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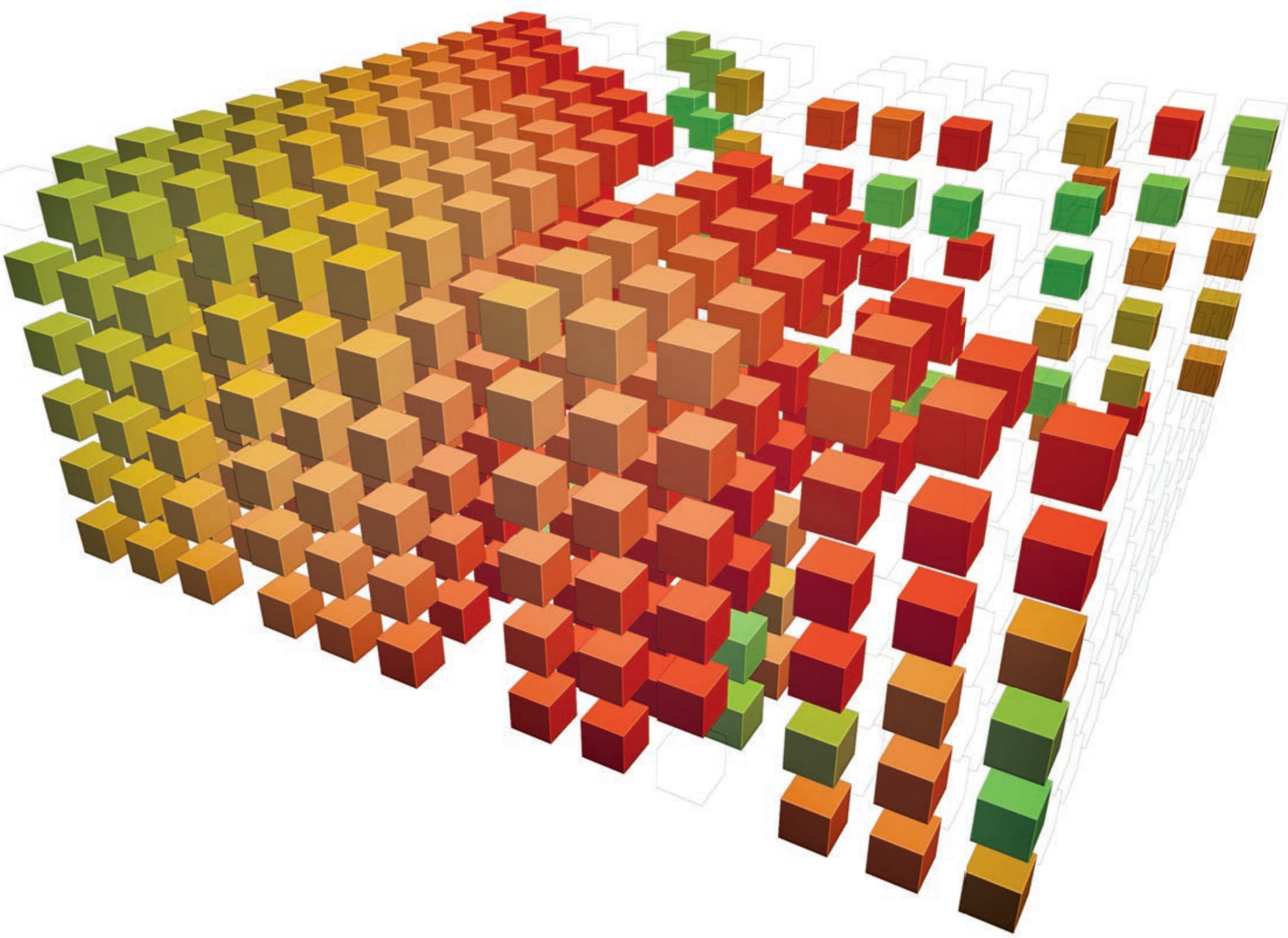

Erlangen National High Performance Computing Center (NHR@FAU)

Annual Report 2024

ANNUAL REPORT 2024

Erlangen National High Performance Computing Center (NHR@FAU)
Friedrich-Alexander-Universität Erlangen-Nürnberg (FAU)

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NHR@FAU Executive Board

Funding

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Gemeinsame Wissenschaftskonferenz GWK

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DFG Deutsche Forschungsgemeinschaft

FAU Friedrich-Alexander-Universität Erlangen-Nürnberg

Dear Reader,

"*Times are changing....*"—is perhaps an appropriate motto for our Erlangen National High-Performance Computing Center (NHR@FAU) in the past year. Originally intended as a year of consolidation and preparation for the first NHR interim report, 2024 turned out to be a year of dynamic developments. We were hit with the full momentum of rapid advances in artificial intelligence (AI) and machine learning (ML), which brought with them new tasks, user groups, and opportunities.

While working closely with our partners in the NHR Alliance we were able to consolidate and improve our national services and processes, and in September the first joint NHR interim report was submitted for evaluation. In parallel, together with our colleagues at the Leibniz Supercomputing Centre (LRZ) in Garching, we developed a concept for establishing a Bavarian AI infrastructure ("BayernKI") and began taking concrete steps toward its implementation. Thanks to substantial funding from the Free State of Bavaria for infrastructure procurement, operations, and the establishment of a joint support team, we are now in a position to firmly embed AI and ML as a key focus area within both our national and Bavarian missions. Researchers across all research funding programs may benefit, and our long-standing partnership with LRZ has been elevated to a new level.

With the installation of the "Helma" system with 384 NVIDIA H100 GPUs FAU entered the illustrious circle of the 100 fastest supercomputers in the world for the first time, achieving 79th place in the Top500 list as of November 2024. In addition, expansion plans are already underway: A further 384 NVIDIA H200 GPUs, funded entirely through Bavarian AI initiatives, have been commissioned for 2025. At the same time, we began to build a dedicated support team for AI applications in 2024, greatly benefiting from FAU's well-programs and broad research activities in AI and ML.

As you can see, 2024 was a year of significant growth and diversification in both our user base and areas of focus. At the same time, we excelled once again in our core competencies of atomistic simulations

Prof. Dr. Gerhard Wellein,
NHR@FAU Director

and performance engineering. This was clearly reflected in the second NHR user survey, where we received consistently excellent ratings. Strengthening the proven while advancing the new: Fittingly, preparations for the construction of the new Northern Bavarian High-Performance Computing Center also progressed on schedule throughout 2024.

It is also a pleasure to see that our activities are highly appreciated by the academic community. More than 150 national projects were active in 2024 and 85 new NHR applications have been accepted. In addition, BayernKI has gained traction before the delivery of the first dedicated hardware, and we could already welcome and help almost 20 new Bavarian user groups.

I would like to extend my sincere thanks to all staff members and our partners who contributed to these achievements in 2024 with outstanding expertise and personal dedication. This 2024 Annual Report aims to provide a comprehensive overview of our joint efforts. To begin, I would like to briefly highlight a few of the most notable achievements from our four departments.

Our *Systems & Services* division has achieved a very stable operation of the systems, which have encountered strong user demands. As already highlighted, the team has installed an internationally visible GPU cluster together with our partner MEGWARE and has performed a procurement to obtain a system of similar size in Q2/2025. Another hot topic in 2024 was the optimization of our storage environment, which was originally designed for classic HPC applications and has been challenged by the diametrical requirements of the AI/ML communities. The first steps towards the incorporation of new powerful hardware and software concepts have been taken and the foundation was laid to structurally adapt the storage environment to the new demands of the AI/ML user community.

The *Training & Support* division has again advanced and strengthened its internationally renowned training program in several dimensions: Our new tutorial on *Performance Engineering for Linear Solvers*, jointly developed with colleagues from TU Munich and TU Delft has been presented at the ISC24 and SC24 conferences, which both have a competitive acceptance process for tutorials. We further continued to improve the quality of existing courses, e.g., by doing a complete makeover of our OpenMP course into a JuypterHub-based format. In addition, another NVIDIA Deep Learning Institute (DLI) training certification has been established for a course on OpenACC programming, now totaling five DLI-certified courses. eyond our regular events, we have also started to offer selected DLI trainings to the EUMaster4HPC program, in which FAU is the only degree-granting university in Germany. From this EU-wide master's program on HPC, the first student started his thesis work at our center in 2024. In addition, the user support team was again heavily involved in consulting the researchers at all stages of their compute-time projects.

The *Software & Tools* division develops, maintains, and supports tools and software for HPC. In 2024, our flagship *LIKWID* tool suite and the OSACA code analyzer have been adapted to the latest AMD and Intel CPU architectures and to the NVIDIA Grace chip. A new tool for retrieving and manipulating system settings was added, substantially expanding the capability of LIKWID. Our in-house HPC account management software, the HPC-Portal, was significantly improved in 2024. It is now fully operational and has received positive feedback and new feature requests from its users. ClusterCockpit (CC), our cluster-wide, job-specific performance and energy monitoring framework, has been further extended. It is a central component in the NHR@FAU-lead BMBF Green-HPC project EE-HPC. Critical new applications of CC for global job-specific power optimization and node settings were developed in 2024. ClusterCockpit is already in use at several major HPC centers in Germany, with many more centers considering its deployment. To continue maintaining and developing our popular Open-Source software products, we were happy to welcome new colleagues to our team in 2024.

The HPC *Research* division pools scientific activities at FAU related to the HPC focus topics of NHR@FAU. PhD students funded by third-party projects are currently pursuing research in the fields of performance modeling, hardware-efficient sparse solvers, or automatic code generation. They are also currently involved in two BMBF SCALEXA projects (*DAREXA* and *StroemungsRaum*). In 2024 we have further strengthened our efforts in the areas of performance, communication, power, and energy modeling with the aim of supporting sustainable computing environments. Several scientific contributions have been published, including a Best Research Poster finalist at SC24. In addition, our work on recursive algebraic coloring techniques for hardware-efficient sparse matrix operations was honored with the *SIAM Activity Group* on *Supercomputing Best Paper Prize*.

"*... and we change in them*"—I am pleased to see that my colleagues at NHR@FAU have met the challenges of the past year, exceeding expectations across the board. We have further developed our center to meet current and future needs in services, training, and research. I am full of confidence that we will continue to facilitate world-leading research in the years to come, despite a dynamic and challenging environment.

Gerhard Wellein
on behalf of the NHR@FAU Executive Board

1 NHR@FAU AT A GLANCE

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1.1 Organization

High performance computing (HPC) has been a key research priority at the Friedrich-Alexander-Universität Erlangen-Nürnberg (FAU). The use of HPC is pivotal to numerous research activities across all faculties; FAU's HPC-related research and teaching/training efforts are recognized internationally, and FAU has continuously developed its HPC infrastructure. In recent years, AI/ML has evolved as another focus topic both at FAU and NHR@FAU.

In 2021, FAU could establish the Erlangen National High Performance Computing Center (NHR@FAU) as one out of nine national centers for HPC (NHR centers) at German universities. The NHR centers receive federal and state funding, and their services are open to all German universities. NHR@FAU closely collaborates and coordinates with the other NHR centers; they jointly operate the *NHR Alliance* (NHR-Verein). Besides fostering coordination and collaboration of the NHR centers, the NHR Alliance also supports the scientific computing and HPC-related research, e.g., by running the *NHR Graduate School.*

Complementing its national duties, NHR@FAU is also responsible for FAU's local infrastructure and services for HPC and AI/ML. These offerings, which were provided by Erlangen Regional Computing Center (RRZE) before 2021, are open to FAU researchers (and the regional RRZE-supported universities) only. Despite being a separate organization within FAU, the NHR@FAU closely collaborates with RRZE in many ways, most notably in the areas of infrastructure maintenance and development, system administration, networks, and Identity Management.

NHR@FAU is a pillar of the HPC activities in the Free State of Bavaria and collaborates closely with the *Leibniz Supercomputing Centre* (LRZ) of the Bavarian Academy of Sciences. It hosts one of the two offices of the *Competence Network for Scientific High Performance Computing* (KONWIHR) in Bavaria. Within KONWIHR, NHR@FAU and LRZ support scientists at Bavarian universities to exploit the potential of the massive computational power available.

NHR@FAU also operates the BayernKI infrastructure jointly with the LRZ. BayernKI is open to all researchers at universities of the Free State of Bavaria and offers a broad spectrum of support and training opportunities.

Reflecting its national (Tier-2), Bavarian, and local (Tier-3) HPC/AI/ML service activities, NHR@FAU receives annual funding from the NHR program, the Free State of Bavaria, and the FAU.

The organizational concept of NHR@FAU covers HPC across all involved fields, including HPC infrastructure design and operation, user support from level one to in-depth collaborations with developers and application scientists, HPC training, HPC research, and application expertise. NHR@FAU aims to be the focal point of FAU's HPC activities to provide high-quality application and user support, up-to-date training and teaching offerings, and efficient and reliable compute capabilities to our users from Erlangen and all over Germany.

1.2 Executive Board, Divisions & Steering Committee

The NHR@FAU director holds the professorship for HPC at the Department of Computer Science and was the lead *principal investigator* (PI) of the NHR@FAU proposal. Together with the other PIs and the technical director of RRZE, the center director forms the NHR@FAU *Executive Board* (see Figure 1.1), which meets regularly to discuss system operations, support and training activities, and budget planning.

NHR@FAU has four divisions: *Systems & Services, Training & Support, Software & Tools,* and *Research*. The research-oriented structure of the center is further supported by a group of *Liaison Scientists,* who establish a sustainable link between NHR services and ongoing research at FAU on the key focus topics of NHR@FAU. The NHR@FAU *Scientific Steering Committee* is responsible for the peer-review-based resource application and allocation process within the NHR funding framework. It is supported by NHR@FAU administrative office and closely coordinates with the executive board and systems administration as well as support activities.

1.3 Services

The main application topics covered by NHR@FAU are in the fields of atomistic simulations and Artificial Intelligence/Machine Learning (AI/ML). FAU's exceptional research profile and its broad application competencies build the foundation for center's activities. NHR@FAU runs an experienced support team which provides specialized user consulting and expert support in the application-focus topics. In atomistic simulations the full spectrum of classical and quantum-mechanical atomistic simulation methods and the most popular application codes can be supported. Large Language Models and Computer Vision are key competencies of NHR@FAU in the field of AI/ML.

The main HPC methodology focus is on node-level performance engineering for CPUs and GPGPUs. The internationally recognized model-driven performance engineering (PE) approach is the foundation

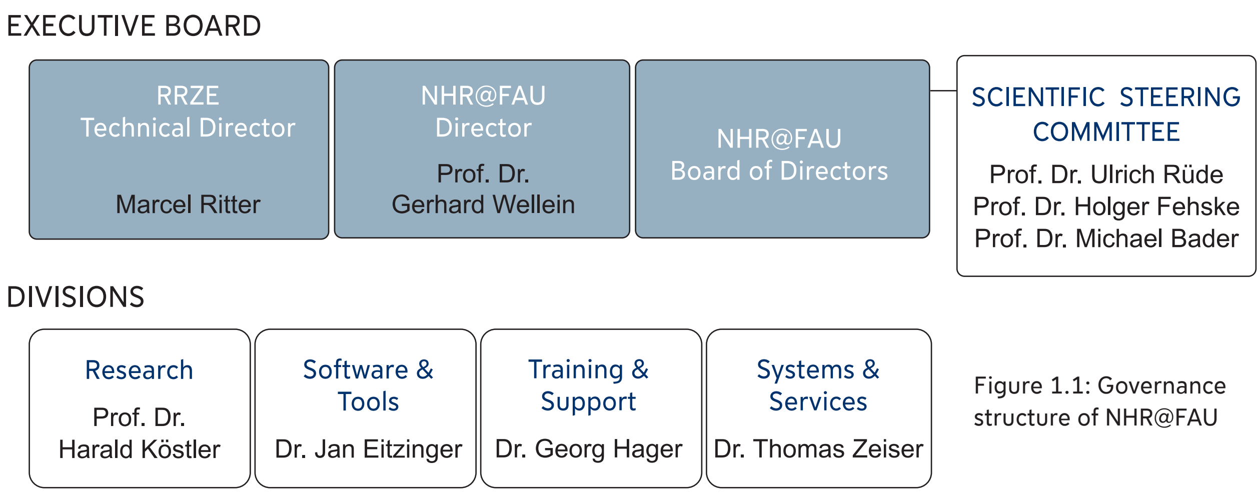


Figure 1.1: Governance structure of NHR@FAU

of performance-related research, user consulting, training, performance monitoring, and all aspects of code optimization and parallelization. Research topics comprise novel performance models, PE concepts, efficient CPU/GPGPU implementation strategies, automatic generation of hardware-efficient codes, and micro-architectural analysis and benchmarking. The PE approach is applicable to a broad range of application fields. These activities are complemented by the development and maintenance of performance tools that support node-level PE.

Continuous job performance monitoring of relevant resource metrics like bandwidths, flop rates, network traffic, I/O utilization, is implemented at NHR@FAU via the job-specific monitoring framework *ClusterCockpit*. In addition, the widely used *LIKWID* tool suite is instrumental in PE activities and a pivotal component in monitoring solutions. NHR@FAU continues to develop and adapt LIKWID to future CPU and GPGPU architectures. LIKWID support is provided as a service to the NHR Alliance and the entire HPC community.

Numerical methods for simulations are focused on scalable iterative solvers, where FAU already had expertise on scalable hardware-efficient sparse solvers, modern matrix-free finite element multigrid methods, and lattice-Boltzmann solvers, including work on adaptive parallel mesh refinement with advanced mesh generation, load balancing, and visualization strategies. The work at NHR@FAU stands out because it integrates the whole method stack ranging from modeling to the hardware-aware and highly optimized implementations for extreme-scale computing on heterogeneous architectures. NHR@FAU has broad experience with building sustainable HPC software and is leading in code generation techniques, where efficient parallel codes are automatically generated from abstract specifications.

Algorithmic user support is offered for these numerical methods, and expert support and training is provided in two directions: (1) manual implementation or automatic generation of hardware-efficient kernels and solvers for CPUs and GPGPUs and (2) defining and implementing maintainable and flexible numerical algorithms and libraries for full-scale applications. An important goal is to foster a software ecosystem of portable and inter-operable applications and libraries for the German HPC community.

NHR@FAU'S
INTERDISCIPLINARY TEAM

operates **state-of-the-art supercomputers**

offers in-depth **user & specialized application support**

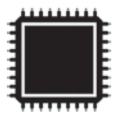
offers dedicated **AI support & a related training program**

provides HPC-related **lectures, tutorials, & training**

develops **performance tools**

NHR@FAU'S
EXPERTISE & RESEARCH includes

node-level performance engineering for CPUs & GPUs



hardware-efficient & scalable **building blocks for sparse solvers**

atomistic simulations in all fields of science

arti cial intelligence & **machine learning**

2 NHR@FAU USAGE REPORT

2 NHR@FAU USAGE REPORT

NHR@FAU Scientific Steering Committee:
Prof. Dr. Michael Bader,
Prof. Dr. Ulrich Rüde,
Prof. Dr. Holger Fehske (f.l.t.r.)

The scientific steering committee of NHR@FAU comprises supercomputing experts from within and outside FAU. The committee advises the NHR@FAU management, and is responsible for important decisions concerning the compute time application process. This includes setting guidelines for the allocation of resources, decisions on accounting formalities, approval of requested resources, and participation in the procurement of hardware and software.

The NHR@FAU scientific steering committee currently consists of the chairperson Prof. Dr. Ulrich Rüde from the Department of Computer Science at FAU, Prof. Dr. Michael Bader from the School of Computation, Information, and Technology at the Technical University of Munich, and Prof. emeritus Dr. Holger Fehske from the Institute of Physics at the University of Greifswald.

2.1 Compute Time Applications

Scientists from German universities are able to gain access to NHR@FAU's resources by submitting a scientific application for compute time.

Project applications can be submitted in different categories. We differentiate test, normal, and large-scale applications, as specified by the NHR Alliance. Starting with call Q3/2024, the *Joint Application, Review and Dispatch Service* (JARDS) is used NHR wide for the application of large-scale projects and has now been extended to all applications. The NHR@FAU steering committee decides on the assignment of expert consultants and on the final allocation of approved resources for all project types.

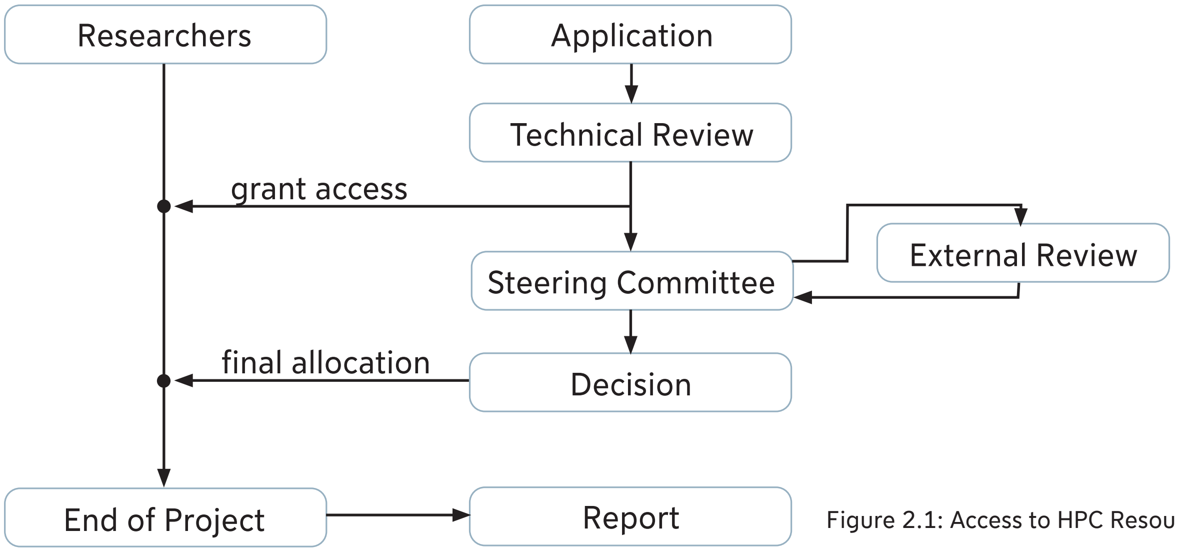


Figure 2.1: Access to HPC Resources

For large-scale projects, the NHR@FAU steering committee makes a recommendation, which is then decided upon quarterly by the central NHR steering committee. The scheme shown in Figure 2.1 summarizes the general application workflow, including the tasks of the steering committee.

Applications for test and normal projects can be submitted at any time. Large-scale project applications are collected on a quarterly basis and are presented in four committee meetings to be decided upon. Test and normal projects are generally able to start using the compute resources within a fortnight and are fully approved within four to six weeks.

Besides the involvement in the application and reviewing process, the local steering committee also supports the NHR@FAU expert advisors in their various activities, such as application porting and optimization. This helps to identify problems in an early phase of the project, far before the first progress report will be available.

2.2 Project Statistics

In the reporting year 2024, a total of 73 normal project and twelve large-scale project applications were received and approved by the local steering committee. Within these project categories, a total of 440.5 million CPU core-hours and 3.75 million GPGPU-hours were awarded.

Of the 85 normal and large-scale project applications approved in the reporting year, 70 came from Bavaria, which corresponds to a share of 82%. A total of 36 applications were received from FAU, as shown in Figure 2.2 below. The remaining 15 applications were spread among nine federal states.

