

Count on NHR@FAU for your Atomistic Simulations

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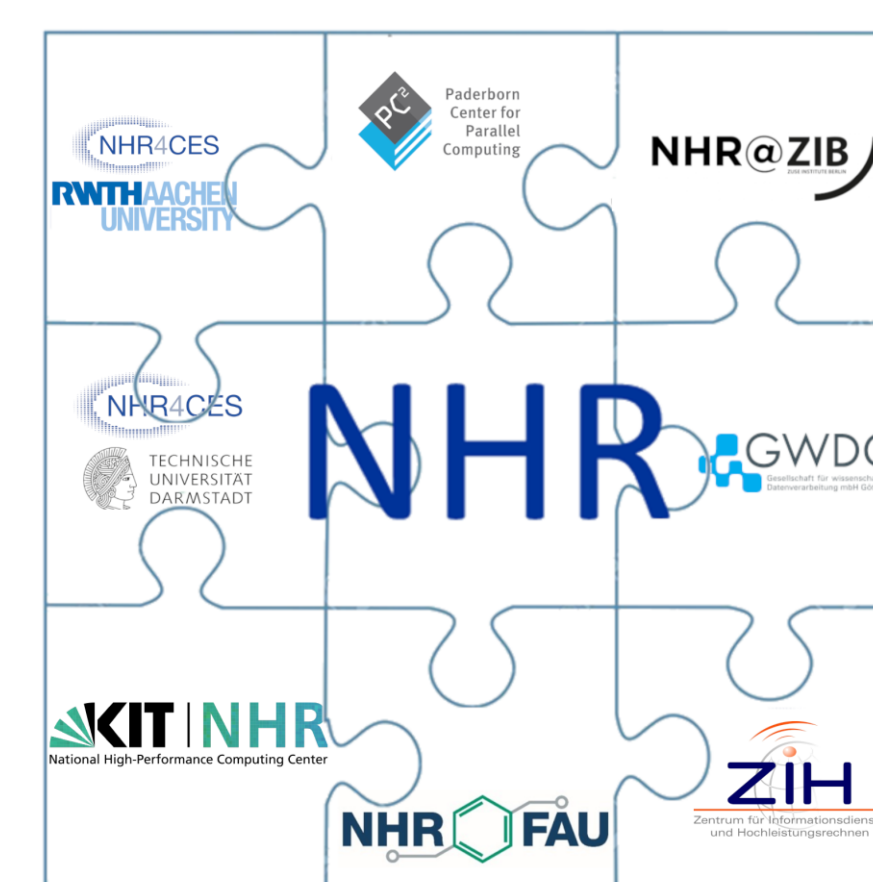
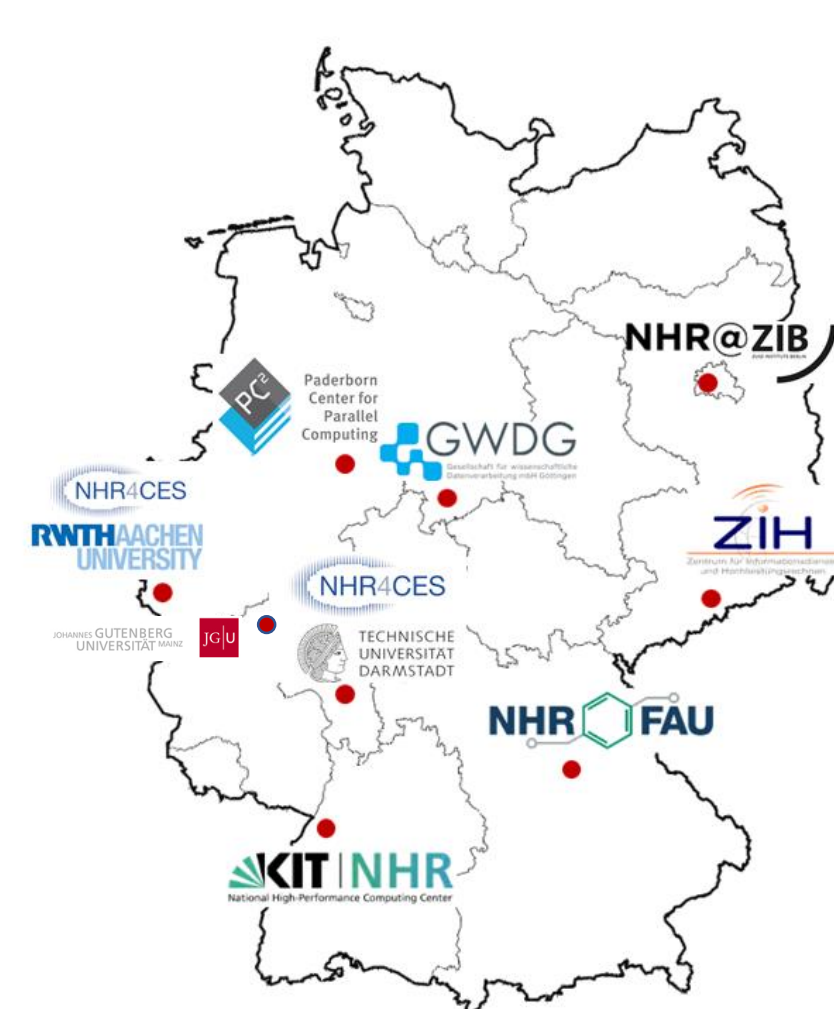
