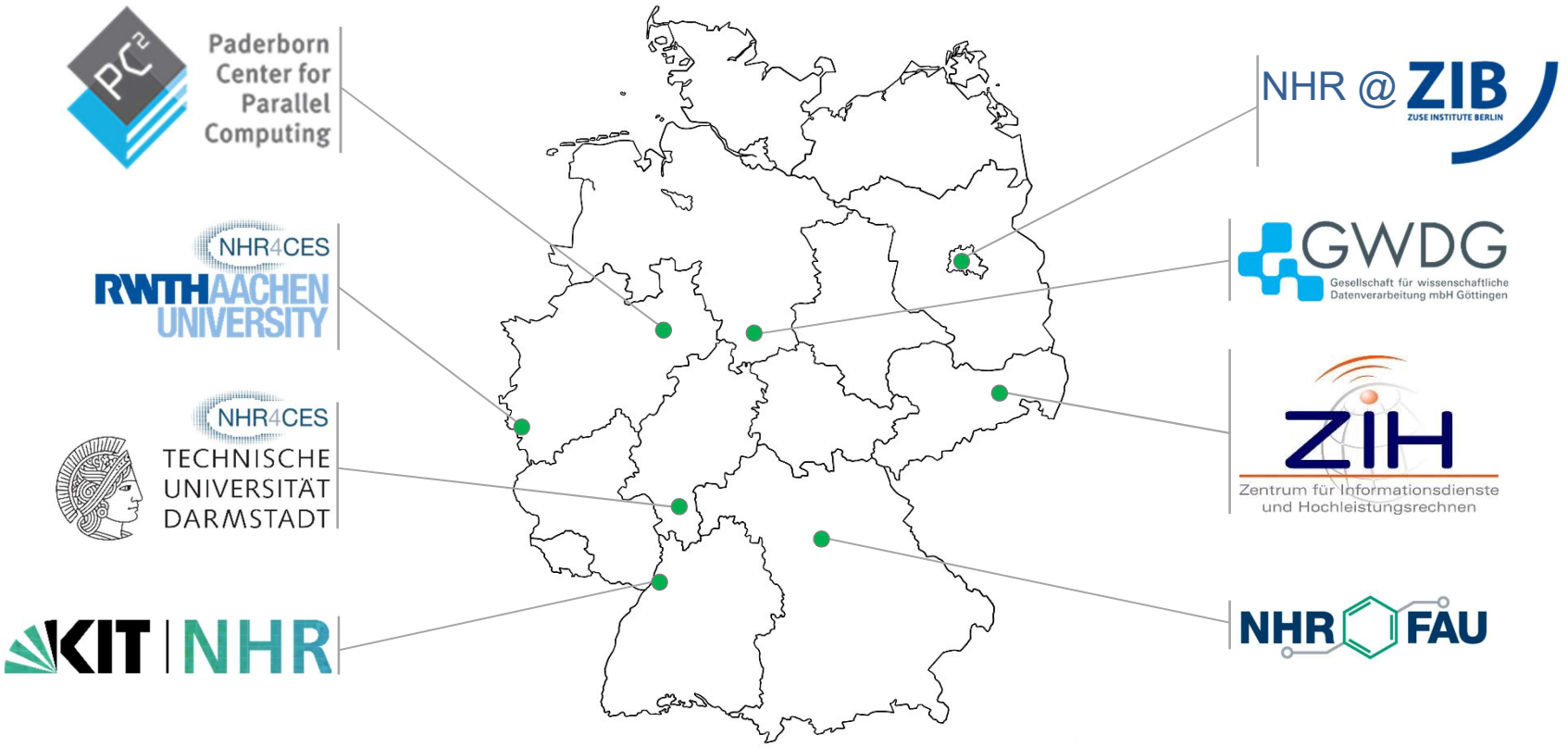
# NHR as part of HPC in Germany

**HPC Supply Pyramid**




- 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: Jan 1st, 2021**

# NHR centers – open for science & research in germany



# First NHR systems – 2021

- NHR@KIT (already installed): „Horeka“
- Univ. Paderborn (Q4/2021): „Nocuta 2“
- NHR@FAU (Q4/2021): „Fritz“ & „Alex“ ???