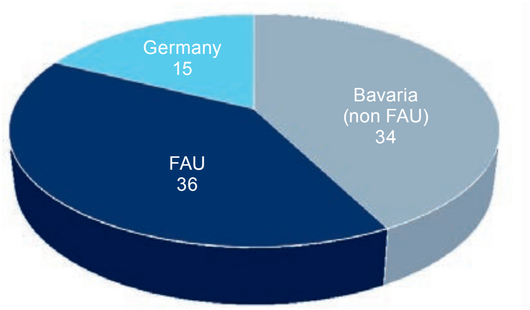


Figure 2.2: Origin of NHR@FAU 2024 approved projects: Geographical distribution of the 85 normal and large-scale NHR compute time projects.

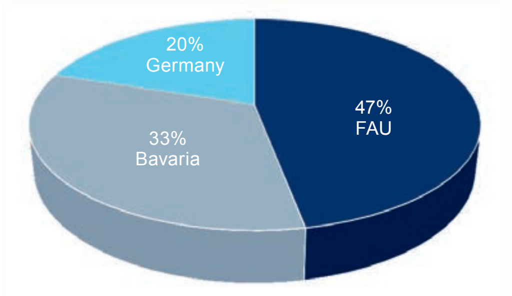


Figure 2.3: Geographical distribution of the CPU core hours awarded to NHR projects in 2024.

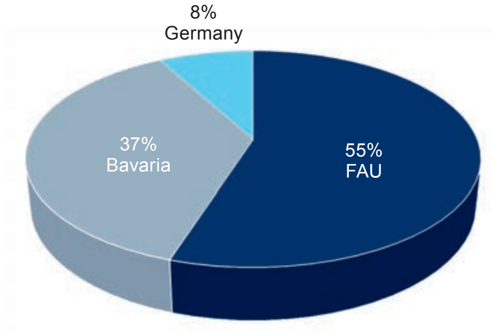


Figure 2.4: Geographical distribution of the GPGPU hours awarded to NHR projects in 2024.

This distribution is consistent with the amount of awarded CPU core hours, as shown in Figure 2.3 (see above). About 47 percent of the CPU resources are assigned to projects from FAU, dominated by atomistic simulation codes for quantum and classical mechanics. 33 percent of the awarded CPU core hours go to other institutions in Bavaria, and 20 percent to institutions in other federal states.

The picture sligthly changes when looking at the distribution of awarded GPGPU hours (see Figure 2.4). Now, 55 percent of these resources were assigned to FAU projects, focussing on artificial intelligence and deep learning topics. In contrast, the GPGPU demand of projects from other federal states decreases to only eight percent.

For testing or porting user-written applications to our NHR systems and for improving performance, researchers can apply for dedicated projects with limited resources via a simplified procedure. These test projects, which only require a technical review, usually serve to prepare a regular NHR application. In the reporting year, 12 working groups made use of this option.

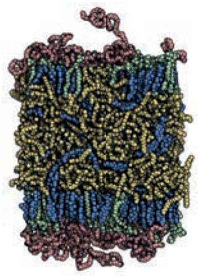
2.3 Resource Usage

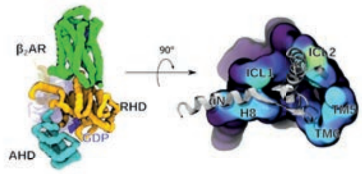
After extensive installation measures and stability tests on both the Fritz and Alex systems in the first two quarters of 2022, regular NHR@FAU user operations started in the third quarter of 2022. In the year 2023, a total of 452 mio CPU core-h and 1.86 mio GPGPU-h were used for NHR projects. Note that the high CPU usage is also caused by the availability of additional Sapphire Rapids nodes with large main memory, which entered production in Q3/2023.

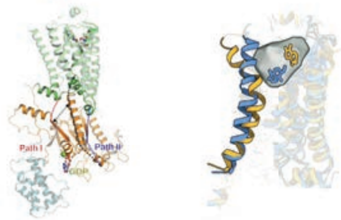
Table 2.1 (see below) presents an overview of available resources for NHR projects at NHR@FAU and their actual utilization in 2024. Both CPU and GPGPU utilization were remarkably high throughout

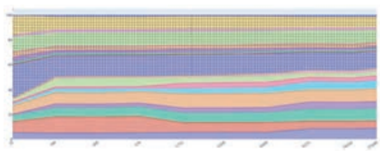
2024	CPU CLUSTER *FRITZ* [mio h]				GPU CLUSTER *ALEX* [mio h]			
	compute nodes	core hours available	core hours used	% usage	GPUs	GPU hours available	GPU hours used	% usage
Q1	812	120.3	116.9	97	462	0.92	0.54	59
Q2	812	120.3	93.5	78	462	0.92	0.69	75
Q3	812	120.3	99.0	82	462	0.92	0.75	82
Q4	812	120.3	97.0	81	462	0.92	0.72	78
total		481.2	406.4			3.68	2.70	

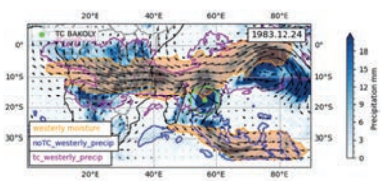
Table 2.1: Overview of available and used resources for NHR projects at NHR@FAU in 2024.

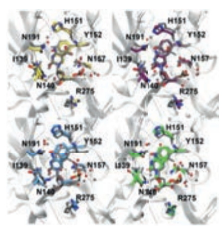












the year. The decrease in CPU usage of about 46 mio core-h compared to 2023 was caused by completion of several large-scale projects. On the other hand, we see an increase in projects requiring GPGPU resources, leading to an additional consumption of 840k GPU hours in 2024. The overall system availability was always satisfactory, achieving values beyond 90 percent.

Figure 2.5 (see below) shows the usage of NHR@FAU's systems in 2024, broken down according to the origin of the application and the research discipline indicated by the applicant, respectively. Test projects were not included. The distribution of the research areas addressed by the applications has not changed significantly compared to 2023. Also in 2024, it clearly shows a focus on life sciences, physics, and chemistry. This maps perfectly to the scientific focus of NHR@FAU, namely atomistic simulations and their use in these areas. Additionally, there is a significant and increasing number of projects applying machine learning techniques, which attests to the current attractiveness of AI-related topics such as image classification, segmentation, large language models, and deep learning.

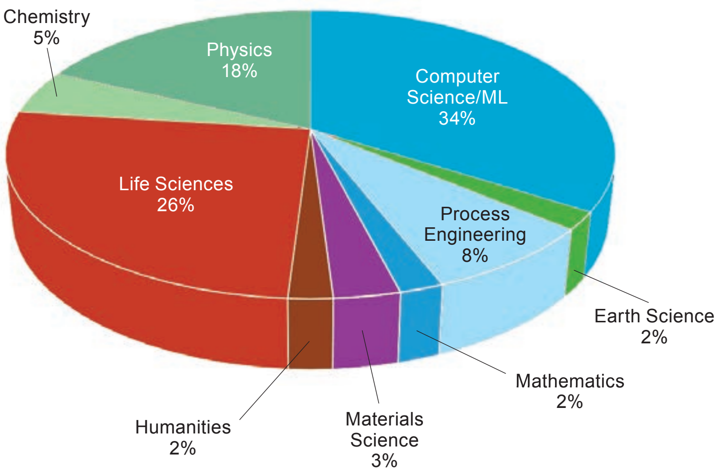


Figure 2.5: Distribution of project research areas of NHR@FAU systems among scientific disciplines in 2024.

Projects active at NHR@FAU in 2024

A list of projects that were actively using the NHR@FAU resources in 2024 is provided in the Appendix (see Chapter 8, page 69).

3 SYSTEMS & SERVICES

3 SYSTEMS & SERVICES

Division head:
Dr. Thomas Zeiser

The *Systems & Services* division at NHR@FAU is responsible for operation of the HPC systems, including procurement and software installation, as well as the required infrastructure, including power and cooling. Many support activities are also carried out or supported by the Systems & Services division. The facility team within the Systems & Services division not only takes care of the current infrastructure but also drives the planning of a new data center building to be completed before the end of the decade.

RRZE has been operating Linux-based HPC clusters as Tier-3 compute resources for users of FAU and regional customers of RRZE since 2003. Centralization of HPC systems and services has been well accepted and the HPC team grew over time. With the inception of NHR@FAU in January 2021, the next level has been reached and all HPC activities and existing systems were technically taken over by NHR@FAU while still relying on the basic services of RRZE. For the Tier-3 operation of the HPC systems and services, dedicated funding is available. However, synergies of NHR and Tier-3 will be exploited wherever possible—including, but not limited to the joint procurement and operation of systems and services. End of 2023, the next step has been started: together with LRZ, NHR@FAU has started to provide basic AI infrastructure “BayernKI” for members of all Bavarian universities and Bavarian Universities of Applied Sciences.

An overview of HPC compute systems, as well as the available architectures and some notable highlights are shown in Table 3.1 on page 19.

From the users’ perspective, there have not been many highlights from the Systems & Services division in 2024. The operation of *Alex* (GPGPU cluster) and *Fritz* (parallel computer) and all other systems was stable with again only minor shortcomings in the storage area. Some new architectures (NVIDIA L4, NVIDIA L40, and NVIDIA L40S GPGPUs; 4-way AMD MI300A GPGPU system, 8-way AMD MI300X GPGPU system; NVIDIA Grace Superchip (2x 72 cores); Dual AMD EPYC 9754 “Bergamo” CPU (2x 128 cores + SMT) @ 2.25GHz; Dual AMD EPYC 9684X “GenoaX” CPU (2x 96 cores) @ 2.55GHz; Dual Intel Xeon “SapphireRapids” Platinum 8470 CPU (2x 52 cores + SMT) @ 2.0GHz) have also been added to the *Testcluster*.

The main activities continued in the background: The next procurement round has already been started in spring last year (2023), and the contract has been signed at the end of 2023. In spring 2024, a second procurement round started for a Bavarian extension of the yet-to-be-provided system. In parallel, infrastructure work was going on in the Kältezentrale. The direct warm-water-cooled H100 nodes of the GPU part of the new HPC system called “Helma” have been delivered in late 2024, and the first early adopters could successfully test the new nodes over winter break. The CPU-only parallel computer is delayed until the second half of 2025 while we hope that the NVMe storage system will already arrive in the first half of 2025.

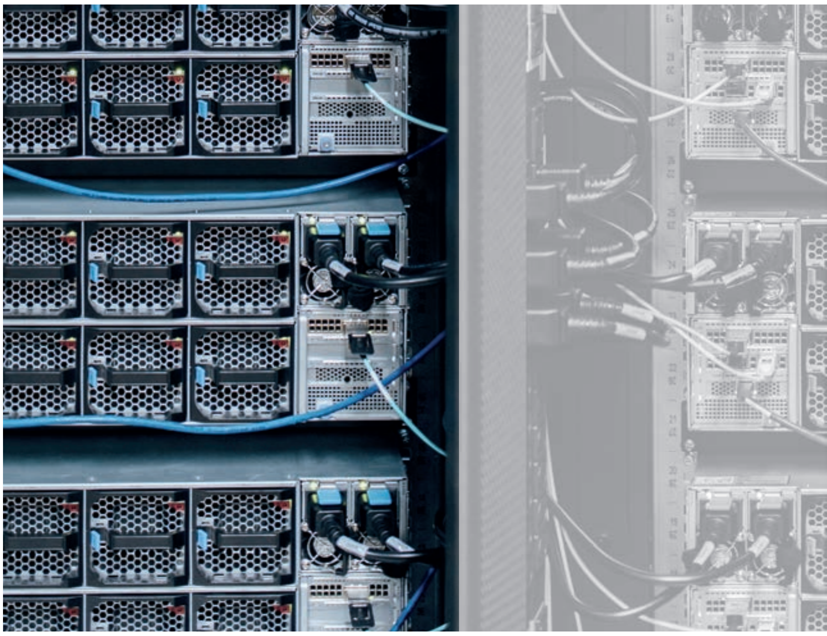


Table 3.1: Overview of the HPC compute systems of NHR@FAU. Tier-2 systems (NHR) are accessible through then NHR application process while Tier-3 systems (FAU) are accessible by researchers from FAU without NHR application.

	SYSTEM	ARCHITECTURE	RESOURCE	ACCESS	HIGHLIGHT
2024	Helma	NVIDIA H100 NDR200-IB	384 GPGPUs	BayernKI, NHR, FAU + 4 other univ.	Top500 11/2024 #79
	Fritz	Intel Ice Lake HDR100-IB	≈ 78,000 cores	NHR FAU	Top500 11/2024 #281
	Alex	NVIDIA A40/100 partially HDR-IB	656 GPGPUs	NHR FAU	Top500 11/2024 #250 Green500 11/2024 #74
	Meggie	Intel Broadwell OmniPath100	> 14,000 cores	FAU	
	Woody	in the meantime mostly Intel IceLake/ throughput	> 2,500 cores	FAU	partially funded by users
	TinyFAT	mostly AMD Rome/ large memory	> 2,400 cores	FAU	all funded by users
	TinyGPU	diverse NVIDIA GPUs/various generations	> 150 GPGPUs	FAU	all funded by users; growing since 2009
	Testcluster	various CPU/GPGPU architectures/generations		NHR FAU	partially early-access hardware provided by vendors

3.1 Compute Resources

3.1.1
Helma-H100 GPGPU parallel computer
NHR & Tier-3 (incl. BayernKI)

Delivery end of 2024; full operation expected for mid-2025

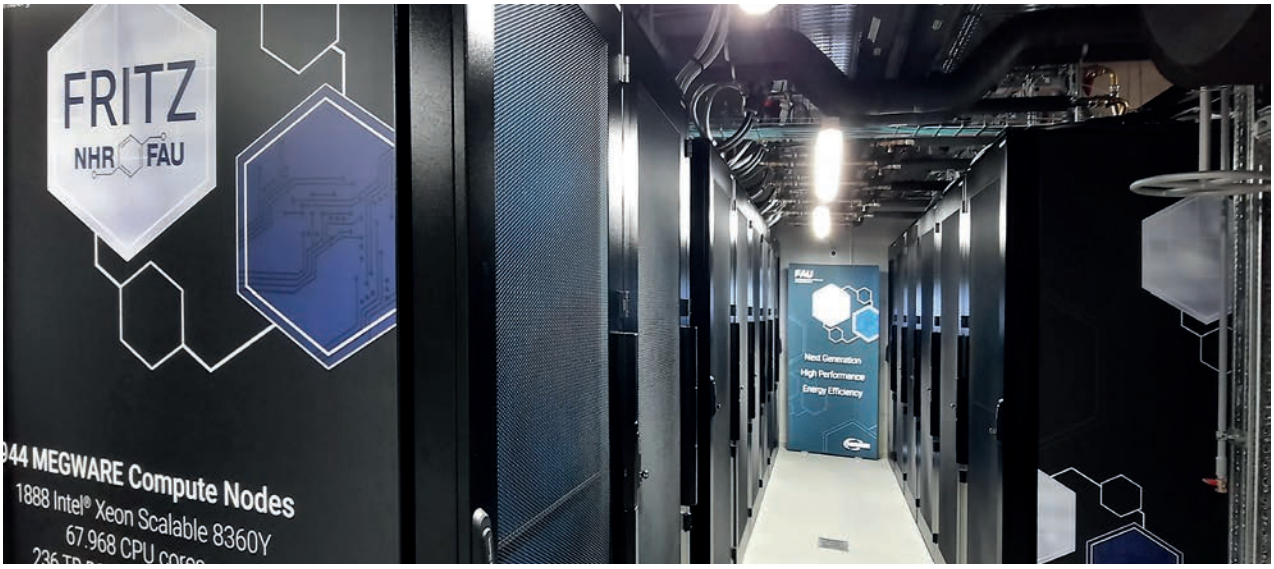
`https://doc.nhr.fau.de/clusters/helma/`

Helma (system integrator: MEGWARE) is a high-performance compute resource with NVIDIA GPGPU accelerators and high-speed interconnect. It is intended for high-end GPGPU workloads, especially in the area of AI. Helma is funded by BayernKI, NHR, Technische Universität Nürnberg (UTN), FAU and three other universities.

The configuration of *Helma-H100* at the end of 2024 is as follows:

- 6 Login nodes (not yet delivered 2024)
- 96 GPGPU nodes, each with two AMD EPYC 9554 *Genoa* CPUs (64 cores per chip) running at 3.1 GHz, 768 GB of DDR5-RAM, four NVIDIA H100 (each 94 GB HBM2e at 2 TB/s; HGX board with NVLink; 34 TFlop/s in FP64 or 67 TFlop/s in FP32), four NDR200 InfiniBand HCAs, 25 GbE, and 14 TB of local NVMe SSDs.
- A dedicated central NVMe storage (not yet delivered 2024)
- Operating system: AlmaLinux 9 (RHEL clone).
- Batch system: Slurm.

A LINPACK performance of 16.94 PFlop/s has been measured resulting in rank 79 on the November 2024 Top500 list.



3.1.2
Fritz parallel computer
NHR & Tier-3

Full operation since mid-2022

https://doc.nhr.fau.de/clusters/fritz/

Fritz (system integrator: MEGWARE) is a high-performance compute resource with high-speed interconnect, i.e., a parallel computer. It is intended for moderately-sized, multi-node parallel workloads. Fritz is funded by NHR and DFG INST 90/1171-1. Thus, it will not only be the main resource for NHR projects at NHR@FAU but, to a certain extent, also serve as FAU's basic Tier-3 resource for high-end demand.

The compute nodes of Fritz have been delivered in late 2021 with additional extensions in fall 2022 and spring/summer 2023. The configuration of Fritz did not change in 2024 and still is as follows:

- Four front-end nodes with the same CPUs as the compute nodes but 512 GB of RAM and 100 GbE connection to RRZE's network backbone.
- One visualization node with the same CPUs as the compute nodes but 1024 GB of RAM, one NVIDIA A16 GPU, 30 TB of local NVMe SSD storage, and a 100 GbE connection to RRZE's network backbone.
- 992 compute nodes with direct liquid cooling (DLC), each with two Intel Xeon Platinum 8360Y Ice Lake CPUs (36 cores per chip) running at a base frequency of 2.4 GHz, 54 MB Shared L3 cache per chip, and 256 GB of DDR4-RAM.
- 48 compute nodes with direct liquid cooling (DLC), each with two Intel Xeon Platinum 8470 Sapphire Rapids CPUs (52 cores per chip) running at a base frequency of 2.0 GHz, 105 MB Shared L3 cache per chip, and 1,024 GB of DDR5-RAM.
- 16 compute nodes with direct liquid cooling (DLC), each with two Intel Xeon Platinum 8470 Sapphire Rapids CPUs (52 cores per chip) running at a base frequency of 2.0 GHz, 105 MB Shared L3 cache per chip, and 2,048 GB of DDR5-RAM.
- Lustre-based parallel file system with a capacity of about 3.5 PB and an aggregated parallel I/O bandwidth of > 20 GB/s.
- Blocking fat-tree HDR100 InfiniBand with up to 100 GBit/s bandwidth per link and direction; there are islands with 64 nodes (i.e. 4,608 cores); the blocking factor between islands is 1:4.
- Operating system: AlmaLinux 8 (RHEL clone)
- Batch system: Slurm.

The LINPACK performance of 3.578 PFlop/s on 986 nodes resulted in rank 151 on the Top500 list in November 2022. The direct liquid cooling of the processors and memory of the compute nodes ensures an efficient operation of Fritz, significantly lowering the operating costs. The annual PUE (power usage efficiency) of the system was better than 1.1; thus, the electrical overhead for cooling was less than 10%.

3.1.3
Alex GPGPU cluster
NHR & Tier 3

Full operation since mid of 2022

`https://doc.nhr.fau.de/clusters/alex/`

Alex (system integrator: MEGWARE) is a high-performance compute resource with NVIDIA GPGPU accelerators and partially high-speed interconnect. It is intended for single- and multi-GPGPU workloads, e.g., from molecular dynamics or machine learning. Alex is funded by NHR and DFG INST 90/1171-1. Thus, Alex serves both as NHR's project resource and as FAU's basic Tier-3 resource.

Most compute nodes of Alex were delivered in October/November 2021. Several extensions have been integrated during the years 2022 and 2023. The configuration of Alex did not change in 2024 and still is as follows:

- Two front-end nodes, each with two AMD EPYC 7713 *Milan* CPUs (64 cores per chip) running at 2.0 GHz with 256 MB Shared L3 cache per chip, 512 GB of RAM, and 100 GbE connection to RRZE's network backbone but no GPGPUs.
- 20 GPGPU nodes, each with two AMD EPYC 7713 Milan CPUs (64 cores per chip) running at 2.0 GHz with 256 MB Shared L3 cache per chip, 1,024 GB of DDR4-RAM, eight NVIDIA A100 (each 40 GB HBM2 at 1,555 GB/s; HGX board with NVLink; 9.7 TFlop/s in FP64 or 19.5 TFlop/s in FP32), two HDR200 InfiniBand HCAs, 25 GbE, and 14 TB of local NVMe SSDs.
- 18 GPGPU nodes, each with two AMD EPYC 7713 Milan CPUs (64 cores per chip) running at 2.0 GHz with 256 MB Shared L3 cache per chip, 2,048 GB of DDR4-RAM, eight NVIDIA A100 (each 80 GB HBM2 at 1,555 GB/s; HGX board with NVLink; 9.7 TFlop/s in FP64 or 19.5 TFlop/s in FP32), two HDR200 InfiniBand HCAs, 25 GbE, and 14 TB on local NVMe SSDs; seven of these nodes belong to HS Coburg and one to FAU Audiolabs/FHG-IIS.
- 44 GPGPU nodes, each with two AMD EPYC 7713 Milan CPUs (64 cores per chip) running at 2.0 GHz with 256 MB Shared L3 cache per chip, 512 GB of DDR4-RAM, eight NVIDIA A40 (each with 48 GB DDR6 at 696 GB/s; 37.42 TFlop/s in FP32), 25 GbE, and 7 TB on local NVMe SSDs.
- Native access to the Lustre-based parallel file system of Fritz through 25/100 GbE.
- A dedicated central NVMe storage with 1 PB of capacity.
- Operating system: AlmaLinux 8 (RHEL clone).
- Batch system: Slurm.

A LINPACK performance of 3.24 PFlop/s has been measured in October 2022, resulting in rank 174 on the November 2022 Top500 list and rank 33 on the Green500 list of November 2022.

For molecular dynamics codes like GROMACS, an NVIDIA A40 GPGPU delivers a performance very similar to a much more expensive NVIDIA A100 GPGPU. Even for many machine learning workloads, the price/performance ratio of the NVIDIA A40 GPGPUs is more than competitive, while applications requiring double precision calculations certainly rely on the NVIDIA A100. The mixture of NVIDIA A40 and A100 allows to maximize the overall cluster performance for a broad range of applications, while still serving very diverse needs.

Meggie parallel cluster

3.1.4
Meggie parallel computer
Tier 3, since 2016

Meggie (system integrator: MEGWARE) is a system that is designed for running parallel programs using significantly more than one node. It is intended for distributed-memory (MPI) or hybrid-parallel programs with medium to high communication requirements and consists of originally 728 compute nodes, each with two Intel Xeon E5-2630v4 *Broadwell* CPUs (10 cores per chip) running at 2.2 GHz, 64 GB of RAM, and OmniPath interconnect. 64 compute nodes and the parallel file system had to be turned off during 2022 due to fatal hardware failure.