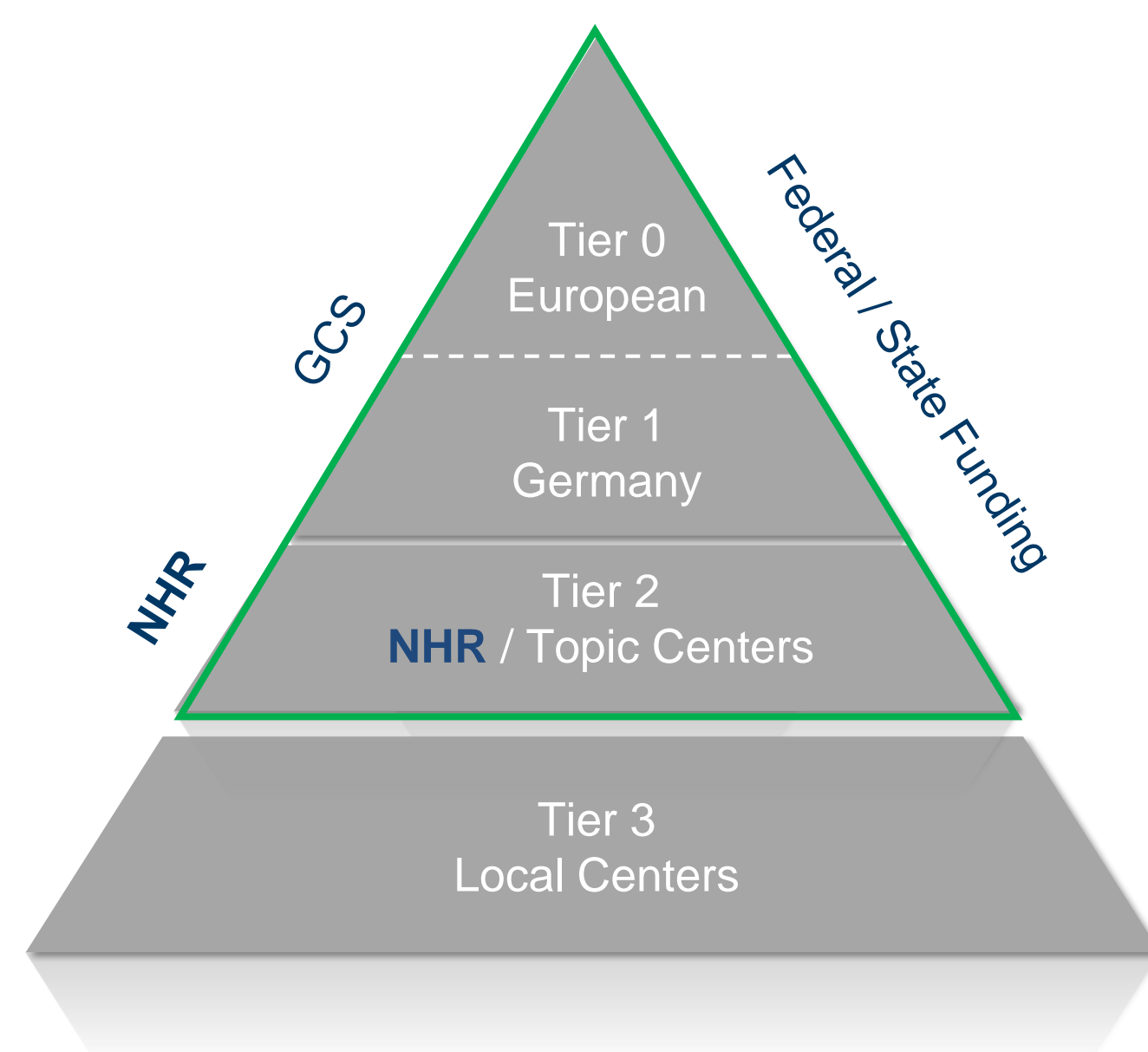
<https://hpc.fau.de>
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NHR (Nationales Hochleistungsrechnen) as Part of High Performance Computing in Germany