HoreKa

KIT | NHR
National High-Performance Computing Center

KIT
Karlsruher Institut für Technologie

* Budget: 15 Million Euro
* Peak-Performance: 17 Pflops

* Burn-In: March 2021 – Full operation: June 2021

* **Green500 Rank 13**
  Top500 EU Top 15 (HoreKa Green: #53)

* 830 kW hot water cooling with re-use
  16 PB Spectrum Scale, InfiniBand HDR

* Future Technologies Partition:
  https://www.nhr.kit.edu/userdocs/ftp/

| | Lenovo SD650 v2 | Lenovo SD650-N v2 |
|---|---|---|
| # Nodes | **570 + 32** | **167** |
| CPUs | **2x Intel „Ice Lake“** | **2x Intel „Ice Lake“** |
| Memory | **256/512 GB** | **512 GB** |
| GPUs | | **4x NVIDIA A100** |
| Interconnect | **InfiniBand HDR (200 Gbit/s)** | |

# Noctua 2 HPC System at Paderborn Center for Parallel Computing

- Atos BullSequana XH2000
- CPU partition
  - 1056 nodes, >140’000 cores, AMD Milan 7763, 2.45 GHz
  - 256 GB memory, 66 nodes with 1024GB
- GPU partition
  - 32 nodes, each with 4 Nvidia A100 GPUs (40 GB HBM2)
  - Nvlink interconnect
- FPGA partition
  - 100 FPGAs (procurement in preparation)
- Network: InfiniBand 100/200 HDR, 1:2 blocking
- Storage
  - DDN Exascaler 7990X with NVMe accelerator
  - 6PB, 60 GB/s
- Installation target: Q4/2021


new HPC center where Noctua 2 will be installed

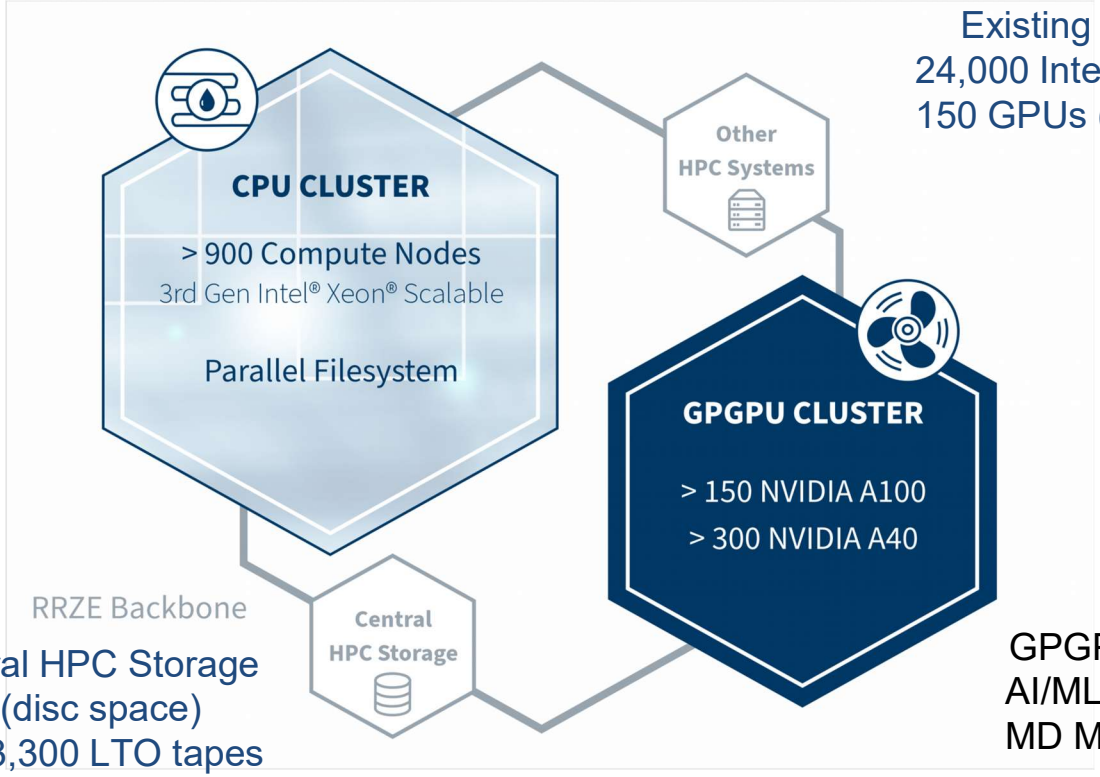
More details: https://pc2.uni-paderborn.de/go/noctua2