Meggie is no longer fully utilized all the time. Therefore, nodes of Meggie are semi-automatically turned on/off depending on demand.

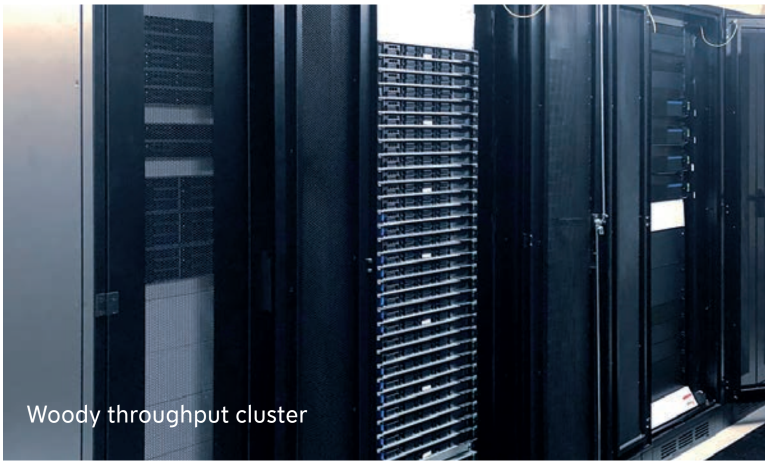
3.1.5
Woody throughput cluster
Tier 3, multiple phases 2013–2022

Woody is the preferred cluster for serial/single-node throughput jobs and has a long history. The nodes changed over time while the name was kept. The currently more than 200 nodes consist of (a) single-socket nodes with rather high-frequency quad-core Intel Xeon E3-12xx processors (E3-1240 v3 Haswell; E3-1240 v5 *Skylake*; E3-1240 v6 *Kaby Lake*) and (b) new dual-socket nodes from 2022 with Intel Ice Lake processors. All nodes have 8 GB of RAM per core and a local HDD/SDD.

While the single-socket nodes only use 1 Gbit Ethernet, the new Ice Lake nodes are connected via 25 Gbit Ethernet. Both node types form a single cluster with quite similar per-core characteristics. Parts of the single-socket nodes are only in operation during high-demand phases.

3.1.6
TinyFAT cluster
Tier 3, 2016/2020

TinyFAT is another small special-purpose cluster. It consists of almost 50 dual-socket Intel *Broadwell* or AMD *Rome* nodes with 256 or 512 GB of main memory and local SSD storage.


Woody throughput cluster

3.1.7
TinyGPU cluster
Tier 3, multiple phases since 2009

TinyGPU started in 2009 as a small special-purpose research test bed. Over the years, TinyGPU grew and no longer is that tiny. It now consists of more than 40 nodes with, in total, more than 200 NVIDIA GPGPUs of different generations (NVIDIA GeForce GTX1080, GeForce GTX1080Ti, GeForce RTX-2080Ti, GeForce RTX3080, Tesla V100, and A100). Almost all nodes have been funded by different research groups across FAU; NHR@FAU only takes care of the proper housing and operation.

The nodes with NVIDIA GeForce GTX1080 and GeForce GTX1080Ti GPUs are no longer powerful enough for regular production workload and are now mainly used for teaching purpose and interactive development work through a JupyterHub web-based service.

3.2 Storage Resources
Tier 3 with dedicated extensions for NHR

NHR@FAU operates several storage systems of different quality but also price/performance ratios serving different needs. Most file servers have 100 Gbit Ethernet connections.

- All throughput and GPGPU/large-memory nodes have local HDDs/SSDs for fast job-local storage.
- Each parallel computer has a parallel file system which is dedicated to that cluster; there are no capacity quotas enforced but high-watermark deletion is applied. The main usage is for checkpoint-restart files.
- `$WORK` consists of several capacity-optimized NFS file servers (more than 4 PB in total); there is no or only very limited backup. These Linux servers can cope rather well with many small files.
- `$VAULT` is a high-quality file system where especially larger files can be kept for longer times; `$VAULT` has a total capacity of 6 PB in a single file system and is served by an IBM Spectrum Scale cluster consisting of six servers (two NDS and four CES nodes; about 700 NL-SAS HDDs plus some SSDs in hardware RAIDs provide the capacity).
- `$HOME` is served by the same IBM Spectrum Scale cluster as `$VAULT`. The main difference is the frequency of snapshots (every 30 minutes vs. once per day).
- For long-term offline storage, an IBM TS4500 tape library with currently eight LTO8 tape drives and two expansion frames for up to 3,370 tapes is available. Archiving data is a manual process.

3.3 System Availability & Usage

There were again no major outages in the year 2024. Table 3.2 shows an overview of core-hours and GPU-hours used. Although many FAU scientists submit NHR applications, the Tier-3 consumption is considerable especially on the GPU-enabled systems!

SYSTEM	NHR	TIER3
Fritz	405 mio core-h	113 mio core-h
Meggie	–	36 mio core-h
Woody	–	13 mio core-h
TinyFAT	–	14 mio core-h
Alex	2.1 mio GPU-h	1.3 mio GPU-h
TinyGPU	–	1.0 mio GPU-h

Table 3.2: Core-hours or GPU-hours used by NHR and Tier-3 (incl. BayernKI), on the different systems in 2024.

4 TRAINING & SUPPORT

4 TRAINING & SUPPORT

Division head:
Dr. Georg Hager

The *Training & Support* division at NHR@FAU is responsible for the HPC training program and support activities. This entails training and event coordination, conducting local courses and user engagement events, organizing invited talks, participation in and organization of external training, application-specific support, performance engineering of user code, expert support for algorithms and libraries, and participation in third-party funded research projects. Due to the cross-cutting nature of many of these activities, members of the Training & Support division are typically active in other divisions as well.

The group offers a wide spectrum of courses and participates in training events organized by other centers, such as LRZ Garching, the Vienna Scientific Cluster (VSC) at TU Wien, and HLRS Stuttgart. Liaison Scientist Sebastian Kuckuk was certified as an NVIDIA DLI Ambassador for the course *Fundamentals of Acclerated Computing with OpenACC* to be held for the first time in 2025. Furthermore, the two-day OpenMP course that was previously conducted in a traditional "slides and hands-on" format was restructured and cast into a JupyterHub-based format in which attendees work interactively with code in Jupyter notebooks, intertwining theory and practice much more tightly. And finally, the new tutorial on *Performance Engineering for Linear Solvers*, which was developed in collaboration with TU Delft and the Innovative Computing Lab at the University of Tennessee, was accepted for both the ISC High Performance and SC24 conferences.

The Training & Support division is further responsible for all HPC user support that requires intense interaction with the customer, such as software configuration, code porting, parallelization, performance analysis and optimization, and the selection of appropriate algorithms and libraries. These services are not only offered to NHR users but also to third party-funded projects conducted by the NHR@FAU Research division and its project partners, and to KONWIHR projects.

4.1. Training

4.1.1 Courses & tutorials

In the following, we list courses and tutorials that were conducted in 2024 and were either organized by NHR@FAU, conducted by others with substantial contributions from NHR@FAU, or performed on invitation by NHR@FAU (see Table 4.1, page 29). Most of these events were conducted online via Zoom.

Node-Level Performance Engineering

This "signature" course covers performance engineering approaches on the compute node level, convey-ing the required knowledge to develop a thorough understanding of the interactions between software and hardware. Pipelining, SIMD, superscalarity, caches, memory interfaces, ccNUMA, etc., are covered. A cornerstone of node-level performance analysis is the Roofline model, which is introduced in due detail and applied to various examples from computational science. This tutorial is designed to be modular and can be given in various formats.

Performance Engineering for Linear Solvers

This new tutorial with hands-on exercises was developed in 2024 as a collaboration among NHR@FAU, TU München, and TU Delft. It covers code analysis, performance modeling, and optimization for (sparse) linear solvers on CPU and GPU nodes. It comprises a brief introduction to parallel node architecture, the Roofline model, and the variants of iterative sparse linear solvers, including preconditioners. Finally, the use of cache blocking for matrix power kernels is demonstrated. The tutorial was presented for the first time at ISC24 and SC24 as a half-day event and received overwhelmingly positive feedback.

Introduction to Parallel Programming with MPI

This new course provides an introduction to the Message Passing Interface (MPI), the dominant distributed-memory programming paradigm in HPC. Developed by Alireza Ghasemi from existing lecture materials, it is a compact two-day event with newly designed hands-on exercises. It covers basic blocking and nonblocking point-to-point and collective communication, derived data types, sub- and intracommunicators, the basics of parallel computer architecture, a glimpse at MPI tracing tools, and typical performance pitfalls.

Introduction to Hybrid Programming

A tutorial conducted by Georg Hager in close collaboration with colleagues from HLRS Stuttgart (Rolf Rabenseifner) and TU Wien (Claudia Blaas-Schenner). Most HPC systems are clusters of shared-memory nodes. To use such systems efficientl , both memory consumption and communication time have to be optimized. Therefore, hybrid programming may combine distributed-memory parallelization on the node interconnect (e.g., with MPI) with the shared-memory parallelization inside each node (e.g., with OpenMP or MPI-3.0 shared memory). This course covers several parallel programming models on clusters of shared-memory nodes, combining MPI with OpenMP, MPI-3.0 shared memory, or accelerators. Numerous case studies and micro-benchmarks demonstrate the performance-related aspects of hybrid programming. Hands-on sessions are included on all days.

Parallel Programming of High Performance Systems (PPHPS)

A three-day introduction to HPC. It is a long-standing collaborative course by NHR@FAU (and previously RRZE) and LRZ Garching. This online course is targeted at students and scientists with interest in programming modern HPC hardware, specifically the large-scale parallel computing systems available in Jülich, Stuttgart, and Munich, but also smaller clusters in Tier-2/-3 centers and departments.

Fundamentals of Accelerated Computing with CUDA Python/with CUDA C/C++

These NVIDIA "Deep Learning Institute" courses are offered by Sebastian Kuckuk, who is a certified NVIDIA DLI University Ambassador. These courses are the foundation for any serious performance-aware accelerator programming.

Performance Analysis on GPUs with NVIDIA tools

This half-day tutorial with hands-on exercises by Dominik Ernst is now offered twice a year at NHR@FAU. It complements the NVIDIA DLI courses (see page 27) since it covers the use of NVIDIA performance tools for the analysis of GPU programs written in CUDA C/C++, OpenACC, or OpenMP.

Introduction to C++ for beginners

Held by Slobodan Dmitrovic, this is a six-day course with a focus on the introduction of the essential language features and the syntax of C++. In addition, it introduced many principles, concepts, idioms, and best practices in C++ software development, which enable programmers to create professional, high-quality code from the very beginning.

Modern C++ Software Design

Held by Klaus Iglberger, this is a three-day course on software development with the C++ programming language. Its focus is on essential C++ software development principles, concepts, idioms, and best practices, which enable programmers to create professional, high-quality code. The course will give insight into the different aspects of C++ (object-oriented programming, functional programming, generic programming) and will teach guidelines to develop mature, robust, maintainable, and efficient C++ code.

Introduction to Parallel Programming with OpenMP

Initially a two-day course with hands-on exercises, designed and conducted by Markus Wittmann, this has been extended to three half-days and converted from a slides presentation with hands-on exercises to a fully interactive, JupyterHub-based experience. It introduces OpenMP from the ground up for developers who have no prior experience with parallel programming. Not only does it cover the basics, but it also touches on advanced concepts like tasking, SIMD, and accelerator programming.

LIKWID

The popular LIKWID tool suite was presented by Thomas Gruber as part of several courses at other sites in 2024. LIKWID (see Section 5.1.1) is in wide use at many computing centers worldwide for affi nity control, performance analysis, and monitoring. It contributes signifi cantly to the visibility and reputation of NHR@FAU within the HPC community. A dedicated full-day online LIKWID tutorial was conducted by Thomas Gruber and Georg Hager in 2024.

Core-Level Performance Engineering

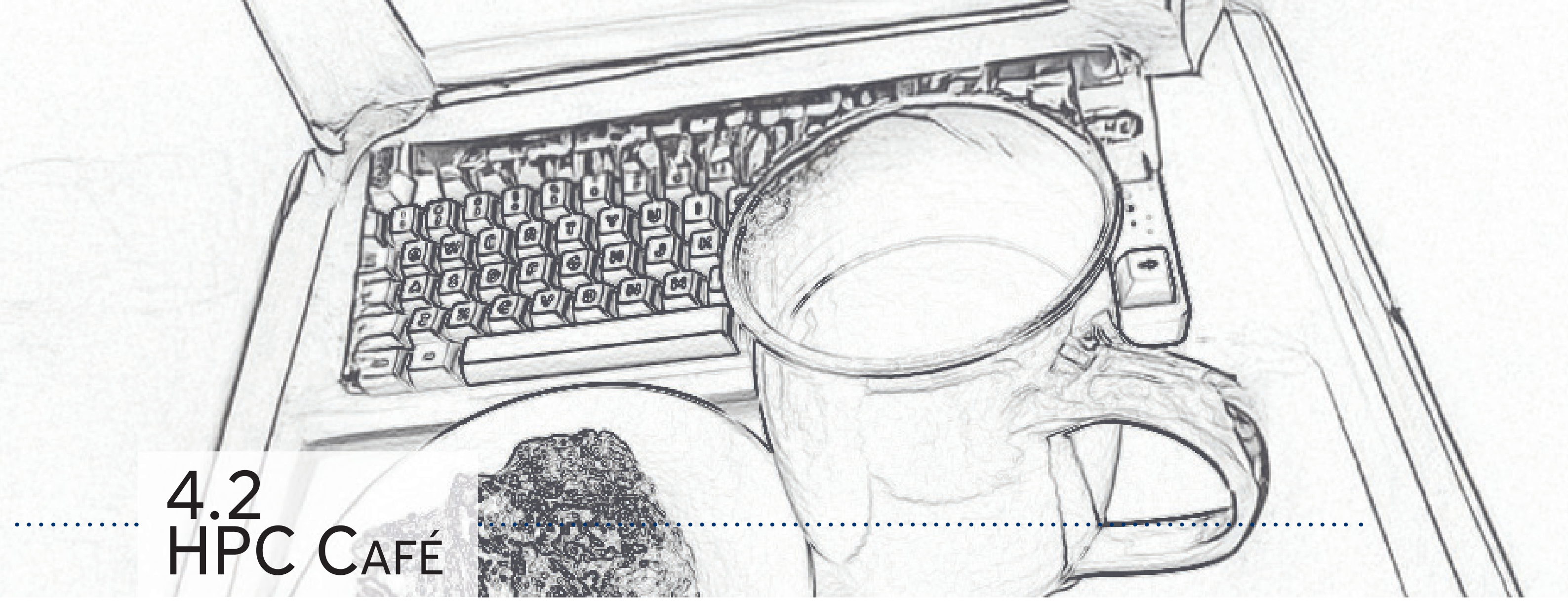
A full-day tutorial with hands-on exercises was designed by Jan Laukemann as part of his work on OSACA, the Open-Source Architecture Code Analyzer. The tutorial conveys the required knowledge to develop a thorough understanding of the interactions between software and hardware on the level of a single CPU core and the lowest memory hierarchy level (the L1 cache). It also covers performance analysis and performance engineering using the Open-Source Architecture Code Analyzer (OSACA) in combination with a dedicated instance of the well-known Compiler Explorer by Matt Godbolt. The tutorial was conducted in person at two conferences and as an online event for NHR@FAU.

COMPLETE LIST

of our entire current course program:
`https://hpc.fau.de/teaching/tutorials-and-courses/`

Table 4.1: Courses and tutorials in 2024; If not stated otherwise, courses were held online.

EVENT	DATE & PLACE	TEACHER(S)
Node-Level Performance Engineering	Dec 3–5 at LRZ	G. Hager
	Jun 18–21, on-site at HLRS	G. Hager with ZIH staff
Performance Engineering for Linear Solvers	Nov 17–22, on-site at SC24, Atlanta, Georgia	C. L. Alappat, G. Hager, J. Thies (TU Delft), H. Anzt (TU München)
	May 12–16, on-site at ISC 2024, Hamburg	C. L. Alappat, G. Hager, J. Thies (TU Delft), H. Anzt (TU München)
Parallel Programming of High Performance Systems (PPHPS24)	Feb 20–22, on-site at NHR@FAU	A. Afzal, M. Wittmann, G. Hager, LRZ staff
Introduction to parallel programming with MPI	Apr 11–12	A. Ghasemi, G. Hager
Introduction to parallel programming with OpenMP	Sep 4–6	S. Kuckuk
	Mar 5/12 (part 1/2)	M. Wittmann
Hybrid Programming in HPC – MPI+X	Jan 23–25, on-site at HLRS	G. Hager, R. Rabenseifner (HLRS), C. Blaas-Schenner (TU Wien).
From Zero to Multi-Node GPU Programming	Sep 18/25 (part 1/2), Oct 2 (part 3)	in collaboration with NHR@TUD
Accelerating CUDA C++ Applications with Multiple GPUs	Feb 8, online	S. Kuckuk
Multi-GPU Programming with CUDA C++	Apr 5/10 (part 1/2)	S. Kuckuk, EUMaster4HPC
Scaling CUDA C++ Applications to Multiple Nodes	Feb 9	S. Kuckuk, EUMaster4HPC
Fundamentals of Accelerated Computing with CUDA C/C++	Mar 4–5	S. Kuckuk, EUMaster4HPC
	Feb 29	S. Kuckuk
Fundamentals of Accelerated Computing with CUDA Python	Oct 24	S. Kuckuk
	Oct 7	S. Kuckuk
	Mar 14	S. Kuckuk
	Mar 6–7	S. Kuckuk, EUMaster4HPC
Core-Level Performance Engineering	Nov 17–22, on-site at SC24, Atlanta, Georgia	J. Laukemann, G. Hager
	Oct 8	J. Laukemann, G. Hager
	Sep 8–11, on-site at PPAM 2024, Ostrava, Czech Republic	J. Laukemann, G. Hager
Performance Analysis on GPUs with NVIDIA tools	Oct 9	S. Kuckuk
	Jul 7–12, on-site at IHPCSS, Kobe, Japan	S. Kuckuk
	Mar 19	D. Ernst
Introduction to the LIKWID Tool Suite	Jul 23	T. Gruber, G. Hager
C++ for beginners	Sep 2/13, 19/20, and 26/27	S. Dimitrovic
Modern C++ Software Design	Sep 30–Oct 2	K. Igelberger



4.2 HPC Café

The HPC Café complements the traditional HPC support channels by providing a deliberately informal setting. Every second Tuesday of a month, all HPC customers are invited to a freestyle Q&A session followed by a short presentation about a "focus topic" of interest. In 2024, the HPC Café was always held as a hybrid event, with HPC customers and speakers attending in person and the option for external attendees to connect via Zoom. Talks were usually recorded and published on the FAU video portal (`https://www.fau.tv/course/id/1146`) and/or the NHR@FAU YouTube channel (`https://www.youtube.com/NHRFAU`).

The following focus topics were covered in 2024:

Slurm batch scheduler best practices & advanced use, G. Hager & T. Gruber, Dec 17.

Exportkontrolle & HPC — ein Leitfaden für PIs & Kontaktpersonen, C. Hoeß & K. Schrüfer, SG Innenrevision (FAU), Nov 12.

File systems & efficient data handling, J. Veh, Oct 8.

Power and Energy Consumption of HPC Systems, G. Hager, Sep 17.

GROMACS 2024 usage and performance on modern CPU and GPU, A. Kahler, Jul 9.

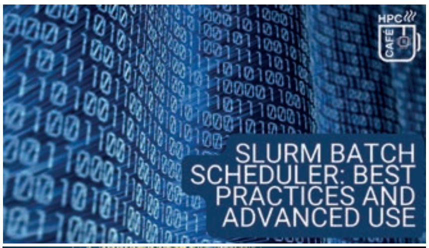
AI Round Table—State & Future of AI-based Research in Bavaria, G. Wellein & N. Hammer (LRZ), Jun 11.

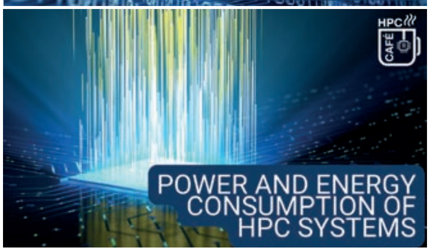
Bridging Domain Science & HPC with Julia, C. Bauer (PC2), May 7.

Secure Login with SSH, G. Hager, Apr 9.

NHR Project Applications & the JARDS System, H. Lanig, Mar 12.

Efficient data handling & data formats, M. Wittmann & H. Reynaud (AIBE), Feb 6.





COMPLETE LIST

with all events and links to slides and video recordings `https://hpc.fau.de/teaching/hpc-cafe/`

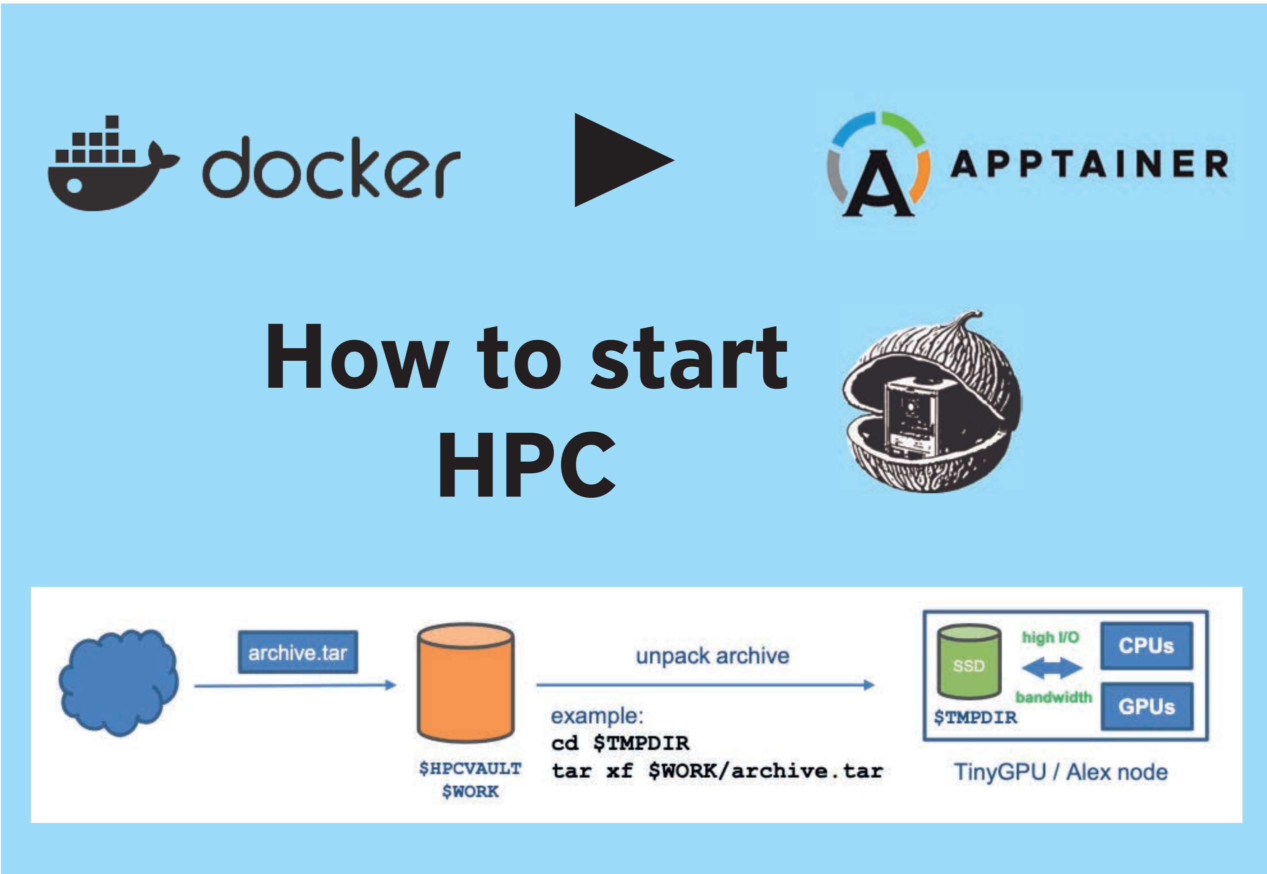
4.3 HPC IN A NUTSHELL BEGINNER'S INTRODUCTION

In November 2024, the beginner's introduction "HPC in a nutshell" was expanded for AI users. Each month, the two days after the HPC Café are specifically dedicated to new users and HPC beginners.