NHR is part of the HPC Supply Pyramid

NHR is more than the sum of the parts

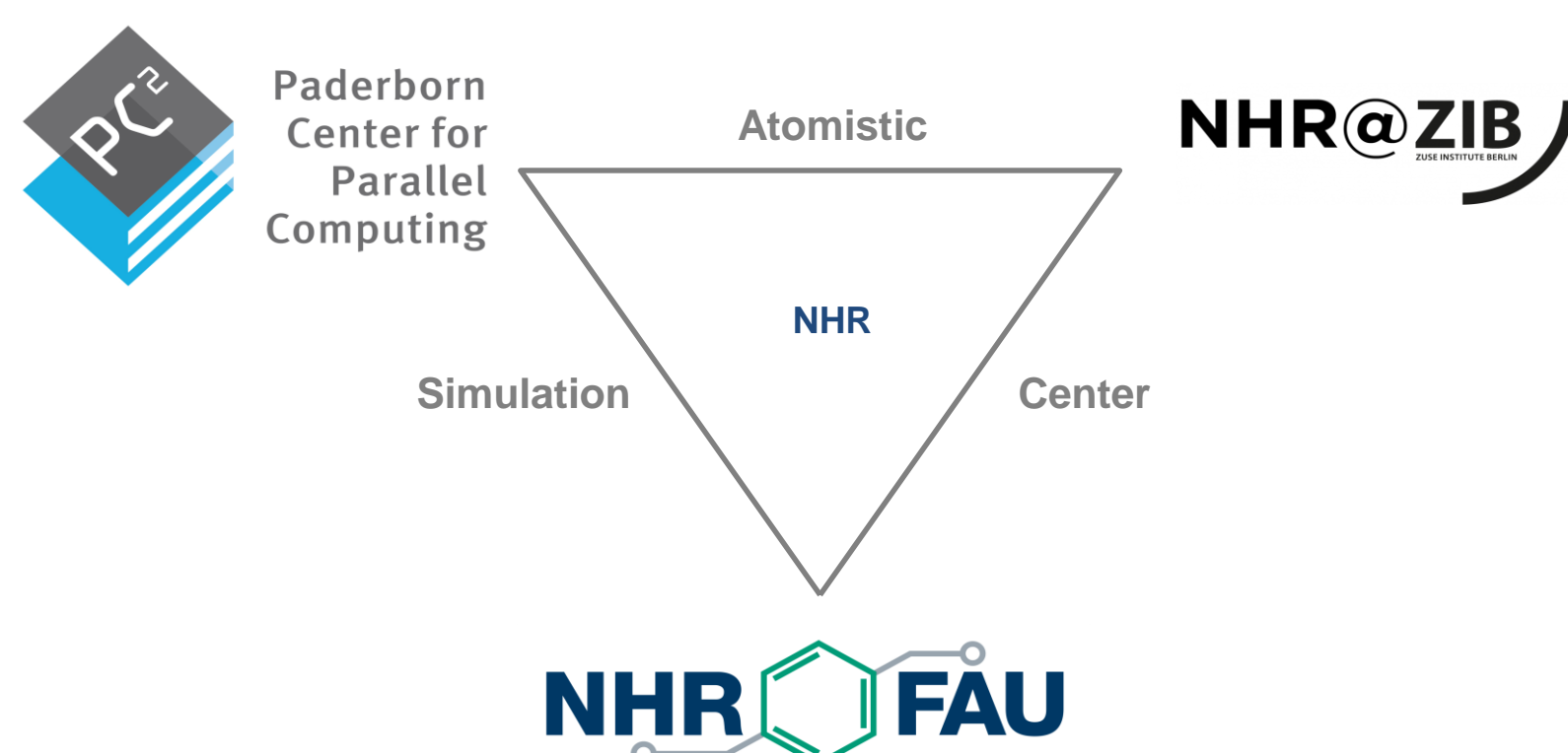


NHR Alliance (NHR-Verein e.V.)