# NHR@FAU: New Compute Facilities 2021/2

CPU Cluster (NEW)
900+ Compute nodes
- 2 * 36 cores per node
- 256 GB per node

Parallel Filesystem
- 3+ PB
- 25+ GB/s

Direct Liquid Cooling:
> 65 KW pro Rack




Existing HPC systems
24,000 Intel cores (2 gens)
150 GPUs (5 gens)

Central HPC Storage
>2 PB (disc space)
Up to 3,300 LTO tapes

GPGPU Cluster (NEW)
AI/ML Module: A100
MD Module: A40

# Is newer / more expensive really much better?

- Gromacs on recent GPGPUs
  - standard all-atom MD simulation (protein in membrane) with explicit water (65,209 atoms in total)
  - Gromacs2019: ~134 ns/day on one RTX2080Ti
  - Gromacs2020: ~229 ns/day on the same RTX2080Ti
  - Gromacs2021: ~233 ns/day on the very same RTX2080Ti => 1.75x faster

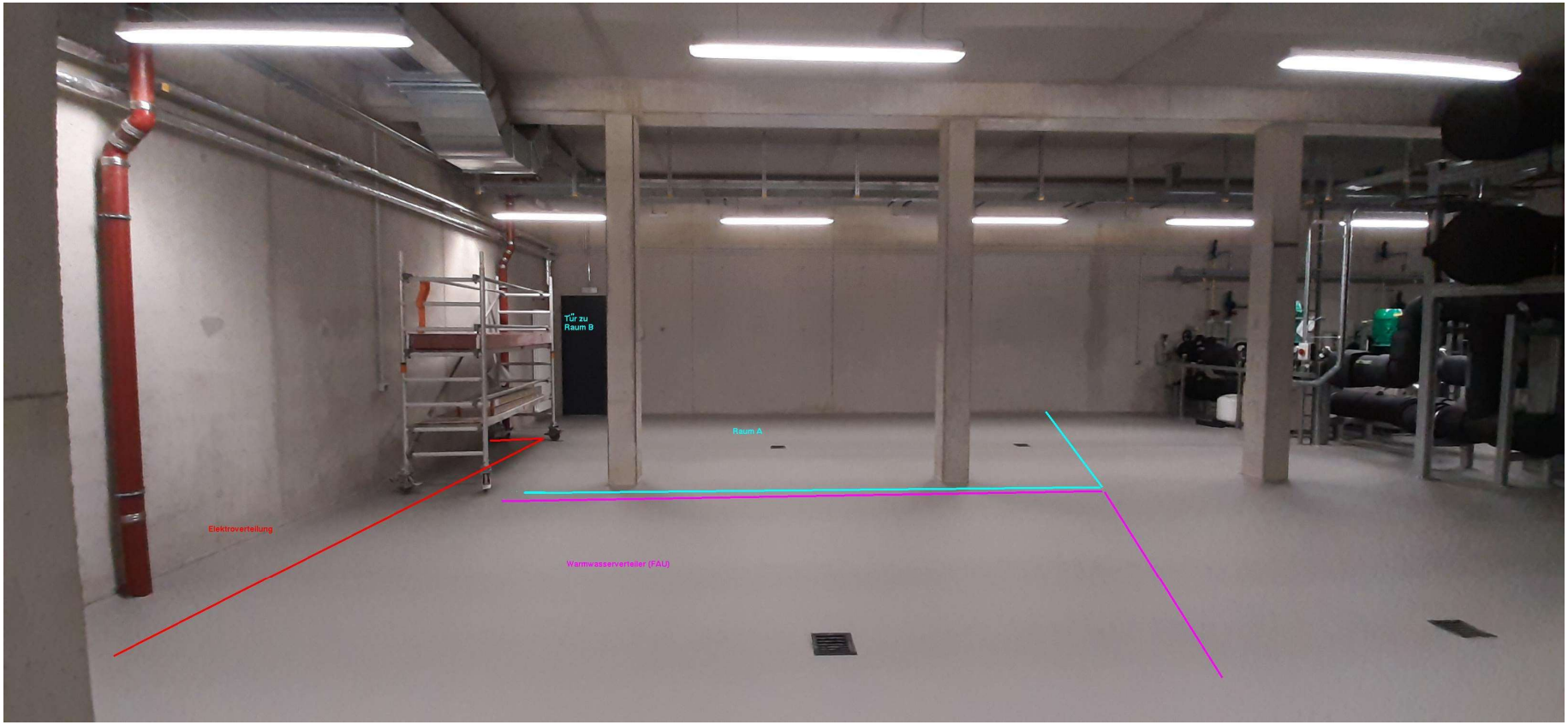
| | RTX2080Ti | RTX3080 (1.000€) | A100 (8.000€) +800% |
|---|---|---|---|
| **adhd-pme** | 223.9 ns/d | 248.5 ns/d +11% | 322.1 ns/d +44% |
| **adhd-rf** | 194.9 ns/d | 198.1 ns/d +2% | 241.1 ns/d +24% |
| rnanvt | 504.6 ns/d | 580.4 ns/d +15% | 637.4 ns/d +26% |
| JK | 167.3 ns/d | 191.2 ns/d +14% | 228.3 ns/d +36% |
| FL | 152.7 ns/d | 172.0 ns/d +13% | 174.7 ns/d +14% |
| **MEM** | 132.3 ns/d | 139.7 ns/d +6% | 153.7 ns/d +16% |