On Wednesday NHR@FAU offers a one-hour "General Introduction" (online) on using the HPC systems, including an overview of HPC clusters, how to connect to the systems, how to use the batch system, and more. This well-received format aims at reducing the entry barrier for new and inexperienced users. The content is continuously updated to reflect recent changes in NHR@FAU systems and access rules.

A one-hour *Introduction for AI Users* (online) on Thursday is aimed at newcomers who plan to run AI workloads on the NHR@FAU systems. Topics covered include file handling for AI workloads, fast storage options, setting up Python environments for AI, and setting up containers with Apptainer.

For more information and upcoming introductions refer to `https://hpc.fau.de/teaching/hpc-cafe/#nutshell`.



HPC in a Nutshell

4.4 NHR PerfLab Seminar

The *NHR PerfLab* is a collaborative effort by the NHR centers at FAU, RWTH Aachen, ZIB Berlin, and the University of Paderborn to combine resources and activities around performance engineering, code analysis, HPC computer architectures, and tools. The *NHR PerfLab Seminar* is a series of public talks about those (and more) topics. Since the inception of the seminar, NHR@FAU has taken on the role of organizing the talks, speaker acquisition, and pre- and post-event dissemination. If possible, all materials like slides and video recordings were published on the NHR@FAU website and YouTube channel. A full list of past seminars with links to slides and video recordings is available at https://hpc.fau.de/research/nhr-perflab-seminar-series/.

The following talks have been given in 2024:

- *A RISC-V vector CPU for High-Performance Computing: architecture, platforms and tools to make it happen* by Filippo Mantovani, Barcelona Supercomputing Center, Dec 10.
- *(Co-)designing a European CPU for HPC/AI* by Estela Suarez, Senior Principal Solution Architect at SiPEARL, Oct 29.
- *Kokkos: Getting Lucky by Design* by Christian Trott, Sandia National Laboratories, Sep 24.
- *How to rapidly deploy and deliver a highly sustainable national Exascale AI research resource* by Sadaf Alam, University of Bristol, Jul 30.
- *Mixing precisions in numerical algorithms: HPC perspective with modern hardware context* by Piotr Luszczek, Innovative Computing Lab (ICL), University of Tennessee, Knoxville, Jul 16.
- *Quantum Computing at DLR—Algorithms and Applications* by Achim Basermann, German Aerospace Center (DLR), Jul 2 (on-site).
- *OpenMP Target Offloading for AMD GPUs and APUs* by Michael Klemm, Advanced Micro Devices (AMD), May 28 (on-site).
- *Breaking through the barrier of time integration for climate and weather simulations* by Martin Schreiber, University of Grenoble, Mar 26.
- *Performance of linear solvers in tensor-train format on current multicore architectures* by Melven Röhrig-Zöllner, German Aerospace Center (DLR), Feb 27.
- *Processing very large image volumes with the adaptive particle representation* by Ivo Sbalzarini, Max Planck Institute of Molecular Cell Biology and Genetics, Dresden, Jan 30.

4.5 PROJECTS

4.5.1 KONWIHR

The main objective of KONWIHR, the *Competence Network for Scientific High-Performance Computing* in Bavaria, is to foster the efficient use of high-performance computers and to increase and broaden their impact on research. KONWIHR supports scientists at Bavarian universities in adapting and developing their numerical applications or other data- or computation-intensive codes for modern parallel computer architectures.

Funding is based on the duration of the project and can amount to a maximum of €10,000 (small project of three months) or up to €50,000 for projects with a duration of twelve months. The projects must be carried out in close cooperation with one of the two computing centers (LRZ and NHR@FAU). In particular, the funded project staff member should spend an extended period at one center.

NHR@FAU receives KONWIHR funding to coordinate KONWIHR activities in the northern part of Bavaria and to support KONWIHR projects in optimizing and adapting their codes and workflows for HPC systems. KONWIHR is currently led by Prof. Bungartz (TU Munich) and Prof. Wellein (FAU).

In 2024, KONWIHR granted the following scientific project applications:

- *Optimization of LuKARS_REACT,* Prof. Gabriele Chiogna (FAU), 2024-2, small project.
- *Development of Distributed, Data parallel Fourier Domain Bloch Simulator*, Prof. Moritz Zaiss (FAU), 2024-2, small project.
- *Boosting the performance of 4C targeting newest HPC hardware*, Prof. Wolfgang A. Wall (TUM), 2024-2, small project.
- *LexicoLLM—Leveraging Large Language Models for Lexicography*, Prof. Peter Uhrig (FAU), 2024-1, small project.
- *GPU Performance and Feature Enhancement of the Earthquake Cycle Simulation Software Tandem*, Prof. Alice-Agnes Gabriel (LMU), 2024-1, long project.
- *Dynamics of Complex Fluids*, Prof. Jens Harting (FAU), 2024-1, small project.
- *Compute Cloud access solutions for FAIR re-use of HPC research data*, Prof. Christian Stemmer (TUM), 2024-1, small project.

In addition, workshops have been organized to allow the KONWIHR projects to present their work and discuss with other projects and with the expert personnel from NHR@FAU and LRZ:

- *KONWIHR workshop for projects from 2024-1*, Oct 11.
- *KONWIHR workshop for projects from 2023/2*, Mar 25.

4.5.2 EoCoE-III

In the EoCoE-III project (Energy-Oriented Center of Excellence), accepted in 2023, NHR@FAU participates with performance engineering activities in various f agship codes. See section 6.2.8, page 49 for details.

4.6 NHR Graduate School

The NHR Graduate School awards up to nine PhD scholarships each year to doctoral students from all over the world. During the program, each student is required to spend six months at one of the other NHR centers. At the end of 2024, four NHR Graduate School fellows worked at FAU.

In 2024, the third cohort of students were admitted. Jorge Amador Balderas, Professorship for Computational Chemistry (Prof. Petra Imhof), received a PhD scholarship at NHR@FAU. He is hosted at the Professorship for Computational Chemistry (Prof. Petra Imhof). His research revolves around DNA recognition by DNA-processing proteins. Using High Performance Computing, he started working on calculating atom-level detailed simulations of DNA glycosylases to understand which interactions are important for damage recognition and specificit . DNA repair is a fundamental process for the conservation of genetic information and prevention of diseases. It must be carried out in a very specific manner, so healthy DNA sequences are not damaged by the repair machinery. Hence, damage recognition is a crucial step, which is carried out by DNA glycosylases.

4.7 EUMaster4HPC

In 2024 the first master student from EUMaster4HPC program started his master thesis at NHR@FAU. The HPC European Consortium Leading Education Activities (EUMaster4HPC) aims to develop a new and innovative European Master program focusing on high-performance solutions to ensure the digital transformation and the sustainability of high-priority economic sectors. The master program catalyzes various aspects of the HPC ecosystem and its applications into different scientific and industrial domains. EUMaster-4HPC students benefit from meeting HPC professionals during the EuroHPC Summit and from annual Summer Schools on top of a variety of workshops. Students are required to spend their second year at one of the partner universities participating in the program. EUMaster4HPC master student Jean-Yves Verhaeghe started his work on investigating innovative ways to visualize MPI program traces with a special focus on idle waves and spontaneous desynchronization. This is an emerging field of research with many surprising insights, as shown in numerous publications by our group in recent years.

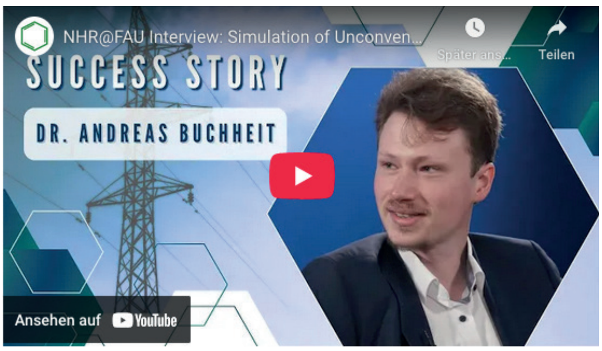
4.8 Dissemination & Outreach

Dissemination of activities and results is an integral part of the NHR@FAU activities. Event and course announcements, success stories from the support (see below), calls for compute time projects, talk recordings, etc., are disseminated via social media channels (YouTube, Linkedin), our bi-monthly newsletter (see below), the NHR@FAU home page, and mailing lists that reach out to NHR@FAU system users, KONWIHR project PIs, and interested subscribers all across the NHR Alliance.

Each semester, a 90-minute online introductory talk on Resources for High Performance Computing at FAU was given at the FAU Graduate Center in order to inform graduate students of the opportunities for using NHR@FAU HPC clusters for their research.

4.8.1 Support success stories

Frequently, customers observe low or fluctuating performance of their jobs, or the cluster monitoring indicates low resource utilization. While most of these cases can be categorized as simple accidental misuse, some require deeper investigation by support staff. The ensuing consultation occasionally results in impressive performance improvements. We document such cases regularly at `https://hpc.fau.de/about-us/success-stories/`.



Simulation of Unconventional Superconductors: Interview with Andreas Buchheit

4.8.2 NHR@FAU newsletter

The bi-monthly NHR@FAU newsletter is a publication that summarizes recent and upcoming events at NHR@FAU and the NHR Alliance. Beyond events, every newsletter highlights special or noteworthy achievements by NHR@FAU scientists and an FAQ corner. Finally, the "newsletter spotlight" introduces an NHR@FAU scientist in some detail. Since October 2024, the NHR@FAU newsletter has featured a new, modern design.

All newsletters are available at `https://hpc.fau.de/about-us/nhrfau-newsletters/`.

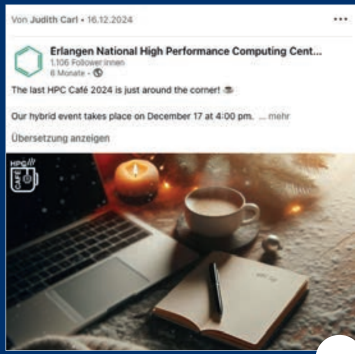
To stay informed about the latest news from the NHR@FAU a mailing list is open for everyone to subscribe at: `https://lists.fau.de/cgi-bin/listinfo/nhr-newsletter`.

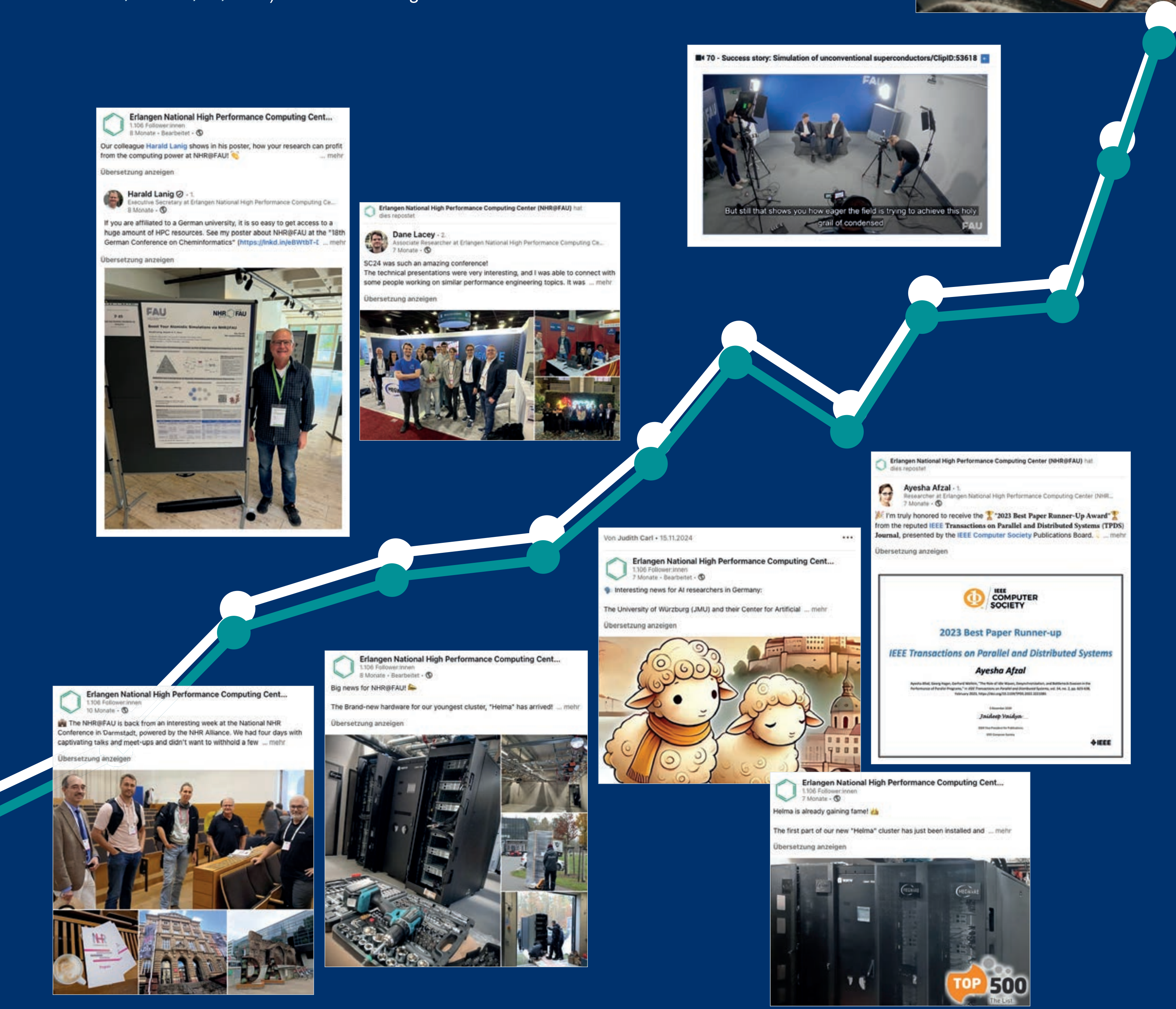
Penguins in the Supercomputer: Interview with biophysicist Alexander Winterl

4.8.3
Social media

In order to widen its reach to potential customers and audiences, NHR@FAU leverages social media channels. Recorded lectures, seminars, and tutorials are published on the NHR@FAU YouTube channel (`https://www.youtube.com/NHRFAU`) and the FAU video portal (`https://www.fau.tv/course/id/1146`). Our recordings of parallel programming lectures are particularly well received and generate considerable feedback in the HPC community and among students.

In 2024 the usage of LinkedIn increased significantly at NHR@FAU. By contributing regular posts, NHR expands its network and actively engages with other national and international experts.





5 SOFTWARE & TOOLS

5 SOFTWARE & TOOLS

Division head:
Dr. Jan Eitzinger

The *Software & Tools* division at NHR@FAU is responsible for the development of Open-Source software and for providing and administrating services for NHR@FAU and the NHR alliance. To this end, the division develops, maintains, and supports Open-Source software that is published on our GitHub account (`https://github.com/RRZE-HPC`): the LIKWID (Like I Knew What I'm Doing) performance tools, the *Open Source Architecture Code Analyzer (OSACA)*, the Loop Kernel Analysis and Performance Modeling Toolkit *Kerncraft*, the *Bandwidth Benchmark*, the *MachineState, and the ClusterCockpit* Monitoring Framework.

The division participates in third-party projects related to performance and monitoring tools, develops and maintains software for internal use at NHR@FAU such as the HPC Portal, and provides and administrates services (NHR Moodle, NHR@FAU HPC Portal, NHR@FAU job-specific monitoring for all cluster systems, Discourse community service, LimeSurvey service). We also host a URL short-link service for usage within the NHR alliance at `go-nhr.de`.

We are a member of the Virtual Institute—High Productivity Supercomputing (VI-HPS) and the SPEC Research Group. In 2023, we contributed our expertise in performance and monitoring tools and software development in the NHR central projects *Automatic Detection of Pathological Jobs for HPC User Support* and *Portable and Efficient Pinning for Hybrid HPC* ("MPI-Wrapper", project lead).

The RRZE HPC group, out of which NHR@FAU has emerged, started to develop the LIKWID Performance Tool Suite already in 2009. From 2013 to 2016, it had the project lead in the BMBF *FEPA* project, which developed a system-wide job-specific monitoring infrastructure. From 2017 to 2020, the group was a partner in the BMBF *Metacca* project and contributed its LIKWID and Kerncraft tools. Also from 2017 to 2020, the RRZE HPC group was the project lead in the DFG *ProPE* project, where, among other activities, the initial development for the ClusterCockpit monitoring framework began. ClusterCockpit is now besides LIKWID the second large Open Source project at NHR@FAU.

Since fall 2022, the BMBF project *EE-HPC* has been strengthening our activities in cluster-wide performance and energy monitoring. NHR@FAU is the project lead with the further partners HLRS Stuttgart, RWTH Aachen, Deutsches Klimarechenzentrum (DKRZ), and Hewlett Packard Enterprise (HPE).

In 2024, ClusterCockpit has further matured and more and more centers are evaluating and deploying it as a tool for their HPC support and an monitoring offering for their users. Two new co-workers joined the group: the new PhD student Aditya Ujeniya, who will be financed as part of the EE-HPC project, and Michael Panzlaff, who will help with LIKWID and ClusterCockpit developments and also act as system administrator for the NHR@FAU ClusterCockpit instance.

5.1 Tool Development

The tool development at NHR@FAU is well integrated with our main research topics of performance engineering and performance modeling. LIKWID and OSACA are important tools used in many of our research and support projects and enable us to adopt and research novel processor architectures at a very early stage. With Kerncraft, analytical performance models (the well-known Roofline model and the ECM model, which was developed at NHR@FAU) are accessible also for non-expert users. The ClusterCockpit monitoring stack bundles our activities in cluster-wide monitoring solutions. A recent addition to our software portfolio is MD-Bench, a performance-focused prototyping harness for state-of-the-art short-range molecular dynamics algorithms.

5.1.1 LIKWID Performance Tool Suite

https://github.com/RRZE-HPC/likwid

LIKWID is an easy-to-use yet powerful command-line performance tool suite for the GNU/Linux operating system. LIKWID is maintained by Thomas Gruber.

Currently, LIKWID consists of seven core tools of which `likwid-perfctr` (counting hardware performance events), `likwid-topology` (display node topology), `likwid-pin` (control thread and process affinity), and `likwid-bench` (microbenchmarking framework) are most prominent. The tools are specific to hardware architecture and currently support x86-64, ARM, and Power processors, and NVIDIA GPUs.

LIKWID is by far our most popular open-source project, and its tools are used worldwide for research, teaching, or in production environments, e.g., at NERSC (Lawrence Berkeley National Laboratory), CSCS (Swiss National Supercomputing Center) in Lugano, the National Supercomputer Center in Guangzhou, the Vienna Scientific Cluster (VSC), or the Barcelona Supercomputing Center (BSC).

In addition, LIKWID is used by the members of the Gauss Center for Supercomputing (GCS)—LRZ Garching, HLRS Stuttgart, and JSC Jülich—and at the IT provider for the Max Planck Society (MPCDF). Some of the Tier-2/3 HPC sites in Germany using LIKWID are RWTH Aachen, TU Dresden, KIT Karlsruhe, University of Paderborn, University of Konstanz, University of Gießen, and the national research center DESY in Hamburg.

In 2024, LIKWID added support for Intel EmeraldRapids and SierraForrest, AMD Zen4 (mobile), AMD Zen4c (Bergamo), and Nvidia Grace chips. The new application `likwid-sysfeatures` and its library backend, which allows the retrieval and manipulation of system settings, were extended. The Nvidia GPU backend was significantly improved.

Also a new bridge to use LIKWID inside of containers was implemented. Together with the TAU development team at the University of Oregon, improved handling of performance groups was added. In a collaborative effort, LIKWID was prepared to implement Uncore measurements in TAU.

5.1.2 OSACA Open Source Architecture Code Analyzer

https://github.com/RRZE-HPC/OSACA
https://godbolt.org/

OSACA is a tool that can analyze x86 and Arm64 assembly code and produce runtime predictions assuming steady-state execution and no cache misses.

By taking data dependencies into account, OSACA provides not only a throughput prediction as the best-case scenario but also the critical path and loop-carried dependencies for loop kernels. OSACA is maintained by Jan Laukemann.

A tool like OSACA is needed for analytic performance modeling, e.g., to formulate ECM or refined Roofline models. While there exist similar tools, such as the Intel Architecture Code Analyzer (IACA), LLVM's Machine Code Analyzer (LLVM-MCA), or the uops.info Code Analyzer (uiCA), they lack accuracy in prediction, are not open source, discontinued in development, or do not provide support for non-x86 architectures. OSACA, on the other hand, can also handle all modern Intel and AMD x86 architectures and several Arm processors. It is available as a Python3 module and a CLI application, but it is also integrated into the Compiler Explorer, which allows using OSACA from a browser without any installation.

In 2024 we added support for Intel Sapphire Rapids and Arm Neoverse V2 (NVIDIA Grace). A large refactoring of the object-oriented code base ensures a stable base for future extensions.

5.1.3 Kerncraft LOOP KERNEL ANALYSIS AND PERFORMANCE MODELING TOOLKIT

Kerncraft is a loop kernel analysis and performance modeling toolkit. It allows automatic analysis of loop kernels using the Execution Cache Memory (ECM) model and the Roofline model, together with their validation via actual benchmarks. Kerncraft provides a framework for investigating the data reuse and cache requirements by static code analysis.

Using Intel IACA or our OSACA tool together with static source code analysis, Kerncraft can give a good overview of both in-core and memory bottlenecks and use these data to construct predictive white-box performance models. Kerncraft was developed and maintained by Julian Hammer, who has left FAU after finishing his PhD. We are currently searching for funding and a new maintainer for the further development of Kerncraft. Please contact Thomas Gruber and Jan Laukemann for any questions or requests regarding Kerncraft.

5.1.4 ClusterCockpit MONITORING FRAMEWORK

https://clustercockpit.org/
https://eehpc.clustercockpit.org/

ClusterCockpit is a full-stack framework for job-specific performance monit oring on HPC clusters. It started as a side project for a web frontend during the DFG ProPE project and has grown into a cooperative effort to provide a customized software stack for job-specific performance monitoring.