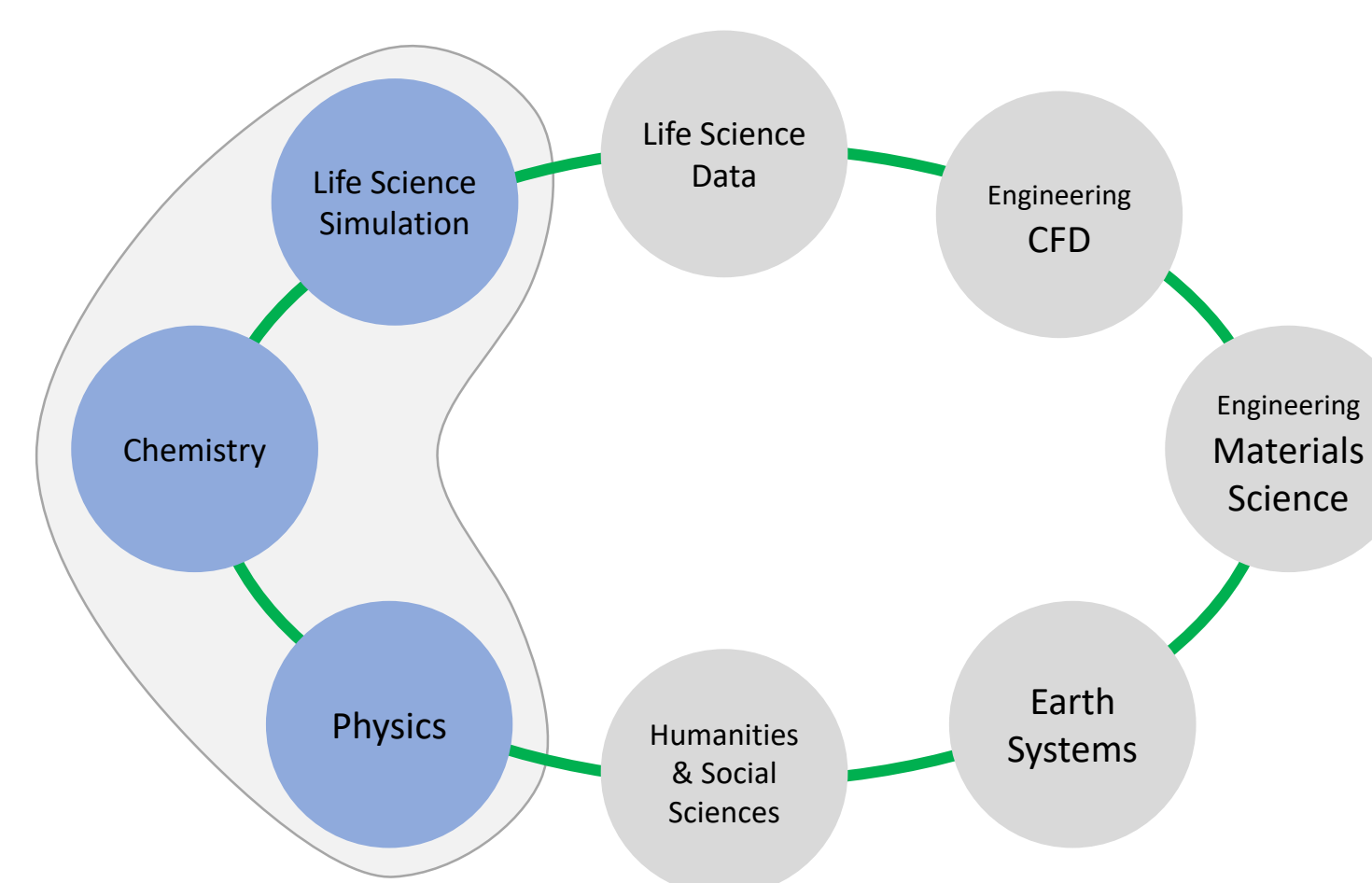
- Coordinated network of NHR centers funded by federal and state governments
- NHR-wide resource application / allocation procedure
- Training and support activities
- Strengthen methodological competences
- Collaborative NHR Future Projects
- NHR Graduate School
- www.nhr-verein.de