# NHR@FAU: New Compute Facilities 2021/2


- Start of operation depends on availability of materials and companies
  - GPU cluster expected to be operational for early users in Q4/2021
  - Parallel computer expected to be available for early users in very late 2021
- Operation system: based on RHEL8
- Batch system: Slurm
- Walltime limits: 24h
- Probably “workspaces” with limited lifetime instead of high watermark deletion on the parallel file system
- Postponed to 2022: fast NVMe storage for GPU cluster

- A100 nodes from TinyGPU will be integrated into the GPU partition (for faster network / storage access); thus, they will be reinstalled with “RHEL8” instead of Ubuntu 20.04

# NF-Technikzentrale: “data center” for the new parallel computer



# NHR alliance / NHR centers

- NHR centers are about to establish a legal entity „NHR Alliance“
- NHR Alliance will establish a central portal for „compute time“ applications
  - Applicants choose hosting „NHR center“
  - Application will be reviewed by „Scientific Steering Committee“ of hosting NHR center
  - Simplified review process for proposals which have been evaluated in scientific review process (e.g. by DFG)
  - Max. time: 3 months

# Compute time NHR@FAU

- Scientific Steering Committee „under construction“
- Application & Review process (GCS-)JARDS
- Accepting application from Q4/2021
- IMPORTANT: Consider NHR@FAU compute time budget already in planned / on-going third-party funding projects (DFG, EU,…)
- Please contact HPC Support for more information: hpc-support@fau.de

# HPC@FAU

- HPC4FAU (Tier-3 for FAU and region)
  - Local HPC services supply (compute + storage + know-how)
  - Low-level admission for FAU researchers and students (and “region”) (simple form, no grant application)
  - Moderate compute requirements (*“Grundversorgung”*)
  - HPC systems Meggie, Emmy, Woody, TinyXYZ + new acquisitions

- NHR@FAU – national HPC supply (Tier-2)
  - Scientific applications are reviewed by an external board (Lenkungsausschuss)
  - Open for all application areas and users from all German academic institutions
  - Thematic focus on „atomistic simulations“ & „performance engineering“ (each NHR center has a different focus)
  - Currently acquisition of CPU + GPU cluster
  - *“Projektversorgung”*

# Admission to NHR systems at FAU

- There will be a central application platform for all NHR funded systems
- Upon submission, you will be asked for your “target center”
- Application will be forwarded to your hosting center:
  - Technical reviewing by NHR@FAU coworkers
  - Scientific reviewing by board of reviewers (local and external)
  - Decision by local “Lenkungsausschuss”
- For large projects: approval by central NHR board necessary *(“zentraler NHR-Nutzungsausschuss”*)
- From application to decision: max 3 months!