ClusterCockpit currently comprises `cc-backend` (web API backend including a web-interface), `cc-metric-collector` (a node agent to measure and forward node metric data), and `cc-metric-store` (a simple metric time series in-memory cache).

A focus of ClusterCockpit is to define standards and interfaces for an interoperable monitoring ecosystem. We document and specify generic data structure descriptions and developed a job archive specification that allows to archive and share job performance data in a portable manner.

Five members of the team (Jan Eitzinger, Thomas Gruber, Christoph Kluge, Aditya Ujeniya and Michael Panzlaff) contributed to the development of ClusterCockpit in 2024, focusing on stability and ease of installation and maintenance. ClusterCockpit is in production use at NHR@FAU, PC2 Paderborn, DKRZ Hamburg, and the University of Bonn. It is funded as part of the BMBF EE-HPC project, which started in fall 2022 (see Section 6.2.6, page 48). Our aim is to establish ClusterCockpit as an attractive open-source offering for job-specific performance monitoring in academic HPC centers.

5.1.4 MachineState

https://github.com/RRZE-HPC/MachineState

MachineState is a Python3 module and CLI application for documenting and comparing hardware and software settings known to affect performance. It is our contribution to enabling deterministic and reproducible benchmark results on today's complex processor and node architectures. MachineState is maintained by Thomas Gruber.

5.1.5 MD-Bench

https://github.com/RRZE-HPC/MD-Bench

MD-Bench is a vehicle for research on performance engineering for molecular dynamics algorithms and strengthens our expertise in this area. Its source code is simple, understandable, and extensible, and therefore well suited for benchmarking, teaching, and researching MD algorithms. A paper about MD-Bench was presented at the PPAM conference 2022 in Gdansk, Poland, where it won the Best Paper Award. MD-Bench is maintained by Rafael Ravedutti.

In 2024, as part of a master thesis, a state-of-the-art MPI parallelization was added to MD-Bench. MD-Bench is used as the central application code in our MuCoSim Seminar.

5.1.6 The Bandwidth Benchmark

https://github.com/RRZE-HPC/TheBandwidthBenchmark
https://github.com/RRZE-HPC/TheBandwidthBenchmark/wiki

The *Bandwidth Benchmark* is inspired by the famous STREAM main memory bandwidth microbenchmark by John McCalpin. It can be seen as "STREAM on steroids" and contains eight streaming kernels with varying data access patterns. Since it is a simple, modular C99 implementation with a simple yet flexible makefile-based build system, it can also be used as a blueprint for other microbenchmarking projects. For teaching purposes, a single-file version of this benchmark is available. The project's Wiki pages feature results for many processor architectures. The Bandwidth Benchmark is maintained by Jan Eitzinger.

5.2 Service & Outreach

5.2.1 HPC Portal

https://portal.hpc.fau.de/

Modern digital workflows are key for efficient project management, handling of user accounts, and resource access. To this end, we are developing the *HPC Portal* web interface, which provides principal investigators with the means for self-administration of approved projects. Access to computational NHR resources are streamlined by utilization of user-supplied public SSH keys, which allows secure, password-less authentication for these accounts.

The HPC Portal supports login via Single-Sign-On (SSO), allowing users to use the credentials of their respective home organization. Since 2024, it has been used in productionas the default user management solution for all Tier-3, external, and teaching accounts. The HPC Portal is maintained by Christoph Kluge.

5.2.2 NHR Moodle learning platform

https://moodle.nhr.fau.de/

Since 2021, we have been hosting and administrating a *Moodle* server for general use within the NHR Alliance. Login is enabled through DFN-AAI Single-Sign-On authentication. All NHR@FAU courses and lectures provide their materials on this platform. The service is deployed as a docker container on a high-availability VM cluster at RRZE and uses the central RRZE SQL database and tape backup services. The NHR Moodle service is maintained by Christoph Kluge.

5.2.3
NHR@FAU ClusterCockpit service

https://monitoring.nhr.fau.de/

For use within the FAU, we provide a central *ClusterCockpit* monitoring server. For this purpose, we procured a dedicated server with large main memory capacity and fast NVMe file storage.

The server is used for all cluster systems and provides job-specific performance monitoring for support personnel and HPC users. FAU HPC users can authenticate via LDAP. External NHR users can delegate their authentication and initiate a ClusterCockpit session with a button in the *HPC Portal*. This service is jointly maintained by Johannes Veh from Systems & Services and Jan Eitzinger, Michaelk Panzlaff, Thomas Gruber, and Christoph Kluge from Software & Tools.

5.2.4
URL short-link service

https://go-nhr.de

For use within the NHR alliance we host and maintain a *URL short-link service*. Every member of the NHR alliance can get access to create short-links for otherwise long URLS.

5.2.5
Services for internal use

The Software & Tools division also hosts and maintains additional services for usage within NHR@FAU:

- A LimeSurvey instance for online surveys (https://survey.nhr.fau.de/)
- A Discourse forum software instance for documentation and knowledge transfer (https://community.nhr.fau.de/)
- A Hedgedoc collaborative Markdown editor (https://pad.nhr.fau.de/)

All services are running as Docker containers on RRZE VMs using a reverse proxy as frontend. They are integrated into the RRZE service infrastructure and use the RRZE database and backup services.

5.3
Talks

J. Eitzinger: *ClusterCockpit—Job specific monitoring framework*, ScalPerf2024 Workshop, Bertinoro, Italy, Sep 24, 2024.

J. Eitzinger: *Developing the ClusterCockpit Monitoring Framework—An Odyssey from PHP to Go* , deRSE24 Conference, Würzburg, Germany, Mar 07, 2024.

T. Gruber: *The LIKWID Performance Tool Suite*. Invited talk for the Server Performance Group at Intel, Jun 27, 2024.

T. Gruber: *ClusterCockpit and EE-HPC: A way to more energy efficiency on HPC systems?* Invited talk at the Durham HPC/AI Days 2024, Durham, UK, May 10, 2024.

T. Gruber: *The LIKWID Performance Tool Suite*. Invited online talk at Los Alamos National Laboratory, Los Alamos, NM, Mar 18, 2024.

T. Gruber and Jakob Fritz (JSC): *Github and Gitlab—Combine the best of both worlds*. Invited talk at dRSE24—Conference for Research Software Engineering in Germany, University of Würzburg, Mar 6, 2024.

T. Gruber: *LIKWID Performance Tool Suite.* Lecture with hands-on exercises at the 44th VI-HPS Tuning Workshop (RWTH Aachen and ZIH, TU Dresden, Germany), Feb 26–Mar 1, 2024.

6 RESEARCH

6 RESEARCH

Division head:
Prof. Dr. Harald Köstler

The overarching goal of the research activities at NHR@FAU is to introduce a systematic and model-guided performance engineering (PE) process into all performance analysis and optimization activities within the field of computing. This process helps developers and performance analysts on all levels of expertise to understand observed performance and find optimization opportunities. Our research is focused on developing and applying analytic performance models, tools, and libraries that support this mission. We participate in projects where we can leverage our expertise to help our partners develop deeper insights into performance issues and how to mitigate them. Additionally, we combine our HPC expertise with software engineering and code generation technology to provide software frameworks for a variety of applications in the field of computational science and engineering.

6.1 Selected Research Activities

6.1.1 Optimizing sparse matrix computations

There is considerable interest in the scientific computing community in methods that separate a sparse matrix A into sub-matrices held in lower-storage data types depending on the magnitude of the data A_{double}, A_{float}, A_{half}, . . . to lower the data volume transferred over the main memory interface during an SpMV. While that work focused only on CRS matrices on CPUs, we found that this technique can potentially destroy the locality when using the GPU-friendly Sell-P format. In this case, one requires row sorting (i.e., Sell-C-σ) on GPUs. We have characterized matrices that exhibit this issue based on the sparsity pattern, and applied our mixed-precision Sell-C-σ SpMV to iterative solvers like CG and GMRES.

Computing $y = A^p x$, is typically implemented as a series of back-to-back SpMVs. This so-called Matrix Power Kernel (MPK) exposes an opportunity for cache blocking—which has recently been exploited using the Recursive Algebraic Coloring Engine (RACE). We extended these cache-blocking techniques beyond shared memory by integrating its level-blocking with an MPI communication scheme. Our distributed level-blocked MPK shows significant performance improvement over a traditional MPK implementation across modern Intel and AMD CPUs and diverse scientific matrices [11].

SpMV performance modeling for shared memory typically uses the Roofline model. For MPI-distributed cases, factors like network latency / bandwidth, halo exchanges, and communication-computation overlap complicate modeling. Existing analytical models were extended to multi-GPU scenarios where libraries like NCCL or NVSHMEM can play a crucial role, and overheads like halo buffer packing become potentially more expensive.

6.1.2 Building blocks for sparse linear algebra and stencil solvers: Adaptive linearized storage of sparse tensor

We continued our collaboration with Intel Labs, University of Oregan, and the Laboratory for Physical Sciences (LPS), and extended the work on the mode-agnostic Adaptive Linearized Tensor Order (ALTO) format for sparse tensor decomposition with focus on new tensor decomposition models such as Alternating Poisson Regression (APR) for fitting CP and reinforcement learning. We expect the results to be published in 2025.

6.1.3 Microarchitectural Analysis

We are constantly exploring new and modern microarchitectures and their behavior with regard to performance. In 2024, this led to a best paper candidate at IPDPS, investigating the proxy app CloverLeaf on Intel Multi-Core CPUs and their capabilities of write-allocate evasion [7], and a short paper at the workshop on *Performance Modeling, Benchmarking and Simulation of High Performance Computer Systems* (PMBS) held during SC24, in which we analyzed the and modeled the in-core part of the state-of-the-art CPUs NVIDIA Grace, Intel Sapphire Rapids, and AMD Genoa [6].

6.2. Ongoing Research Projects

Oue developments and research in the field of performance related tools are bundled in the *Software & Tools* division (for details, see page 38), which collaborates closely with the Research division.

6.2.1 KONWIHR OMI4papps: Optimization, Modeling and Implementation for highly parallel applications

As part of the KONWIHR project, our previous research focused on the development of advanced performance models for parallel computing systems. A significant area of study was idle waves, which are delays originating from one part of a parallel program that propagate throughout the system, affecting overall performance. We examined how factors such as system noise, topology, and load imbalances influence the behavior of idle waves and their impact on execution efficiency. Additionally, the project explored the effects of memory bandwidth bottlenecks and their role in enabling asynchronous communication. Our findings suggested that, under specific conditions, these factors could actually enhance code execution speeds.

In 2024, the focus shifted towards the development of DisCostiC (Distributed Cost in Clusters). DisCostiC is a cross-architecture parallel simulation framework that predicts the performance of real or hypothetical, massively parallel MPI programs on current and future supercomputer systems. It allows us to simulate research insights and performance dynamics for MPI-based parallel applications, providing a controlled, noise-free experimental environment where various factors, from code characteristics to communication parameters and contention effects, can be influenced at will. Unlike conventional networking simulators, which often fail to account for resource sharing beyond the network level, DisCostiC incorporates a separate analytical, first-principle performance model at full scale, including cores, chips, nodes, and networks, while being aware of bottlenecks such as memory bandwidth. DisCostiC uses application skeletons in a Domain-Specific Embedded Language (DSEL), which encodes interprocess dependencies and any number of system and code properties, enabling flexible design space exploration. As a consequence of the model-based design, DisCostiC requires much less time and resources than traditional simulators because the application code is never actually run. This is in contrast to state-of-the-art solutions, which are based on trace data and/or simulated code execution and may thus need considerable resources. The resulting traces can be visualized using Chromium Browser, ITAC, or Vampir. For more, visit: `https://github.com/RRZE-HPC/DisCostiC-Sim`.

6.2.2 NHR Central Project EEC: Energy Efficiency and operational Costs in NHR

Launched in November 2024, the project addresses rising energy costs and growing demand for HPC computing power by creating standardized methods and KPIs for measuring energy consumption. Focused on energy efficienc , infrastructure, and software optimization, it aims to improve benchmarking and optimization across HPC centers. The project offers benefits like energy consumption benchmarks, reduced costs, and alignment with sustainability goals, while enhancing software performance and increasing computing power for more sustainable HPC operations. Within the project, we are is responsible for developing energy efficiency assessment methods for HPC centers, including energy-consumption KPIs, measurement techniques, and analytic power models. We will also apply these methods to measure energy use at NHR centers, creating profiles for idle and load conditions to guide optimizations. Additionally, we will focus on minimizing energy consumption during idle times, optimizing usage under load with the benchmarks, and improving energy efficiency in infrastructure like network and storage.

Tool: Wattlytics

Wattlytics (`https://wattlytics.netlify.app/`) is a tool designed to optimize cluster configurations by considering both investment and operational costs. It takes performance data for applications like GROMACS or AMBER as input and compares clusters based on key metrics such as performance per TCO, power per TCO, and performance per watt per TCO. The tool tracks live GPU prices, offers sensitivity analysis to assess the impact of factors like clock speeds and energy costs on TCO, and provides power management insights to stay within energy budgets. It includes advanced visualizations for comparing GPU setups and offers detailed TCO breakdowns to identify where cost arise. It is designed for data center planners, computational scientists, and IT managers who need scenario-based decision-making tools to ensure optimal GPU performance and cost management over a system's lifetime. Currently, Wattlytics evaluates the impact of various parameters on performance, power, and cost. For instance, it compares scenarios where a slower but more power-efficient GPU outperforms a faster but less power-efficient GPU by deploying more units within the same budget and system lifetime. In 2025, it will be expanded to analyze the impact of adjusting GPU and (un-)core CPU clock frequencies, helping users decide whether to prioritize raw performance or optimize performance per watt.

6.2.3 JHPCN Heterogeneous Computing Project

The JHPCN Heterogeneous Computing Project with collaborators Kengo Nakajima and Shinji Sumimoto was overseen by Ayesha Afzal et al. In this project, FAU was responsible for exploring the possibility of extending the DisCostiC simulator to simulate the performance of MPI programs, moving from homogeneous systems with similar CPUs and networks to heterogeneous systems with different CPUs per node. This work identified performance bottlenecks in heterogeneous HPC architectures—including Intel CPUs, Fujitsu A64FX CPUs, and networks like InfiniBand, Omni-Path, and Tofu D—and extended the simulator to effectively model performance in such heterogeneous environments. n October 2024, Ayesha Afzal et. al submitted the midterm project report, which was later published as a comprehensive report *Innovative Computational Science by Integration of Simulation/Data/Learning on Heterogeneous Supercomputers.* The report featured all project partners: University Tokyo, Hokkaido University, Nagoya University, Kyushu University, University Hyogo, RIKEN, NIES, CliMTECH, CEA (France), JSC (Germany), FAU (Germany), BUW (Germany), TUM (Germany), University Cologne (Germany), RBI (Croatia), Fujitsu, and Hitachi. It is available at `https://jhpcn-kyoten.itc.u-tokyo.ac.jp/abstract/jh240029`.

6.2.4
JHPCN Non-blocking Collectives Project

The JHPCN Non-blocking Collectives Project with collaborators Takeshi Nanri et. al was overseen by Ayesha Afzal and Gerhard Wellein. In this project, FAU's role focuses on investigating non-blocking MPI operations, aiming to improve performance by overlapping communication and computation in HPC applications. This builds on FAU's earlier work, including the MPIBench benchmark suite developed during Asghar's master's thesis, supervised by Ayesha Afzal et. al. in 2019, providing a flexible framework to study point-to-point and collective communications with Intel MPI and OpenMPI across multi-core systems. Benchmarks like PingPong and PingPing were used to measure intra-node and inter-node communication, revealing that Asynchronous Progress Threads allow for overlap, though the benefits vary across different MPI routines.

In 2024, the focus shifted to studying non-blocking routines in real applications, such as the Parallel Optical Flow Solver, with an emphasis on optimizing memory bandwidth and improving communication overlap as part of a master thesis supervised by Ayesha Afzal et. al. The goal was to better understand how communication overlap affects the performance of applications and how MPI non-blocking routines play a role for such scenarios.

In October 2024, Ayesha Afzal et al. submitted the midterm project report, which was later published as a report and research poster, titled *Study on the real effect of non-blocking collective communications*. The report featured all project partners—Kyushu University, University Tokyo, Hokkaido University, Tohoku University, University Tsukuba, Institute of Science Tokyo, Nagoya University, Kyoto University, University Osaka, Teikyo University, NVIDIA Co., TU Munich, Ohio State University, TU Darmstadt, and NHR and is available at `https://jhpcn-kyoten.itc.u-tokyo.ac.jp/abstract/jh240058`.

6.2.5
DAREXA-F: Data reduction for exascale applications in fusion research

For the efficient usage of HPC applications in the exascale era, we need to improve the scalability on large and heterogeneous systems. This requires a variety of components, such as efficient processing, data storage, software, and algorithms. The goal of this BMBF-funded project is to develop new methods for reducing data traffic between compute nodes with distributed memory and storage in file systems on supercomputers.

For this purpose, a co-design approach will be used to develop solutions for variable-precision computation, data compression, and novel data formats. These solutions will be used to improve GENE, a program used worldwide for the simulation of plasma turbulence, and will be validated using GENE (`https://genecode.org/`). This would be a breakthrough in plasma physics with global visibility and many novel application possibilities, resulting in an acceleration of fusion research. Furthermore, new insight and methods of the DAREXA-F project can be transferred to other research areas and be made available for teaching and research of a broad audience. 2024 marks the second of the three-year project, and we had a closer look at compression algorithms with a focus on ZFP, lower-precision computation, and enhanced collective communications on GPU systems, and presented our work as a poster at Supercomputing 25 (https://sc24.supercomputing.org/proceedings/poster/poster_files/post109s2-file2.pdf). The project is a collaboration between Max Planck Computing and Data Facility (MPCDF)/Garching, Max-Planck-Institut für Plasmaphysik (IPP)/Garching, Technische Universität München/Garching, Friedrich-Alexander-Universität Erlangen-Nürnberg/Erlangen, and ParTec AG/ München.

6.2.6 EE-HPC: Energy-efficient HPC

https://eehpc.clustercockpit.org/

The energy consumption of HPC data centers is a decisive factor in the procurement and operation of the systems. EE-HPCachieves a more efficient energy use of HPC systems by targeted job-specific control and optimization of the hardware configuration as well as of settings of the runtime environments.

The aim of the project is the automated optimization of the energy efficiency of HPC systems. An innovative monitoring system is to contribute to reducing energy consumption while simultaneously increasing computing performance. This goal is to be achieved by new software-based control mechanisms of system parameters. The adjustment of system parameters, such as the utilization of computing nodes, is to take place automatically. A monitoring software coupled with a novel user interface shall provide the user with a transparent platform to also decide on the energy efficiency part of the computing load. This holistic approach ensures flexible and broad use for a wide range of applications.

In 2024, a number of experiments with Gromacs on CPU and GPU targets on both Fritz and Alex superclusters were conducted. The experiments focused on evaluating the energy efficiency of Gromacs in many scenarios and benchmarks, also changing the frequency and power capping settings of the machines. Apart from that, there were some improvements and fixes in MD-Bench, a performance-focused prototyping harness application, which was used as the base application, for the MuCoSim seminar where students could engage and work on challenging parallelization and performance engineering problems. Tutoring activities were also provided for the students and also assisted them in obtaining interesting insights on Molecular Dynamics, SIMD, and GPU performance in general.

6.2.7 StrömungsRaum: Novel Exascale-Architectures with Heterogeneous Hardware Components for Computational Fluid Dynamics Simulations

https://gauss-allianz.de/de/project/title/StroemungsRaum

For applications to efficiently exploit the power of exascale systems, scalability must be improved on very large and heterogeneous systems. A variety of components are required for modern high-performance computing: from processors to data storage and file systems to software and algorithms. All of these components also require new technologies and adaptations to specific applications and interfaces. The goal of the project StrömungsRaum is to improve the scalability of the open-source software FEATFLOW from the field of computational fluid dynamics (CFD) for application on exascale architectures with heterogeneous hardware components. This should enable fi-er resolution and more complex computations and improve energy efficiency by reducing computation time. The core of the work consists of the development of novel numerical solution methods, such as so-called multigrid solvers and highly scalable domain decomposition methods, which will be tested and validated within the project. The innovative core is a novel, scalable solution for flow simulations with subsequent implementation in modern heterogeneous (exascale) architectures. Due to the improved scalability with simultaneous increase in efficienc , high-resolution simulations can be generated for industrial use. One example is flow simulations in chemical reactors to achieve the most complete reaction and high yield. The open-source approach additionally provides a high degree of broad-scale effectiveness.

In 2024, our work centered on performance engineering for codes used in productionscale CFD applications, namely: FROSch, a parallel overlapping Schwarz solver framework in Trilinos, and FEAT, a finite element analysis toolbox supporting iterative and multigrid solvers.

FROSch will generate a preconditioner of the form: $M^{-1} = \Phi A_0^{-1} \Phi^T + \sum_{i=1}^{N} R_i^T A_i R_i$. Scalability limitations in the three-level recursive application of FROSch at high core counts are well documented. Using Intel's trace analyzer ITAC, we identified inefficient communication patterns stemming from Trilinos' Import/Export mechanism when applying the final Φ matrix to the triple product $\Phi A_0^{-1} \Phi^T$. We are collaborating with FROSch developers to resolve this.

One of the main applications of FEAT is to solve the saddle-point system that derives from the discretization of a d-dimensional (Navier-)Stokes system, where $v\colon \Omega \to \mathbb{R}^d$ is the velocity vector field and $p\colon \Omega \to \mathbb{R}$ is the pressure function:

$$\begin{bmatrix} A & B \\ D & 0 \end{bmatrix} \begin{bmatrix} v \\ p \end{bmatrix} \begin{matrix} = \\ = \end{matrix} \begin{bmatrix} f \\ 0 \end{bmatrix}$$

The sub-matrices B and D exhibit unsymmetric $n \times m$ block structures in their block-CSR representations (e.g., 2 × 3, 1 × 4), which severely limits the performance of vendor-optimized libraries like cuSPARSE. This has led to ongoing efforts to develop custom Sparse Matrix-Vector Multiplication (SpMV) kernels tailored for such block layouts. At high MPI-rank counts, communication within the Vanka multigrid smoothers emerges as the primary bottleneck. We mitigated this by eliminating global synchronization via delayed status checking and restructuring of MPI_Wait operations. At lower ranks, performance remains bounded by block-CSR SpMV in the smoother operations.

6.2.8 EoCoE-III

Many pressing questions about the future global energy supply lead to highly complex scientific problems that are increasingly being researched with the help of simulations on supercomputers. The scientific topics range from photovoltaics to the use of geothermal energy or the design of wind farms to plasma physics for the possible future use of fusion energy. Simulations replace and complement expensive and lengthy experiments. Together with several partners from different European countries (France, Germany, Italy, Belgium, Great Britain, Spain, Poland), a continuation application to the expiring EU project "EoCoE" (Energy oriented Centre of Excellence) was submitted in 2018, funded by the Horizon 2020 project (`https://www.eocoe.eu/`). After a first extension EoCoE-II the second extension EoCoE-III started in 2024.

EoCoE-III is anchored both in the High Performance Computing (HPC) community and in the energy field. It channels its efforts into 5 exascale lighthouse applications covering the key domains of Energy Materials, Water, Wind and Fusion.

The multidisciplinary effort of the consortium partners harnesses innovations in computer science and mathematical algorithms within a tightly integrated co-design approach to overcome performance bottlenecks, to deploy the lighthouse applications on the coming European exascale infrastructure and to anticipate future HPC hardware developments.