NHR@FAU has a strong focus on Atomistic Simulations and Performance Engineering

Atomistic Simulation Center ASC



NHR Alliance Scientific Focus Areas



MMWS2023: PROMO-NHR@FAU

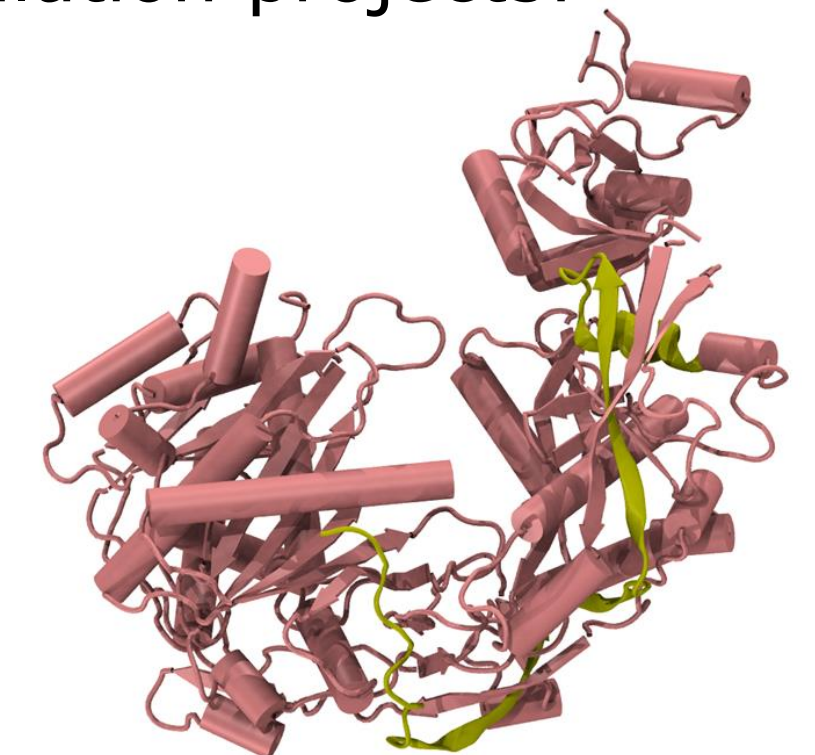
Get **free access** to NHR@FAU resources:

- 1,500 GPU-h (Alex)
- 250,000 CPU-h (Fritz)

Check out the compute clusters' feasibility for your own MD simulation projects!



Scan me



Inauguration Symposium (26/27-Oct-2021)

Recorded talks available via conference website
tiny.cc/ASC-NHR-2021

NHR@FAU Resources and how to access them

Application Focus

Atomistic simulations by Quantum mechanical (QM) and classical molecular dynamics (MD) methods for computational chemistry, life sciences, and materials science.
www.atomistic-simlab.hpc.fau.de

HPC Methodology

Node-level performance analysis, modelling, and engineering for CPUs and GPUs & effective code generation techniques.
www.perf-lab.hpc.fau.de

Access to NHR@FAU Resources

- Open to researchers at all German Universities
- Peer-reviewed application process
- Simplified procedure for projects reviewed by DFG and others
- Application by word template – portal available Q3/2023
- General user/project support available through NHR-centers
- Special project support via liaison scientists at NHR@FAU

Project type	GPU limits	CPU limits	Review	Deadlines		# Nodes	Node configuration	Storage	Typical job sizes	Peak (FP64)
Test projects	up to 3.000 GPU hours (A40 or A100)	up to 500.000 core hours	technical review	Rolling call						
Normal projects	6.000 – 60.000 GPU hours (A40) 4.000 – 40.000 GPU hours (A100)	1 – 10 mio core hours	technical + two external scientific reviews	Rolling call	CPU Fritz	992 Intel ICL (71,424 cores)	2 * 36 c (8360Y) 256 GB 1 x HDR100	Shared PFS • 3.5 PB • 80 GB/s	1 – 64 nodes	5.2 PF/s
Pre-reviewed normal projects			technical + one simplified scientific review	Rolling call	GPU Alex	35 NVIDIA A100 (280 A100)	8 * A100 2 * 64 c (AMD) 1 TB 2 x HDR200	Node local 14 TB NVMe	1 – 8 GPUs	5.0 PF/s
Large scale projects	60.000 – 180.000 GPU hours (A40) 40.000 – 120.000 GPU hours (A100)	10 – 30 mio core hours	technical + two external scientific reviews	Cut-off 1st of each quarter	GPU Alex	38 NVIDIA A40 (304 A40)	8 * A40 2 * 64 c (AMD) 0.5 TB	Node local 7 TB NVMe	1 – 8 GPUs	---

<https://hpc.fau.de/systems-services/systems-documentation-instructions/nhr-application-rules/>

Installed **Molecular Dynamics simulation codes** (working out of the box): Amber, Gromacs, LAMMPS, NAMD