# Project categories

- Test or development projects
  - Approval by local NHR center without reviewing
- Normal projects
  - Apply when you are ready, no deadlines
  - Local reviewing and approval at your target NHR center
- Large-scale projects (more than one NHR center)
  - Limits to be defined (~10 M core-hrs p.a.)
  - Application deadline every three months
  - Scientific reviewing by local reviewing board(s)
  - Approval by central NHR board (*zentraler Nutzerausschuss*)

# Normal- and large-scale projects

- Standard project timeframe
  - One year
  - Continuation application with „reduced effort“ possible
  - Grants for more than one year (e.g. coupled to third party funding) will be tested
- Scientific reviewing
  - Two reviews for each application
  - Waived when the scientific quality of your project is already proved by DFG reviewing
  - Amount of CPU time and methods reviewed by local staff
- For DFG and other big projects applications, please contact us already BEFORE submitting your proposal to the funding agency!

# Application for NHR Resources

**1. Allgemeine Angaben**

- Projektmanager = technische*r Ansprechpartner*in (nur dienstliche Kontaktdaten)
- Verantwortliche*r Wissenschaftler*in - in der Regel Professor*in, mindestens PostDoc (dienstliche Kontaktdaten)
- Institution, Bundesland
- Wissenschaftsfeld (DFG-Systematik)
- Falls Wissenschaftler*innen anderer Einrichtungen Rechnerkapazitäten dieses Projektes nutzen: Angabe des Bundeslandes
- Angaben zu HPC-Anträgen mit gleichem Thema an anderen HPC-Zentren

- * HPC-Erfahrung der am Antrag beteiligten Personen (z.B. relevante Veröffentlichungen der letzten 5 Jahre, genutzte Beratungsangebote)

* Not necessary for test projects

# Application for NHR Resources

**2. Projekt-Formalia**

- „gewünschtes Zentrum“, mögliche alternative Zentren bei Kapazitätsengpässen
- geplanter Projektzeitraum (insgesamt und mit diesem Antrag beantragter Zeitraum)
- Neu- oder Folgeprojekt (im NHR-Verbund) – wenn Folgeprojekt Projekt ID
- Projekttyp nach Größe
- bereits vorhandenes Gutachten für das Projekt (NHR-Verbund, oder externes Gutachten, z.B. BMBF, DFG)
- Angaben über Geheimhaltung/Sensibilität von Projektdaten
- Ist ein ähnlicher Antrag an anderen Rechenzentren eingereicht worden? Ggf. die Unterschiede und woanders beantragte Rechenzeit angeben

# Application for NHR Resources

**3. Technische Projektbeschreibung**

- beantragte Ressourcen
- benötigte Bibliotheken, Lizenzen
- Technische Anforderungen und Randbedingungen (Architektur, Speicherplatz, Jobgrößen, Bandbreiten, Bibliotheken, Softwarelizenzen…)
- Nennung oder Beschreibung der Software, die auf dem Hochleistungsrechner im Batchbetrieb genutzt werden soll

- * Begründung der Notwendigkeit der Nutzung von HPC-Ressourcen, inkl. Nutzungszeitplan mit Bezug zu den Projektzielen und mathematischer Abschätzung der beantragten Ressourcen
- * Nachweis der HPC-Eignung des Projektes (Skalierungsnachweis etc.)