Goals are to demonstrate the benefits to the energy industry, such as accelerated design of photovoltaic devices, high-resolution wind farm modelling over complex terrains and quantitative understanding of plasma core-edge interactions in ITER-scale tokamaks.

At FAU, in addition to the NHR@FAU, the *Chair of System Simulation* (Prof. Rüde) is also involved. The HPC group supports the application developers from the other project parts in the area of performance engineering. This includes, besides performance analysis and optimization, also the organization of courses, tutorials and "hackathons", where project collaborators can apply advanced performance analysis techniques to their own simulation codes.

6.3 Awards, Talks & Publications

6.3.1 Research Awards

2024 SIAM Activity Group on Supercomputing Best Paper Prize

On March 7, 2024, the paper A Recursive Algebraic Coloring Technique for Hardware-Efficient Symmetric Sparse Matrix-Vector Multiplication by Christie L. Alappat, Georg Hager, Olaf Schenk, Jonas Thies, Achim Basermann, Alan R. Bishop, Holger Fehske, and Gerhard Wellein was awarded the 2024 SIAG/SC Best Paper Prize. This paper was published in June 2020 in the renowned journal ACM Transactions on Parallel Computing. It is a collaboration among researchers from several institutions: NHR@FAU, the University of Lugano (Switzerland), German Aerospace Center (DLR), Los Alamos National Laboratory (USA), and the University of Greifswald (Germany).The work introduced a novel algorithm and library, the Recursive Algebraic Coloring Engine (RACE). It can adapt the parallelism in symmetric SpMV to the underlying hardware while retaining good load balancing and cache-friendly data access patterns. It thus solves a long-standing problem in computational science. Lead author Christie L. Alappat presented the paper at the SIAM Conference on Parallel Processing for Scientific Computing (PP24) in Baltimore, MD.

IEEE Transactions on Parallel and Distributed Systems Journal Best Paper Runner-Up Award

In December 2024, our paper titled *The Role of Idle Waves, Desynchronization, and Bottleneck Evasion in the Performance of Parallel Programs* [1], authored by Ayesha Afzal, Georg Hager, and Gerhard Wellein, was recognized with the 2023 *Best Paper Runner-Up Award* by the prestigious *IEEE Transactions on Parallel and Distributed Systems journal*. This achievement underscores the impact of our research on the field of parallel program performance and highlights our ongoing commitment to advancing computational research.

Extended Paper Submission for PMBS Best Short Paper to Paralel Computing Journal

In November 2024, following the recognition of our paper *Physical Oscillator Model for Supercomputing* by Ayesha Afzal, Georg Hager, and Gerhard Wellein—which received the *Best Short Paper Award* at the 14th *IEEE/ACM Workshop on Performance Modeling, Benchmarking and Simulation of High Performance Computer Systems* (PMBS23)—we were invited to submit an extended version to the *Journal of Parallel Computing*.

SC24 Poster

In November 17–22, 2024, the research poster, *DisCostiC: Simulating MPI Applications Without Executing Code,* by Ayesha Afzal, Georg Hager, and Gerhard Wellein presented at the *International Conference for High Performance Computing, Networking, Storage, and Analysis* (SC24) in Atlanta, GA, was nominated as *Best Research Poster Award Candidate and Finalist*. The poster showcased the capabilities of DisCostiC to simulate MPI applications without the need for code execution, providing a tool for performance analysis in parallel programming.

6.3.2 Talks

A. Afzal. *Predicting Parallel Applications Performance using Automated Analytic First-principles Models in DisCostiC*. Invited at TU Darmstadt, as part of the *Parallel Programming Group seminar series*, Mar 25, 2024.

A. Afzal: *Predicting Parallel Applications Performance using Automated Analytic First-principles Models in DisCostiC*. Invited talk at TU Darmstadt, Parallel Programming Group, Darmstadt, Mar 25, 2024.

C. L. Alappat: *Performance optimisation of sparse iterative solvers using temporal cache blocking*. Talk at the Minisyposium “Parallel in time methods for High-Performance Computing” at Algorithmy 2024, High Tatra Mountains, Slovakia, Mar 17, 2024.

C. L. Alappat: *Accelerating Sparse Iterative Solvers and Preconditioners Using RACE*. Best Paper Prize talk at SIAM PP24, Baltimore, MD, Mar 7, 2024.

C. L. Alappat: *Accelerating Sparse Solvers with Cache-Optimized Matrix Power Kernels*. Talk at the Minisyposium “Advancements in Sparse Linear Algebra: Hardware-Aware Algorithms and Optimization Techniques” at SIAM PP24, Baltimore, MD, Mar 7, 2024.

D. Ernst: *Performance Engineering of the Navier-Stokes Finite Element Assembly of Alya on GPUs*. Talk at the Minisymposium “Advances in Highly Parallel Solvers for Partial Differential Equations” at SIAM PP24, Baltimore, MD, Mar 8, 2024.

G. Hager: Analytic Performance Modeling for HPC Workloads. Invited talk at the Sino-German Workshop on Multiphysics Device Simulation and Hardware-Aware Computing, Xi’An, China, Oct 10-16, 2024.

G. Hager: *Hardware Evolution from an HPC Point of View*. Invited talk at “20 ans du Groupe Calcul,” Paris, France, Jun 3, 2024.

G. Hager: *Performance Engineering with Resource-Based Metrics*. Invited talk at the Zentralinstitut für Technische Informatik (ZITI), University of Heidelberg, Feb 5, 2024.

A. Kahler: *Performance Improvements through In-Depth Hardware Knowledge.* Talk at the 1st Proud and Strong in Computing Conference, Jun 24, 2024.

Dane Lacey. *Adaptive-Precision SpMV on modern multicore CPUs and GPUs – A Roofline Perspective.* ScalPerf24, Bertinoro, Italy, Sep 23, 2024.

Dane Lacey. *Adaptive Precision Sparse Matrix- Vector Products*. University of Bayreuth, Jul 22, 2024.

Jan Laukemann. *Brave New World? A closer look at Intel’s and NVIDIA’s newest CPUs*. Leogang Workshop, Mar 11–13, 2024.

Gerhard Wellein: *Performance Engineering for High Performance Computing*. Los Alamos National Laboratory, Los Alamos, NM, USA, Nov 13, 2024

6.3.3 Publications

[1] A. Afzal, G. Hager, and G. Wellein: *The Role of Idle Waves, Desynchronization, and Bottleneck Evasion in the Performance of Parallel Programs*. IEEE Transactions on Parallel and Distributed Systems 34(2), 623-638 (2023), DOI: https://doi.org/10.1109/TPDS.2022.3221085. 2023 Best Paper Runner-up in IEEE TPDS.

C. Alappat, J. Thies, G. Hager, H. Fehske, and G. Wellein: *Algebraic Temporal Blocking for Sparse Iterative Solvers on Multi-Core CPUs*. The International Journal of High Performance Computing Applications, 2024;0(0). Available with Open Access. DOI: https://doi.org/10.1177/10943420241283828.
Preprint: https://arxiv.org/abs/2309.02228

M. Chakraborty and H. Fehske: *Quantum transport in an environment parametrized by dispersive bosons*. Phys. Rev. B 109, 085125 (2024). DOI: https://doi.org/10.1103/PhysRevB.109.085125

[11] D. C. Lacey, C. L. Alappat, F. Lange, G. Hager, H. Fehske, and G. Wellein: *Cache Blocking of Distributed-Memory Parallel Matrix Power Kernels*. The International Journal of High Performance Computing Applications (IJHPCA), 2025. DOI: https://doi.org/10.1177/10943420251319332. Available with Open Access.

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R. Ravedutti Lucio Machado, J, Eitzinger, and H. Köstler: *P4irs: An Intermediate Representation and Compiler for Parallel and Performance-Portable Particle Simulations*. SSRN, 4714072 (2024).
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DOI: https://doi.org/10.1038/s42004-024-01369-y

H. Owen, D. Ernst, T. Gruber, O. Lemkuhl, G. Houzeaux, L. Gasparino, and Gerhard Wellein: *Alya towards Exascale: Optimal OpenACC Performance of the Navier-Stokes Finite Element Assembly on GPUs*. In 2024 IEEE International Parallel and Distributed Processing Symposium (IPDPS), San Francisco, CA, USA, 2024 pp. 408-416. DOI: https://doi.org/10.1109/IPDPS57955.2024.00043
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7 NHR@FAU APPLICATION FOCUS

7 NHR@FAU APPLICATION FOCUS

NHR@FAU offers the whole spectrum of both atomistic simulation methods and their fields of application: Scientists at FAU use methods from classical MD to quantum chemistry, and everything in between. Atomistic simulation methods are applied in chemistry, biology, physics, medicine, materials science, and engineering.

We have established a Germany-wide unique interdisciplinary competence center that helps users to select and use atomistic simulation methods in an HPC environment and actively accompanies and coordinates the development of high-performance simulation codes. An interdisciplinary approach promises not only synergy effects through the exchange and joint development of simulation and evaluation tools but a cross-fertilization of materials and life sciences, which often use the same or very similar simulation techniques. Software for simulations and data analysis is thus readily available at production quality when the corresponding HPC installations start their operation. In turn, liaison scientists aware about the actual computational requirements can recommend optimized workflows of current simulation-based research.

A further core project is the education and lifelong training of scientists and engineers. The close cooperation between theory, simulation, and experiment ensures that the training is not aimed specifically at modelers but that it is made available to experimental colleagues as well. NHR@FAU makes an important contribution to the key technologies of scientific computing and software development through sustained concentration of methodological competence both in application and development of computer codes and their hardware-related optimization.

7.1 Atomistic Simulation Center (ASC)

The NHR centers in Paderborn, Berlin, and Erlangen have a strong focus on atomistic simulations. Researchers develop methods for and perform interdisciplinary simulations with various applications in the materials and the life sciences, spanning the areas of physics, biology, and chemistry. In order to join forces, share expertise, and bundle competence, the centers have formed the *Atomistic Simulation Center*. This umbrella organization serves as a platform providing guidance in tackling research questions by simulations.

Liaison scientists at the three centers, who are local experts in software and application domains, assist in providing individual support through advice and training on methods, software, tricks, and pitfalls, best-suited architectures, and best practices.

The CECAM node *Mathematics and Computation in Molecular Simulation* enhances European cooperation in computational research in biology, chemistry, engineering, and physics. In 2024 a flagship workshop about *Perspectives and challenges of future HPC installations for atomistic and molecular simulations* provided a platform for scientific researchers, software engineers, and hardware specialists to exchange about recent successes and demands for the future in the field of atomistic and molecular simulations using HPC and to communicate early technological innovations to scientific researchers

7.2 Activities of Liaison Scientists

Dr. Frank Beierlein

Computer-Chemie-Centrum (CCC) & NHR@FAU

NHR activities, projects, and support

Frank Beierlein was part of the organizing team for the 36th Molecular Modeling Workshop, which took place as a hybrid event in Erlangen from March 4-6, 2024. Together with Petra Imhof, Frank Beierlein organized the Computational Chemistry part of the "Tag der offenen Labortür", which took place on March 26, 2024. The regular NHR liaison scientist seminars and the AG Imhof group seminar serve as further opportunity to present and discuss current and planned activities. Close contact with the RRZE HPC group is further ensured by regularly attending the RRZE HPC Café.

As one of the two liaison scientists (LS) responsible for AMBER, Frank Beierlein provides support for AMBER customers of NHR@FAU, together with Anselm Horn. Frank Beierlein trained scientists for performing standard MD and thermodynamic integration free energy simulations with AMBER on the NHR@FAU GPU cluster Alex. The Imhof group members use Frank Beierlein's scripts and protocol to investigate e.g. DNA-repair mechanisms, the Gmeiner group (NHR project "`Medchem-Dynamics`", Susanne Gleich, Nico Staffen, Eduard Neu) was also supported in their effort to perform high-throughput docking of a large ligand database into the NK1 receptor, looking for agonists (using the DOCK software). The NAMD software was benchmarked and tested on Alex, with the result that the GPU-resident mode of NAMD 3.0.1 works on our Alex GPU cluster as advertised by the developers. This software is used by NHR project `b235bb`, which was also supported. Following the AMBER list and the AMBER literature ensures being up-to-date on what happens in the AMBER community. Together with the RRZE HPC group, Frank Beierlein continues optimizing the setup of AMBER simulations for efficient use on the GPU cluster Alex.

Frank Beierlein is an expert in parameterizing nonstandard residues and ligands for AMBER. Together with Anselm Horn (Sticht group), Frank Beierlein compares different approaches for the parameterization of non-standard amino acids, nucleic acids, and ligands. As a result of a close collaboration with Anselm Horn, Heinrich Sticht, Andriy Mokhir, and others a joint paper on cancer-specific activation of pro-drugs was published in January 2024 (*Biomolecules* 2024, 14, 153.).

In his current research on DNA repair mechanisms, Frank Beierlein carries on performing conventional, unbiased MD as well as alchemistic free energy methods, like thermodynamic integration, a technique that is increasingly used in pharmaceutical research. The first funding period of Frank Beierlein's NHR proposal (`b106dc/DNARepairTDG`) for computing time and storage on Alex was successfully completed, which provided valuable insights into the mechanisms of DNA repair by Thymine DNA Glycosylase. The results obtained from this NHR project are very promising and will likely be published shortly. An extension of this NHR project was applied for in August 2024 and granted in February 2025. Additionally, Frank Beierlein supports Petra Imhof's NHR project `b186dc` (DNA glycosylase—DNA base excision repair) and Petra Imhof's DFG project on DNA repair (IM141/1-3).

Frank Beierlein also closely collaborates with Janet Lovett (School of Physics and Astronomy, University of St Andrews) and Edward Anderson (Organic Chemistry, University of Oxford) in a project on spin-labeled RNA:DNA hybrids. Here, comparison of simulations with experiment allows a direct interpretation of the EPR experiments conducted in St Andrews and also an assessment of the quality of the force fields used in the simulations.

In their teaching (see page 56) and research activities Frank Beierlein and Petra Imhof take care that documentation, scripts, and inputs are as user-friendly as possible to ensure that even unexperienced users or potential NHR customers can use advanced simulation techniques on HPC systems.

Teaching & training

Frank Beierlein is closely involved in teaching computational chemistry courses/hands on user trainings for the FAU students at the Computer-Chemistry-Center (CCC). These were, in 2024, *Datenmanagement-Anwendungen—Data-PR*, *Bio-Organic & Bio-Inorganic—Lab BioIOC-LAB*, *Drug Discovery—LAB DD-LAB*, and *Bio-Organic & Bio-Inorganic Chemistry—Lab BioIOC-LAB*.

Publications

I. Klemt, V. Reshetnikov, S. Dutta, G. Bila, R. Bilyy, I. C. Cuartero, A. Hidalgo, A. Wünsche, M. Böhm, M. Wondrak, L. A. Kunz-Schughart, R. Tietze, F. Beierlein, P. Imhof, S. Gensberger-Reigl, M. Pischetsrieder, M. Körber, T. Jost, A. Mokhir. *A concept of dual-responsive prodrugs based on oligomerization-controlled reactivity of ester groups: an improvement of cancer cells versus neutrophils selectivity of camptothecin*, *RSC Med. Chem. 2024*, 15, 1189-1197.
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(also presented as a "research highlight" in the NHR@FAU newsletter on Apr 19, 2024)

F. Beierlein, A. H.C. Horn, H. Sticht, A. Mokhir, P. Imhof. *In Silico Study of Binding of Camptothecin-Based Pro-Drugs to Human Carboxylesterase 2*, *Biomolecules 2024*, 14, 153.
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DOI: https://doi.org/10.3390/ijms252413725

Posters

J. A. A. Balderas, F. Beierlein, P. Imhof. *Insight into the active site conformation of DNA repair enzyme MBD4 from molecular simulations*, 36th *Molecular Modeling Workshop*, Erlangen, Mar 4–6, 2024.

F. Beierlein, A. H. C. Horn, H. Sticht, A. Mokhir, P. Imhof. *In Silico Study of Binding of Camptothecin-Based Pro-Drugs to Human Carboxylesterase 2*, 36th *Molecular Modeling Workshop*, Erlangen, Mar 4–6, 2024.

Outreach

The Molecular Modeling Workshop, which is annually organized in Erlangen by the Molecular Graphics and Modeling Society—Deutschsprachige Sektion e.V., took place from March 4-6, 2024. Frank Beierlein is an active member of this society and supports the managing board as helping hand and cash auditor („Kassenprüfer"). He also contributed scientifically by presenting posters; at this opportunity, the excellent computing facilities and support of NHR@FAU were emphasized, in addition to the scientific results. At the „Tag der offenen Labortür" on March 26, 2024, the Imhof group presented the field of computational chemistry to potential new FAU students. The research in the Imhof group was also presented at the event „Unser Department—Unsere Forschung (UDUF)" on June 10, 2024. A "research highlight" on our two papers on *Cancer-Specific Activation of Prodrugs* (*Biomolecules* 2024, 14, 153; RSC Med. Chem. 2024, 15, 1189-1197.) was presented in the NHR@FAU newsletter on April 19, 2024, and a "Spotlight" on Frank Beierlein in the same newsletter on February 18, 2024.

Collaboration with other Liaison Scientists and HPC staff

Together with Anselm Horn, Frank Beierlein is the responsible liaison scientist for AMBER. Frank Beierlein also closely collaborates with Anselm Horn on the parameterization of non-standard amino acids, nucleic acids, and ligands, which resulted in the publication of a joint paper in January 2024. Together with the HPC group, the AMBER performance is optimized on the NHR@FAU HPC systems.

PD Dr. Anselm Horn

Department of Medicine (Professorship for Bioinformatics) and NHR@FAU

Projects and support

Anselm Horn had applied his expertise in generating force field parameters to support two projects studying protein-ligand interactions.[1,2] The parameters obtained are now publicly available to the scientific community.

Since the AI-driven structure prediction software AlphaFold2 has been installed locally on the NHR@FAU cluster, it is now possible to run protein structure predictions on a larger scale. Anselm Horn thus entered a collaboration with the group of Prof. Dr. Soba (DFG-Heisenberg-Professor für zelluläre und molekulare Neurophysiologie, FAU Erlangen-Nürnberg). Within this project, the local AlphaFold installation is utilized to optimize strategies for targeted protein engineering, the results of which are then to be evaluated experimentally. Building on this, a more comprehensive systematic design approach is envisaged, which will then require a designated NHR-project.

Additionally, Anselm Horn applied his skills in atomistic molecular modeling to collaborate with other research groups: a research project together with the Comprehensive Cancer Center Erlangen (FAU Erlangen-Nürnberg) resulted in a joint publication.[4] Furthermore, supporting the group of Dr. Henry Oppermann (Institut für Humangenetik, Universität Leipzig) by the use of computational methods also yielded a joint publication.[5]

In an emergency data project, Anselm Horn supported a graduate student from the Institute of Anatomy (FAU Erlangen-Nürnberg) in rescuing all his generated R research data. As the file size was too large to be processed on normal desktop computers, the huge-memory facilities of NHR@FAU were utilized to split up the data and make them accessible again.

Performance Tests

Anselm Horn continued to run simulations with the AMBER-specific coarse-grained force field Sirah to obtain further experience. Although the Martini force field shipped with the Gromacs molecular dynamics package is the most used and best-known method, the AMBER-approach Sirah is an alternative with a different parameterization focus.

Teaching and Training

Anselm Horn further pursued his work on AMBER training and started to conceptualize an introductory workshop for molecular dynamics (beginners' level) together with Frank Beierlein. The underlying concepts were already applied for the training of a new PhD student Silvana Zurmühl, who joined the Research Training Group 2950 SyMoCADS ("Synthetic Molecular Communications Across Different Scales: From Theory to Experiments")[6] in 2024. First scientific results were presented at the NHR conference in Darmstadt [7], supported by an NHR travel grant to Ms Zurmühl. Additionally, Anselm Horn continued his training of PhD student Olena Denysenko (RTG 2504)[8], resulting in a conference contribution at the MMWS in Erlangen [9].

At the technical level, Anselm Horn participated in a project of Dr. Georg Hager (NHR@FAU), to provide MS Windows users with alternative access to the HPC systems after the former HPC-service running NoMachine was retired. His suggestions where then incorporated into the updated online help.

Exchange and Collaboration with other Liaison Scientists

Anselm Horn is engaged in ongoing collaboration projects with liaison scientist Frank Beierlein, where he applies his expertise in force field parameter generation. The results from these collaborations are part of two publications in 2024.[1,2] The work was also presented at the Molecular Modelling Workshop (MMWS) in Erlangen[3].

He participated in the regular, mostly informal online meeting of the Liaison Scientists once a week. This Zoom meeting every Wednesday was organized by Dr. Lanig (NHR@FAU executive secretary) and provided a platform for mutual exchange about many organisational, technical, and scientific aspects. Scientifically, atomistic simulations played a major role.

A further important opportunity for the exchange with both, NHR@FAU staff and the other Liaison Scientists, was the monthly HPC café, and more specifically the coffee session right before the talk. The technical and scientific input provided by the respective speakers, either internal or external, additionally widened the general HPC knowledge and inspired further ideas.

Outreach

Anselm Horn was part of the organisational committee of the MMWS 2024 in Erlangen that provided a special HPC section ("HPC meets Molecular Modelling").[10] He presented a poster about the NHR@FAU computational facilities informing potential users about the application procedure, again advertising "free" small-scale test projects.[11] This opportunity offers access to the NHR@FAU clusters without the formalities of a full application process, but allowing users to test both the cluster hardware and the software environment for their own research problems. As member of the German Chemical Society (GDCh), he also wrote a conference review about the MMWS and the NHR involvement in the GDCh members' journal.[12] Since the GDCh has more than 28,000 members from all areas of chemistry, such contributions may strongly add to the visibility of NHR. In turn, the poster informing about the NHR@FAU facilities, the NHR initiative, and the small-scale project offer was also presented at the German Conference of Cheminformatics, which was organized by a subdivision of the GDCh.[13]

He further continued support on the AMBER Mailing List supporting national and international users to address problems, especially in the area of parameter generation. Thus, he helped to increase the visibility of NHR@FAU both, as a local brand and as part of the nationwide NHR initiative.[14]

The joint publication with Frank Beierlein [1] was presented in the NHR@FAU newsletter (April).[15] An earlier publication of the Bioinformatics group, which Anselm Horn supported by tailor-made force field parameters, was summarized in the first quartl volume that year.[16]

Administrative tasks

Anselm Horn acted as scientific and technical reviewer for several NHR@FAU proposals and as advisor in NHR@FAU projects.

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Marius Trollmann

Computational Biology, Department of Biology and NHR@FAU

NHR activities

Projects & Support

Marius Trollmann is a liaison scientist in the field of molecular dynamics (MD) simulations with a special focus on the software package *GROMACS*. His expertise extends to simulating biomolecular systems using both GPUs and CPUs. In his role, Marius Trollmann has provided support to NHR-funded projects, ensuring optimal utilization of available resources: For two NHR large-scale projects (ID: b223dc and ID: b224dc), he provided benchmark data during the application process, and supported the users during the lifetime of the projects in the performance of their simulations. In close collaboration with the NHR@FAU support staff, Marius Trollmann helps to ensure an e cient application of GROMACS on the Fritz (CPU), and Alex (GPU) clusters regarding parameter choices or submission scripts. Since the end of 2024, he is particpating in the early-access phase of the new GPU cluster Helma.

Scientific results

As a PhD-student, Marius Trollmann applies and enhances his expertise by utilizing available resources in his own research projects. Notably, he contributed sign cantly to the development of the Python-ba sed software tool *DomHMM* that (semi-)automates the detection process of ordered domains in lipid bilayers utilizing machine-learning [1]. The open-source project is available as so-called "MDAKit" as part of the popular MDAnalysis ecosystem [7, 6]. He further uses state-of-the-art constant-pH molecular dynamics (cpHMD) simulations to investigate the protonation behavior of pharmaceutical-relevant aminolipids in lipid nanoparticle (LNP) formulations. The ability to model dynamic (de-)protonation events during classical MD simulations allows for a more realistic representation of the processes crucial for delivering bioactive mRNA into human cells to protect the body against severe infections or certain cancer types [2, 5]. To support other researchers in the MD community in setting up their own constantpH simulations of lipid nanoparticles, he summarized the most important steps and practical guidelines in a book chapter [4].

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Outreach

Throughout the year, Marius participated in several national and international scientific conferences. His work on the modeling of full lipid nanoparticles [3] was featured in the *Best of Biophysical Journal* Symposium at the annual meeting of the American Biophysical Society in Philadelphia (USA). For his poster presentation at the Heraeus Seminar 2024 on *Physical Modes of Action of Membrane-Active Compounds* in Bad

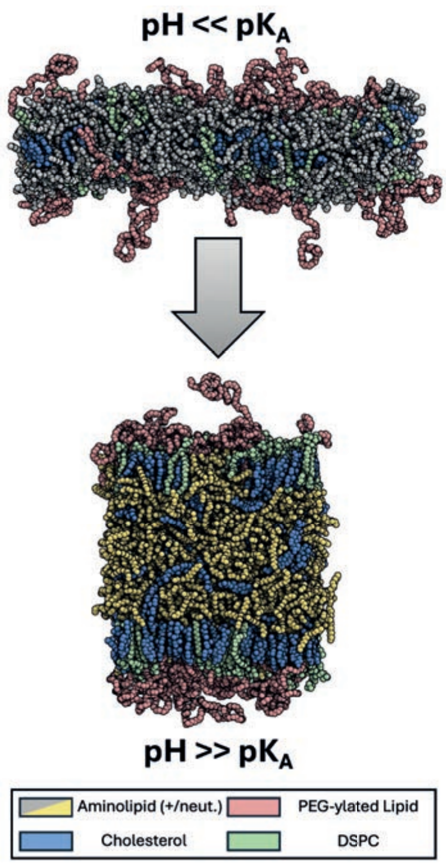

Figure 1: Lipid nanoparticle (LNP) formulations at low and high pH containing the aminolipid ALC-0315. At pH levels below the apparent pK$_A$ of the aminolipids, the protonated form is the dominant species of ALC-0315, forming a very exible lipid bilayer. Raising the pH level, leads to a phase transition characterized by a migration of deprotonated ALC-0315 into the membrane core forming a hydrophobic slab sandwiched between two polar monolayers. Figure was taken from Trollmann *et al.* [5].

Honnef (Germany), he received the *Best Poster Prize*. In the context of the NHR, he presented a poster about his current research at the second NHR conference in Darmstadt. A more comprehensive list of his additional outreach activities can be found below.

Teaching & training

Marius Trollmann actively contributes to the education and training of both new and existing users of HPC systems. Working with students on cutting-edge scientific topics using state-of-the-art simulation codes requires the integration of HPC resources into the tutorials. To achieve this, he utilizes the JupyterHub instances provided by NHR@FAU in various tutorials, giving students access to NHR resources within a realistic HPC environment. This approach allows students to apply highly optimized software on HPC systems early in their academic journey, introducing them to the NHR association already during their undergraduate studies. The knowledge and experience acquired during these tutorials have subsequently been shared with other research groups to facilitate the organization of similar hands-on tutorials.

- *Orientierungsmodul Strukturbiologie I*, Master Zell- und Molekularbiologie/Integrated Life Sciences
- *Orientierungsmodul Strukturbiologie II*, Master Zell- und Molekularbiologie/Integrated Life Sciences
- *Orientierungsmodul Computational Immunobiology*, Master Zell- und Molekularbiologie/Integrated Life Sciences
- *Fachmodul Strukturbiologie*, Bachelor Biologie/Integrated Life Sciences

In the *Orientierungsmodul Strukturbiologie I*, *Orientierungsmodul Strukturbiologie II*, and *Orientierungsmodul Computational Immunobiology* courses, students are given the opportunity to prepare and conduct their own molecular dynamics (MD) simulations to work on a realistic and biologicalrelevant research hypothesis. The *Fachmodul Strukturbiologie* is a more general introduction into the MD engine GROMACS, and the subsequent post-processing/analysis of biomolecular systems.

Meetings, travel, and community outreach

- Weekly virtual NHR@FAU liaison scientist meeting
- Annual Meeting of the American Biophysical Society, Feb 10–14, 2024, Pennsylvania (Poster Presentation)
- Heraeus Seminar on *Physical Modes of Action of Membrane-Active Compounds*, Apr 7–10, 2024, Bad Honnef, (Poster Presentation)
- Workshop on *Computer Simulation and Theory of Macromolecules,* Apr 19–20, 2024, Hünfeld, (Contributed Talk)
- International Membrane Biophysics Meeting, May 6–8, 2024, Drübeck, (Contributed Talk)
- NHR Conference '24 (Scientic Conference), Sep 9–10, 2024, Darmstadt, (Poster Presentation)
- NHR Conference '24 (NHR Networking Event), Sep 11–12, 2024, Darmstadt

Awards

- *Best of Biophysical Journal* with *mRNA Lipid Nano-particle Phase Transition*
  DOI: `https://doi.org/10.1016/j.bpj.2022.08.037`
- *Best Poster Prize*—Hereaus Seminar on *Physical Modes of Action of Membrane-Active Compounds*

Dr. Egor Trushin

Chair of Theoretical Chemistry and NHR@FAU

NHR activities, projects, and support

Egor Trushin is a *liaison scientist* in the field of *ab initio* methods for electronic structure calculations, with a special focus on the development of novel density-functional and quantum chemistry methods. He is actively involved in the implementation of new quantum chemistry and density-functional methods in several computational quantum chemistry software packages, such as *Molpro* [1], *PySCF* [2], and *PySCFAD* [3]. Furthermore, Egor maintains his own code, *sigma-4pyscf* [4], which is interfaced with PySCF and enables highly accurate density functional theory calculations using the *σ-functional method* [5] that was developed at the Theoretical Chemistry Department at FAU.

Teaching & training

Egor is involved in teaching and mentoring young researchers in scientific programming and in using modern quantum chemistry software. He has also developed a series of Jupyter notebook tutorials that demonstrate how to apply quantum chemical methods developed at the Theoretical Chemistry Department at FAU.

Scientific results

As a postdoc at the Chair of Theoretical Chemistry, Egor applies and deepens his knowledge and skills in computational chemistry and scientific programming. His recent study on the self-consistent random phase approximation method resulted in a publication as first author in Physical Review Letters, which is considered one of the most prestigious in the field of physics. Furthermore, a number of other research projects were published in Q1 journals.

Publications

R. Mandalia, S. Fauser, E. Trushin, A. Görling. *Assessment of RPA and σ-functional methods for the calculation of dipole moments and static polarizabilities and hyperpolarizabilities*—J. Chem. Phys. 162, 184106 (2025).

S. Fauser, E. Trushin, A. Görling. *Highly precise values for the energy ratios underlying the Lieb–Oxford bound and the convexity conjecture for the adiabatic connection*—J. Chem. Phys. 162, 164108 (2025).

E. Trushin, A. Görling. *Improving Exchange-Correlation Potentials of Standard Density Functionals with the Optimized-Effective-Potential Method for Higher Accuracy of Excitation Energies*—J. Chem. Theory Comput. 21, 4, 1667–1683 (2025).

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8 APPENDIX

8 APPENDIX

8.1 Publications which used NHR@FAU Resources

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J. A. Amador Balderas, F. Beierlein, A. Horn, S. Volkenandt, L. Völcker, N. Mokhtari, J. C. Epee Ndongue, and P. Imhof. 2024. *Mode of Metal Ligation Governs Inhibition of Carboxypeptidase A*. *International Journal of Molecular Sciences 25*, 13725. DOI: https://doi.org/10.3390/ijms252413725. (Alex, TinyGPU)

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8.2
NHR Compute Time Projects

In this section we list all compute projects that used the NHR@FAU resources GPGPU parallel computer *Helma*, parallel computer *Fritz*, and GPGPU cluster *Alex* in 2024, sorted by fields of science. To give a short overview of the diverse scientific disciplines, the projects are listed according to DFG subject areas—information that is added to the application by the *Principal Investigators* (PIs). Abstracts are truncated as indicated by square brackets; full-length abstracts can be found at `https://hpc.fau.de/about-us/nhr-compute-time-projects/`.

Humanities and Social Sciences

Fine Arts, Music, Theatre and Media Studies

bildsynth: Bildsynthese als Methode des kunsthistorischen Erkenntnisgewinns (10/2024–10/2025)
[…] AI-driven generative models to transform the study of art history by creating new digital images that visually represent complex concepts such as style, composition, and pose. […] enhances both art interpretation and the analysis of large image datasets […] new insights into image understanding and visual content analysis in cultural heritage.
PI: Prof. Dr. Björn Ommer, Ludwig-Maximilians-Universität München
Target system: Alex

Linguistics

MULTIDATA: Skills and resources for the multimodal turn: Unlocking audiovisual datasets for research and learning (10/2024–09/2027)
[…] transition from analog or textual approaches to digital, audiovisual, and statistical skills for the study of language, communication, cognition, and their technological and social applications. […] obtain speech and gesture data from video files, offer didactic and learning resources. […] develop a free online platform with an open-source multimodal processing pipeline to analyze speech and gesture data from videos. […]
PI: Prof. Dr. Peter Uhrig, FAU
Target systems: Fritz & Alex

MultiGest24: Multimodal models of Co-Speech Gesture (05/2024–04/2025)
[…] studying the mechanisms used for disinformation, in particular viewpoint manipulation, by Russian state-sponsored media. […] use the dataset created in the first stage of the project (NHR-project Pose-22) to build a multimodal transformer that allows us to improve performance of downstream tasks such as gesture detection, segmentation and annotation.
PI: Prof. Dr. Peter Uhrig, FAU
Target systems: Fritz & Alex

Literary Studies

LitCharAnnot: Annotation of Characterizations in Literary Texts (07/2024–06/2025)
[…] investigate the textual description of character's internal and external features, actions […] develop a character-attentive, "literary" language model ("LitBERT") for automatic literary analysis. […] improve the handling of longer texts like novels by advancing the capabilities of language models to represent knowledge, like representation and types of characters in the text world (i.e., the world described in the text).
PI: Prof. Dr. Fotis Jannidis, Julius-Maximilians-Universität Würzburg
Target system: Alex

Life Sciences

Basic Research in Biology and Medicine

PDZpeptide: How phosphorylation affects peptide interaction with adaptor domains (10/2024–12/2025)
[…] use plain molecular dynamics simulations and non-equilibrium alchemical molecular dynamics simulations to study how adaptor domains interact with

phosphorylated vs. non-phosphorylated peptides. […] want to understand mechanistically why phosphorylation can favor or disfavor binding of peptides to these two PDZ domains depending on where it is placed along the peptide sequence.
PI: Prof. Dr. Volkhard Helms, Saarland University
Target system: Alex

ALsim: Rendering Antibody Light Chains Amyloidogenic: Insight into Systemic Amyloidosis from Molecular Dynamics Simulations (10/2024–12/2025)
[…] systematically introduce a large variety of mutations and posttranslational modifications in amyloidogenic LCs derived from patients diagnosed with AL. […] enable us to connect the molecular insights from our simulations with the pathological course of the disease. […] resolve the molecular principles of misfolding […] serve as foundation for improved diagnostics and treatment.
PI: Prof. Dr. Nadine Schwierz, Augsburg University
Target system: Alex & Fritz

Athena: A multimodal intelligent agent for general-purpose protein design (07/2024–06/2025)
[…] develop a multi-task intelligent agent capable of efficiently engineering functional proteins tailored to user-defined specifications. […] the agent will be trained using available sequence, structural, functional, and dynamic data to perform multiple protein engineering tasks. The model will be freely accessible through user-friendly interfaces, empowering researchers worldwide with an easy-to-use tool for tailored protein design.
PI: Dr. Noelia Ferruz, Universität Bayreuth
Target system: Alex

ReceptorCrosstalk: Understanding the Mincle-FcγR crosstalk in the regulation of autoantibody-dependent inflammation (07/2024–06/2025; LARGE SCALE)
[…] explore the competitive binding of activating FcγRs and of the C-type lectin receptor Mincle to the common FcRγ-chain, characterize the receptor-specific lipid environment and their impact on receptor dimerization, receptor clustering and signaling, and the modulation of autoantibody-driven inflammation. […] enhance our understanding of the complex mechanisms underlying Mincle-dependent modulation […]
PI: Prof. Dr. Rainer Böckmann, FAU
Target systems: Fritz & Alex

MK2P97: Allosteric Mechanism of the ATPase p97 (06/2024–09/2025; LARGE SCALE)
The ATPase p97 is a hexameric protein complex that pulls out other proteins from complexes or membranes for further processing, e.g. degredation. […] During pulling, the substrate is pushed through a pore in the center of p97 by moving its subunits in a ladder motion […] formulate a hypothesis through studying the collective coupled motions with molecular dynamics simulations.
PI: Dr. Martin Kulke, Technical University of Munich
Target system: Alex

ProtDynDesign: Probing the effects of evolution-guided atomistic design on the dynamics of periplasmic binding proteins (06/2024–06/2026; NHR STARTER)
[…] elucidate the conformational dynamics underlying protein switching behavior upon interaction with target molecules, thereby advancing our ability to engineer functional nanoswitches. […] insights into the mechanisms governing protein conformational rearrangements, facilitating the rational design of responsive biosensors and other innovative nanotechnologies.
PI: Prof. Dr. Birte Höcker, Universität Bayreuth
Target systems: Fritz & Alex

AMPel: High-resolution analysis of synergistic effects between membrane active peptides and classical antibiotics on bacterial membranes (04/2024–03/2027)
[…] The aim of the proposed project is to use membrane-active peptides to influence bacterial membranes such that (i) classical antibiotics become more effective, and (ii) substances with a high affinity for the target structure but a low or even non-existent membrane permeability can efficiently reach their target. […]
PI: Prof. Dr. Rainer Böckmann, FAU
Target systems: Fritz & Alex

GlyMoProt: Molecular dynamics Simulations of glycan-modulated protein interactions in dense cellular environments—Impact of cancerous glycan types on cell adhesion (04/2024–09/2025; LARGE SCALE)
[…] A crucial process in metastasis is the disruption of cell adhesion, enabling cancer cells to detach and invade surrounding tissues. This transition involves the upregulation of N-cadherin, enhancing cell motility and invasiveness. […] Glycosylation of cadherins modulates these interactions, impacting protein folding, trafficking, and dynamic shielding. […]
PI: Dr. Isabell Louise Grothaus, Universität Bremen
Target systems: Fritz & Alex

DynaTaste: Molecular dynamics simulations of taste molecular systems (02/2024–01/2025)
Bitter and sweet taste modalities are mediated by chemosensory receptors […] Sweet and bitter receptors recognize chemically diverse molecules. […] investigate the dynamics of sweet and bitter taste receptors in complex with peptide modulators.
PI: Prof. Dr. Antonella Di Pizio, Technical University of Munich
Target system: Alex

CaSRMD: Molecular Dynamics Investigation of Calcium-sensing Receptor Dynamics (01/2024–06/2025; LARGE SCALE)
[…] In light of new Cryo-EM structures of the CaSR, we intend to explore VFT/CRR activation dynamics by permutating occupancy of binding sites, and further simulate the full-length and G-protein bound CaSR dimer. Additional analysis by e.g. allosteric network analysis of this multi-regulated system featuring various allosteric modulators, helps to uncover the activation dynamics of the CaSR.
PI: Prof. Dr. Peter W. Hildebrand, Freie Universität Berlin
Target systems: Fritz & Alex

ORmd: Systematic molecular dynamics simulations of the odorant receptor family (10/2023–03/2026; LARGE SCALE)
ORmd aims to explore the dynamics of all the odorant receptors [...] [with] cutting-edge High-Throughput Molecular Dynamics simulations starting from receptor models in the active and inactive states. [...] analyses of the trajectories will allow us to outline structural features relevant to the activation [...]
PI: Prof. Dr. Antonella Di Pizio, Technical University of Munich
Target system: Alex

ChannelProtonation: Investigating the Influence of Protonation States on Cation Conductivity in Ion Channels through Molecular Dynamics Simulations (10/2023–06/2025)
[...] investigating the dynamics of proton-coupled cation permeation in ion channels, with a specific emphasis on comprehending how pH influences the channel's cation conduction and selectivity. [...]
PI: Prof. Dr. Han Sun, Technical University of Berlin
Target system: Alex

AmPeL: Interaction of Antimicrobial Peptide Lugdunin with Membranes (Large Scale, 07/2023–09/2024)
[...] understanding of the novel antimicrobial peptide lugdunin by characterizing its interaction with various bacterial and eukaryotic membrane models. [...] mechanisms of action underlying lugdunin's antimicrobial properties against bacteria, [...] reasons for its lack of activity against erythrocytes. [...]
PI: Prof. Dr. Rainer Böckmann, FAU
Target systems: Fritz & Alex

DNA-glycosylase: DNA Base excision repair (06/2023–06/2026)
[...] machinery of enzymes, recognising and removing damaged/wrong bases and replacing them [...] some [glycosylases] also have lyase activity [...] revealing the mechanism of this strand incision, [...] [relation to] specificity of glycosylases with dual activity compared to [...] mono-functional glycosylases.
PI: Prof. Dr. Petra Imhof, FAU
Target system: Alex

Dynasome3: Exploring Protein Dynamics Space to Improve Protein Function Prediction (10/2022–09/2025; LARGE SCALE)
The function of proteins is determined by their amino acid sequence and tertiary structure, but nevertheless the particular function of most proteins is unknown.

[...] we explore to what extent protein function can be predicted by protein dynamics, and explore the space of protein dynamics in general. [...]
PI: Prof. Dr. Helmut Grubmüller, Georg-August-Universität Göttingen
Target system: Fritz

GPCRSCOMPEVO: Computational models of structure, dynamics and evolution of GPCRs (07/2022–01/2028; LARGE SCALE)
[...] R*-Gs/i/o arrestin complexes resolved so far do not provide a clear explanation for G protein coupling specificity. [...] existence of transient complexes between the R* and GTP-bound G protein [...] several novel intermediates on the way to the formation of GαsGTP and may contribute to coupling specificity.
PI: Prof. Dr. Peter W. Hildebrand, Leipzig University
Target systems: Fritz & Alex

CoupledFoldBind: Conformational presentation switching processes studied by Molecular Simulations (07/2022–05/2025)
[...] follow conformational changes in proteins at atomic resolution and at high time resolution. [...] Especially in case of conformational switching processes such as binding induced folding an understanding of the process requires the analysis of intermediate states and driving forces for conformational changes. [...]
PI: Prof. Dr. Martin Zacharias, Techn. Univ. of Munich
Target system: Alex

SimMediSoft: Biomolecular simulations for the efficient design of lipid nanoparticles (07/2022–12/2024)
[...] tool to deliver RNA to target cells thereby providing promising perspectives to combat life-threatening diseases such as Amyloidosis or COVID-19. [...] to resolve the structure of these clinically relevant particles and [provide] molecular insights how the RNA cargo is distributed inside the [lipid nanoparticles] LNPs. [...]
PI: Prof. Dr. Nadine Schwierz, Augsburg University
Target systems: Fritz & Alex

DNARepairTDG—DNA Repair by Thymine DNA Glycosylase (06/2022–09/2025)
Thymine DNA glycosylase [...] involved in DNA repair [...] removes mispaired or modified DNA bases [...] ensures genetic integrity. [...] investigate the possible role of imino-tautomeric forms [...] [and the] effect of different protonation states [...] [and the effect of] an important histidine residue in the binding pocket.
PI: Dr. Frank Beierlein, FAU
Target system: Alex

Antivirals: Structure-based design and optimization of ligands for novel antiviral strategies (04/2022–03/2027)
[...] complexes between antibodies and the viral fusion proteins from HIV-1 and CoV-2 are analyzed to identify energetic hot-spots of the interaction. [...] design of antibody-derived peptides that bind to viral fusion proteins thereby blocking viral infection. [...]
PI: Prof. Dr. Heinrich Sticht, FAU
Target system: Alex

Medicine

LLM4MMD: Large language models to process multimodal medical data (09/2024–08/2026)
[…] clinicians consider an array of multimodal data, such as demographic and genomic information, patient interviews, laboratory test results and biomedical images. […] we will build upon these abilities of LLMs—tunability, processing of multimodal data and causal reasoning—to create clinical decision support systems that can process multimodal healthcare data.
PI: Dr. Martin Menten, Julius-Maxim.-Univ. Würzburg
Target system: Alex

PANDORA: FOR2886 PANDORA Pathways triggering Autoimmunity and Defining Onset of early Reumatoid Arthritis (04/2024–07/2025)
[…] understand the influence of the natural bacterial flora or the microbiome as well as a number of environmental factors (including nutrition and salt consumption) on our immune system and […] their impact on immune tolerance. […] are combined with state-of-the-art deep learning algorithms to map the cellular and molecular landscape of the synovial tissue during onset of inflammation.
PI: Prof. Dr. Katharina Breininger, Julius-Maximilians-Universität Würzburg
Target system: Alex

MIA-NORMAL: Medical Image Analysis with Normative Machine Learning (10/2023–09/2028; LARGE SCALE)
[...] develop normative representation learning as a new machine learning paradigm for medical imaging, providing patient-specific computational tools for robust confirmation of normality, image quality control, health screening, and prevention of disease before onset. [...]
PI: Prof. Dr. Bernhard Kainz, FAU
Target system: Alex

Medchem-Dynamics: Molecular Dynamics and Docking Studies with Multifunctional Receptor-Ligand Complexes (01/2023–06/2025; LARGE SCALE)
[...] understand relationships of structure and function, including the interactions of the individual modules. Modeling will also guide ligand optimization. [...] support the rationalization of the observed biological responses and integrate novel structural information obtained by biophysical methods. [...]
PI: Prof. Dr. Peter Gmeiner, FAU
Target system: Fritz

PatRo-MRI-2: Pathology-robust image reconstruction in Magnetic Resonance Imaging (10/2022–09/2026)
[...] beneficial for speedy imaging protocols that prioritize patient comfort. However, this reduction in data acquisition could cause generic image reconstruction techniques to obscure disease markers, replacing pathological features with typical healthy image features derived from the training data.
Principal Investigator: Prof. Dr. Bernhard Kainz, FAU
Target system: Alex

FPRMetaD: Investigating binding pathways for a diverse set of ligands with biased and unbiased simulation of the Formyl Peptide Receptor (08/2022–12/2025)
Our project includes unbiased and biased molecular dynamics simulations of the FPR receptor class and its vast array of ligands that include modified peptides as well as non-modified peptides and small molecules like Lipoxin A4 or the circular peptide Ciclosporin A. [...]
PI: Prof. Dr. Oliver Koch, Universität Münster
Target systems: Fritz & Alex

InTimeVRSimulPatMod: In-time Virtual Reality Simulation Patient Models: Machine Learning and immersive-interactive Modeling of Virtual Patient Bodies (06/2022–05/2025)
[...] provide high-quality body models given medical imaging data by the segmentation of relevant structures.[...] current machine learning methods and atlas-based methods are to be compared for their segmentation proposals [...]
PI: Prof. Dr. Andre Mastmeyer, Aalen University
Target systems: Fritz & Alex

Neurosciences

SFB 1540: Exploring Brain mechanics (EBM) Understanding, engineering, and exploiting mechanical properties and signals in central nervous system development, physiology and pathology (01/2024–12/2026)
[…] explores mechanical influences on the central nervous system (CNS), of which many processes are not yet fully understood. Mechanical signals have shown to impact CNS cell function, emphasizing mechanics' crucial role. EBM aims to enhance CNS understanding for improved neurological disorder diagnosis and treatment. […] employs advanced machine learning for domain adaptation and generalization.
PI: Prof. Dr. Katharina Breininger, Julius-Maximilians- Universität Würzburg
Target system: Alex

charite_mlcn: Aligned preprocessing of structural and functional neuroimaging data of the NAKO (National German Cohort) and UK Biobank (01/2024–06/2025)
[…] align the preprocessing of two large MRI datasets from the UK Biobank and NAKO Gesundheitsstudie, predominantly comprising healthy individuals. […] predicting various phenotypes from neuroimaging data modalities and a comparative analysis of the results between the two datasets will be conducted based on robustness and reproducibility criteria.
PI: Dr. Marc-André Schulz, Charité, Universitätsmedizin Berlin
Target system: Fritz

HPC-MarkovModelling: Single-channel Markov modelling of voltage-gated ion channels with simulations and implementation of the 2D-Fit algorithm on High Performance Computing Cluster (08/2022–05/2025)

[...] modelling single-channel patch-clamp data with Markov models. The 2D-Dwell-Time fit with simulations of time series captures gating kinetics with a high background of noise and can extract rate constants beyond the recording bandwidth. [...] exceptionally valuable for relating ion-channel kinetics [...]