# Application for NHR Resources

**4. Wissenschaftliche Projektbeschreibung**

- Projektübersicht (Kurzbeschreibung)

- * Stand der Forschung
- * Eigene Vorarbeiten
- * Projektziele, zu erwartender wissenschaftlicher Einfluss und Abgrenzung zu existierenden Projekten
- * Detaillierte wissenschaftliche Projektbeschreibung inkl. numerischer Methoden sowie der technischen Umsetzung
- * Projektplan mit Arbeitspaketen, inkl. wissenschaftliche, projektbasierte Begründung der Ressourcenschätzung, nachvollziehbar
- * Bibliographische Übersicht projektrelevanter Publikationen

# Application for NHR Resources

**5. Bei Folgeprojekten im NHR-Verbund**

- Darstellung der bisher im Projekt genutzten Ressourcen
- Allgemeinverständlicher Zwischenbericht (zur Veröffentlichung auf NHR-Verbund Webseite)
- Darstellung bisher erzielter Ergebnisse, z.B. durch Publikationen
- Begründung des Folgeantrags (unter Berücksichtigung des ursprünglichen Antrags)

# Application for NHR Resources

**6. Erklärungen**

- Verpflichtungserklärung in Publikationen die Nutzung der NHR-Ressourcen zu würdigen
- Datenschutzerklärung, inkl. Genehmigung zur Weitergabe der Daten an Gutachter*innen und an andere NHR-Zentren
- Erklärung, dass zum Projektabschluss ein Bericht erstellt wird

- * Bitte: Erklärung zur Bereitschaft als Gutachter*in zu fungieren und um Erlaubnis zum Eintrag in Gutachter*innen-Datenbank (mindestens Dr./PhD) – mit dazugehöriger Erklärung zum Datenschutz

**7. Optional**

- Vorschlag von Gutachter*inne*n
- Zentrumsspezifische Angaben

# NHR@FAU focus areas

**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

# Expert advisors (Fachberater) within the HPC group

- Application-specific user support and training by **Expert advisors** and **Liaison scientists** from specific disciplines
- **Tight binding** to the FAU **application scientists**

- Anna Kahler – Life Science
- Tobias Klöffel – Chemistry
- Markus Wittmann – Code optimization and SIMD vectorization
- Sebastian Kuckuk – Code generation and iterative solvers
- Ayesha Afzal – MPI/Analysis
- Thomas Gruber – LIKWID & MachineState
- Dominik Ernst – GPGPU Programming and Optimization
- *(Katrin Nusser – KONWHIR, CFD)*
- *(Johannes Veh – Physics, Storage Systems)*

# The NHR@FAU Liaison Scientist (LS) Concept

- Liaison means connection
  - NHR@FAU relies on tight **interweaving of expert science with application consulting** via liaison scientists, who can handle complex support requests
  - LS hold **shared positions** between NHR@FAU and FAU application PI groups
  - LS are affiliated to the
    - **Atomistic Structure Simulation-Lab** (PIs Bitzek, Böckmann, Görling, Imhof, Sticht)
    - **Performance-Lab** (PIs Rüde, Wellein)
  - LS provide **high-quality expert support** to NHR@FAU users
- Scientific services
  - LS involved in **teaching, training, and user support**
  - Provide **knowledge transfer** between expert research groups and NHR@FAU users by user support and training
  - LS will establish a **sustainable link** between NHR services and on-going research in relevant fields

# Liaison Scientists - Areas of Expertise

- Frank Beierlein (PI Petra Imhof)
  - Support: MD with various simulation packages
  - Training: MD first steps / combining QM with MM
- Anselm Horn (PI Heinrich Sticht)
  - Support: MolMod with AMBER (parameters, setup, performance, analysis)
  - Training: MD simulations with AMBER / introduction into parameterisation
- Sebastian Kuckuck (PI Ulrich Rüde)
  - Support: code generation, iterative solvers, C++, Scala, MPI, CUDA
  - Training: Performance engineering on GPUs / code generation for HPC

# Liaison Scientists - Areas of Expertise

- Rafael Ravedutti (PI Harald Köstler / Gerhard Wellein)
  - Support: Performance Engineering of MD codes
  - Training: Performance Engineering of MD codes
- Marius Trollmann (PI Rainer Böckmann)
  - Support: Setup and analysis on biomembrane simulation with GROMACS
  - Training: MD simulations on biomembranes / Intro on Python Programming
- Egor Trushin (PI Andreas Görling)
  - Support: VASP simulation setup and analysis
  - Training: Simulations with VASP / advanced DFT aspects