PI: PD Dr. Dr. Tobias Huth, FAU

Target systems: Fritz & Alex

Natural Sciences

Molecular Chemistry

SiAl-Reactivity: Reactivity of low-valent/low-oxidation-state Si- and Al-based molecular compounds (10/2024–10/2025; NHR STARTER)

[…] studying in detail the properties of the low-valent/low-oxidation-state main-group-element-based molecular compounds, with special focus on silicon and aluminum. […] study computationally the mechanisms of reactions of low-valent Si and Al based molecular compounds. […] develop novel chemical transformations and applications based on low-valent main group species.

PI: Dr. Arseni Kostenko, Technical University of Munich

Target system: Fritz

SpectroscopicProperties: Spectroscopic properties of molecules with unusual electronic structures (07/2022–12/2025)

[...] predicted how to harness the peculiar properties of carbene decorated diradicals in solar cells and demonstrated their use as singlet fission molecules. Thus, our calculations helped to discover a new class of molecules of use for solar energy conversion, quantum computing, or organic light emitting diodes (OLEDs).

PI: Prof. Dr. Dominik Munz, Saarland University

Target system: Fritz

MoTrNanoMat: Molecular transport in nanoporous materials (07/2022–10/2025)

[...] interconnected channels can be used for "flow-through" applications such as purification of drinking water or nanoseparation of proteins or organic solvents. Here, we will evaluate the impact of (i) nanomaterial kind, (ii) pore size, (iii) pore shape, and (iv) solvent polarity on the material's permeability [...]

PI: Dr. Kristyna Pluhackova, University of Stuttgart

Target systems: Fritz & Alex

Chemical Solid State and Surface Research

CIMSSNB: Computational Investigation of Materials for Solid State Na-Based Batteries (05/2024–04/2025)

[…] investigate the potential of NaxV2(PO4)2F3, a polyanionic compound, as a promising material for sodium-ion batteries. […] understand the mechanisms limiting sodium extraction in fluorophosphate cathodes, with a focus on expanding the compositional range and introducing transition metals for enhanced performance. […] explore the stability and electrochemical proprieties of these materials.

PI: Prof. Dr. Matteo Bianchini, Universität Bayreuth

Target system: Fritz

Crystal23: Prediction of new ferroelectric metal fluorides (04/2024–06/2025; NHR STARTER)

[…] predict new ferroelectric metal fluorides. To this end, we will compile an overview of polar metal fluorides, which we will investigate using crystallographic and quantum chemical methods. The starting point is a database screening that yields fluorides in 105 structure types that potentially crystallize in polar space groups. […]

PI: Prof. Dr. Florian Kraus, Philipps-Universität Marburg

Target system: Fritz

Lg_SurfCatal_AIMD_MLFF: Computational modeling of new surface catalysis systems by means of ab initio methods as well as novel machine-learning force-field approaches (07/2022–12/2025; LARGE SCALE)

[...] Periodic DFT simulations are able to shed a light on the exact processes taking place at the catalyst.

Recently, a new machine-learning force-field (ML-FF) was developed which is able to efficiently learn on the fly from DFT data, leading to a high-level FF for metal surfaces in contact with other phases [...]
PI: Prof. Dr. Andreas Görling, FAU
Target system: Fritz

Physical and Theoretical Chemistry

MultiTransBatt: Correlated ion and electron transport in Li-ion battery cathode materials (09/2024–09/2027)
[…] discovering the interactions of charge carriers in battery materials. […] localize electrons in the form of polarons, which in turn have been shown to also influence ionic movement. […] compute the energies and transport properties of symmetry inequivalent polaron configurations for different degrees of doping, and lithiation, and different defect concentrations, to unravel […] the correlation between polarons and ions.
PI: Prof. Dr. Harald Oberhofer, Universität Bayreuth
Target system: Fritz

PolarBatt: Polaronic Influences on the Charge Transport Properties of Battery Anodes (08/2024–04/2026)
[…] test the hypothesis that many of the […] experimentally observed properties of lithium titanium oxide, can be explained considering the occurrence of polarons. […] examine the possibly correlated motion of either charge carrier at different degrees of lithiation of the material (i.e. charging of the battery) […] point the way towards rational design criteria for improved battery anodes, e.g. in the form [of] certain defect patterns.
PI: Prof. Dr. Harald Oberhofer, Universität Bayreuth
Target system: Fritz

Ion-catch: Molecular Modelling based design of ligand shells to functionalize magnetic nanoparticles for the removal of heavy metal pollutants from water (07/2022–05/2025)
[...] designing tailor-made functionalization of magnetite nanoparticles to bind heavy metal ions and related organometallic compounds by means of molecular modelling and simulation. [...] developing a model-based search strategy for identifying suitable constituents and structures as guides to syntheses. [...]
PI: Prof. Dr. Dirk Zahn, FAU
Target systems: Fritz & Alex

Condensed Matter Physics

MLQT: Machine Learning for Quantum Technology (09/2024–08/2027)
[…] exploit the known strengths of machine learning approaches in dimensional reduction and pattern recognition for the advancement of near-term quantum technology. […] push the boundaries of classical simulations for the certification of quantum simulators […] exploit the new capabilities in order to investigate otherwise inaccessible terrain in the realm of correlated matter.
PI: Dr. Markus Schmitt, University of Regensburg
Target system: Alex

MLTCM: Machine Learning to Tailor Correlated States of Matter (09/2024–08/2025)
[…] propose to overcome some of the current limitations by combining techniques from machine learning with ideas from quantum many-body physics. Within this project, we will develop simulation methods for periodically driven systems based on neural quantum states (NQS), and a new interpretable framework for tensor-networks- based reinforcement learning (RL) to optimize control of quantum matter.
PI: Dr. Markus Schmitt, University of Regensburg
Target system: Alex

Hitma: Hydrogen in transition-metal alloys (08/2024–08/2025)
[…] major materials-science challenges in the transition from fossil to hydrogen-based fuels. […] thorough understanding of the interplay between H atoms and the local geometric and chemical details of the microstructure. This project addresses the impact of H on single-crystal Ni-based superalloys and on grain boundaries in ferritic alloys. […]
PI: PD Dr. habil. Thomas Hammerschmidt, Ruhr-Universität Bochum
Target system: Fritz

ion_solvation: Ion solvation free energies in molten salts electrolytes (08/2024–07/2025)
[…] focus on the computation and prediction of ion formation energies in molten chloride electrolytes, such as LiCl, KCl, NaCl, CaCl2, and MgCl2. This work founds the base to enable selective metal extraction by providing theoretical guidance that complements experimental efforts.
PI: Prof. Dr. Lucio Colombi Ciacchi, Universität Bremen
Target system: Alex

A07SFB1277: Quantum transport and time-dependent dynamics of Dirac fermions (05/2024–07/2025)
[…] employ complementary quantum mechanical wave packet-based techniques and semiclassical path integral methods, with emphasis on reaching the regimes of parameters where the well-established so-called three-step-method may break down and non-classical mechanisms are responsible for the emission process.
PI: apl. Prof. Dr. Juan Diego Urbina, University of Regensburg
Target system: Alex

SuperSEM: Simulation of unconventional superconductors with long-range interactions beyond the mean-field approximation (10/2023–09/2025)
[...] use the T-matrix approach to derive a generalized gap equation that goes beyond the mean-field approximation. [...] investigate how the phase diagram of a 2D superconductor changes as higher-order quantum corrections are included. [...] explore whether the Higgs mode [...] stabilized due to long-range interactions in the mean field limit, remains stable in the T-matrix approach.
PI: Dr. Andreas Buchheit, Saarland University
Target system: Fritz

PCL-topology: Optical and vibrational signatures of structural and electronic topology in planar carbon lattices (07/2023–06/2026)
[...] In this project, we will investigate the physical properties of such PCLs [planar carbon lattices] by numerical methods and predict new PCL structures with intriguing topological and correlated electronic properties.
PI: Prof. Dr. Janina Maultzsch,FAU
Target system: Fritz

FRASCAL P12: Quantum-to-Continuum Model of Thermoset Fracture (06/2023–05/2026)
[...] understanding of fracture in brittle heterogeneous materials by developing simulation methods able to capture the multiscale nature of failure. [...] focus on the influence of heterogeneities on fracture at different length and time scales [...] [in this] cross-sectional topic in mechanics of materials. [...]
PI: Prof. Dr. Ana-Sunčana Smith, FAU
Target system: Fritz & Alex

SELRIQS: Series expansions for long-range interacting quantum systems (06/2023–02/2026)
[...] understanding of quantum phases and quantum phase transitions, where competing long-range interactions [...] result in unconventional correlations and interesting entanglement properties. [...] [determine] complicated quantum-critical properties in quantum many-body systems with long-range interactions.
PI: Prof. Dr. Kai Phillip Schmidt, FAU
Target system: Fritz

UltrafastDyn: Ultrafast electron dynamics and Kerr rotations (01/2023–06/2025)
This project focuses on simulating and understanding topological materials and their excitations under ultrafast laser driving; it is motivated by experimental activities towards “lightwave spintronics” in Dirac systems. [...]
PI: Dr. Jan Wilhelm, University of Regensburg
Target system: Fritz

DMFT2TBLG: DMFT study of a heavy-fermion model for twisted bilayer graphene (12/2022–03/2026)
Twisted bilayer graphene (TBLG) has recently captivated the interest of the condensed matter community, for its capability of hosting a wide variety of peculiar phenomena such as superconductive and correlated insulating phases, as well as topological features. [...]
PI: Dr. Lorenzo Crippa, Julius-Maximilians-Universität Würzburg
Target system: Fritz

nqsQuMat: Neural quantum states for strongly correlated quantum matter (12/2022–12/2025, LARGE SCALE)
[...] we employ a modern method named neural quantum states which has shown great potential in studying various quantum problems. [...] target both ground states as well as the time evolution of cutting-edge quantum models to gain new insights on novel quantum phenomena.
PI: Prof. Dr. Markus Heyl, Augsburg University
Target system: Alex

FRG: Functional Renormalization Group calculations for material analysis (11/2022–06/2025)
Current ab-initio theory for solid state materials excels in the prediction of electronic band structures. The secondary part of any full description—the interaction between electrons—is beyond the scope of those methods. [...] (FRG) has the expressed goal of deriving effective low-energy interaction models. [...]
PI: Prof. Dr. Carsten Honerkamp, RWTH Aachen Univ.
Target system: Fritz

ALFQMCsim: Emergent and critical phenomena in correlated electron systems: Quantum Monte Carlo simulations (10/2022–03/2026; LARGE SCALE)
[...] a general implementation of the so called auxiliary field quantum Monte Carlo algorithm. [...] triggered at solving systems of correlated electrons that couple to bosonic modes such as lattice vibrations. [...] allows us to compute properties of systems in thermodynamic equilibrium at polynomial cost. [...]
PI: Prof. Dr. Fakher Assaad, Julius-Maximilians-Universität Würzburg
Target system: Fritz

Optics, Quantum Optics and Physics of Atoms, Molecules and Plasmas

DelayLineDetectors: Deep Learning-Based Spatiotemporal Multi-Event Reconstruction for Delay Line Detectors (06/2024–05/2025; NHR STARTER)
[…] present a new spatiotemporal machine learning model to identify and reconstruct the position and time of such multi-hit particle signals. […] much better resolution for nearby particle hits compared to the classical approach, removing some of the artifacts and reducing the dead radius by half. We show that machine learning models can be effective in improving the spatiotemporal performance of delay line detectors.
PI: Dr. Marco Knipfer, FAU
Target system: Alex

DAREXA-F: Datenreduktion für Exascale-Anwendungen in der Fusionsforschung (06/2023–11/2025)
[...] develop new methods for reducing data traffic between compute nodes with distributed memory and storage in file systems on supercomputers. For this purpose, a co-design approach will be used to develop solutions for variable-precision computation, data compression and novel data formats. [...]
PI: Prof. Dr. Gerhard Wellein, FAU
Target systems: Fritz & Alex

Particles, Nuclei, and Fields

GAMMAML: Deep learning with the H.E.S.S., CTA, and SWGO gamma-ray telescopes (01/2024–12/2025)
[…] H.E.S.S. operates by observing the Cherenkov light emitted when such a gamma-ray creates a particle cascade in the atmosphere; the nature, origin, and energy of the incident particle can be determined using image processing techniques. State-of-the-art deep learning methods allow for high-sensitivity image analysis at high-speed, by exploiting patterns in the data which are currently not being exploited […]
PI: Dr. Jonas Glombitza, FAU
Target system: Alex

CLS3pt: Hadron structure observables on lattices at low pion masses (10/2023–06/2025; LARGE SCALE)
[...] Using this [lattice QuantumChromoDynamics] method we propose to compute (and improve on) the matrix elements related to Beyond-the-Standard-Model (BSM) interactions (which are not accessible experimentally) and (lower) moments of the parton distribution functions.
PI: PD Dr. Wolfgang Söldner, University of Regensburg
Target system: Fritz

ETH: SU(2) real time evolution on a classical computer (04/2023–11/2025)
[...] we want to find out whether SU(2) (as prototype for all SU(N) gauge theories) fulfills the Eigenstate Thermalization Hypothesis (ETH). [...] It can be addressed on small lattice volumes and thus is one of the best candidates for an early demonstration of quantum supremacy. [...]
PI: Prof. Dr. Andreas Schäfer, University of Regensburg
Target system: Fritz

DPDa: Quark Double Parton Distributions of the Nucleon (04/2023–06/2025; LARGE SCALE)
A better understanding of Double-Parton Distributions (DPDs) in the proton is vital to make full usage of the discovery potential of the LHC (CERN). [...] we want to perform additional simulations with different lattice constants, which will allow for a continuum extrapolation. [...]
PI: Prof. Dr. Andreas Schäfer, University of Regensburg
Target system: Fritz

addlight: The spectrum of charmonium and glueballs: adding the light hadrons (01/2023–04/2026; LARGE SCALE)
[...] In this project we plan to study charmonium and glueballs by simulations of QCD on a lattice. The novelty of our study is the inclusion of light hadrons into which these states can decay. Our software has excellent scaling behavior on HPC systems.
PI: Prof. Dr. Francesco Knechtli, Bergische Universität Wuppertal
Target system: Fritz

Statistical Physics, Soft Matter, Biological Physics, Nonlinear Dynamics

ArrhythmiaControl: Investigating termination mechanisms of chaotic spiral and scroll wave dynamics underlying cardiac arrhythmias by using hypothesis-driven and AI-driven termination approaches (02/2024–03/2027)
Sudden Cardiac Death caused by, for example, malignant ventricular arrhythmias, results in an estimated 600.000 deaths per year in the European Community alone. […] Current clinical treatment consists of the application of a high-energy defibrillation shock […] alternative control strategies, with the aim to significantly reduce these side effects while reliably terminating the arrhythmia and restoring sinus rhythm. […]
PI: Prof. Dr. Thomas Lilienkamp, Technische Hochschule Nürnberg
Target system: Alex

CLINT-M02: Multiscale modelling of SILP and SCILL catalysis (07/2023–06/2025)
[…] developing an understanding of the structural and transport properties of functionalised ILs and reactant molecules within the film using molecular dynamics simulations. […] boost the spatial coordination of the reactants with the solid and the gas interfaces, and address issues of solubility, viscosity as well as wetting. […]
PI: Prof. Dr. Ana-Sunčana Smith, FAU
Target system: Alex

CRC1411D04: Design of Particulate Products: Modelling particle aggregation and assembly into optimal structures (03/2023–12/2026)
[…] develops and applies new methods to study not only the self-assembly process itself but also the properties of the self-assembled nanostructures. The computations in this proposal closely interact with experimental work that is conducted in the framework of the Collaborative Research Centre Design of Particulate Products.
PI: Prof. Dr. Michael Engel, FAU
Target systems: Fritz & Alex

EnSimTurb: Towards ensemble simulations of fully developed turbulence (12/2022–04/2026)
[…] investigate the statistical properties of fully developed turbulence. […] aim at developing new theoretical and computational approaches to better understand and model fully developed turbulence. […] capture the large-scale dynamics of turbulent flows. Both projects use our code TurTLE, a pseudo-spectral solver of the Navier-Stokes equations which also features particle tracking capabilities.
PI: Prof. Dr. Michael Wilczek, Universität Bayreuth
Target systems: Fritz & Alex

Astrophysics and Astronomy

FISHNET: Fisher Information Surrogates for High-energy NEutrino Telescopes (07/2024–06/2025)
[…] Our surrogate model will learn to parametrize detector responses, enabling more efficient event simulations. Additionally, it will facilitate design studies for next-generation detectors like P-ONE and IceCube-Gen2. By leveraging statistical tools, our framework will optimize detector design without the need for limiting the design parameter space or developing event selection and reconstruction algorithms.
PI: Prof. Dr. Claudio Kopper, FAU
Target system: Alex

AREPOStar1: 'First light' of the AREPO-Star project: A grid of global 3D moving-mesh radiation hydrodynamic simulations of red supergiant envelopes (07/2024–06/2025)
[…] perform a suite of global 3D radiation hydrodynamic simulations of red supergiant envelopes with updated physics. […] most up-to-date models to be compared with observations of red supergiants. [… enable …] simulations of wind launching, shock breakout, common envelope, and binary mass transfer, which pose major uncertainties in our predictions of some transient events and gravitational wave sources.
PI: Prof. Dr. Selma E. de Mink, Ludwig-Maximilians-Universität München
Target system: Fritz

3Dmasstransfer: 3D hydrodynamics simulations of mass transfer in interacting binaries (04/2024–06/2025)
[…] by adopting a novel approach to hydrodynamics calculations, we attempt to simulate the mass transfer process, focusing on understanding the properties of transferred mass, using detailed hydrodynamics simulations. […] implications for the stability of mass transfer […] build an accurate prescription for mass transfer, implement it into stellar evolution codes, and investigate the binary evolution.
PI: Prof. Dr. Selma E. de Mink, Ludwig-Maximilians-Universität München
Target system: Fritz

ECOGAL_MW: Full disk modeling of the Milky Way (05/2023–04/2025)
[…] create the essential synergic framework where the extensive observational datasets available for our Galaxy can be analyzed back-to-back with state-of-the-art theoretical simulations of all Galactic environments, also using innovative machine-learning and decision-making tools. […] build a unifying predictive model of the Milky Way ecosystem […] interweaves the unique expertise of four European research groups […]
PI: Dr. Noé Brucy, Heidelberg University
Target system: Fritz

Mathematics

FOR5134-HPC: Nonlinear finite element simulations of thermoelasticity/thermoplasticity equations in laser beam welding processes (08/2024–08/2025)
[…] In our project we consider a laser beam welding process. […] due to the high cooling rate inherent in the process solidification cracks can occur. […] provide a complete simulation of this process that will gives us indicators under which conditions a crack can appear. A multiscale approach is needed to represent the properties and the behavior of the material and moreover efficient solver strategies are indispensable. […]
PI: Prof. Dr. Axel Klawonn, University of Cologne
Target system: Fritz

PDExa-CFD: Efficient simulation of fluid flow with high-order finite element methods (02/2024–09/2025)
[…] new understanding of the flow behavior near boundaries and support future method development. […] uses high-order discontinuous Galerkin finite element discretizations in space and splitting implicit/explicit methods in time to discretize the incompressible Navier-Stokes equations. […] direct numerical simulation of the flow over a periodic hill will be computed at a Reynolds number Re=19,000 as well as limit studies […]
PI: Prof. Dr. Martin Kronbichler, Ruhr-Univ. Bochum
Target systems: Fritz & Alex

Bio-FROSch: Modeling and simulation of pharmaco-mechanical FSI for an enhanced treatment of cardiovascular diseases and non-Newtonian micro-macro blood flow simulations (07/2023–06/2025)
[...] develop a robust numerical framework including suitable models [...] of the effects of drugs on the complex bio-chemo-mechanical processes in arterial walls. [...] improve computational efficiency of the multiscale model by identifying and implementing areas where advanced ML techniques can be applied. [...]
PI: Prof. Dr. Axel Klawonn, University of Cologne
Target systems: Fritz & Alex

StroemungsRaum: Neuartige Exascale-Architekturen mit heterogenen Hardwarekomponenten für Strömungssimulationen (03/2023–09/2025)
[...] the open-source software FEATFLOW, is a central component of the StroemungsRaum platform that is successfully used by the industrial partner of the project IANUS for years. In the context of the whole project, FEATFLOW will be extended methodologically and by parallel near-hardware implementations.
PI: Prof. Dr. Stefan Turek, TU Dortmund University
Target systems: Fritz & Alex

Atmospheric Science, Oceanography and Climate Research

BigDataGeo2: From data to action–Increasing the resilience of the agricultural sector in north Bavaria with artificial intelligence and web solutions (03/2024–08/2025)
[…] increase the resilience of farms in the northern Bavarian agricultural sector […] development of new modules […] that translate changing climate indicators such as heat stress, UV exposure and late frost into operationally relevant metrics such as crop stress factors, risk exposure and crop yields. […] develop data-driven climate models with Deep Learning […]
PI: Prof. Dr. Andreas Hotho, Julius-Maximilians-Universität Würzburg
Target system: Alex

EEA_TC: The Influence of Tropical Cyclones on Kilimanjaro's Glaciers (12/2023–01/2026)
Glaciers […] provide valuable long-term records of environmental change in the tropics […] understanding how large-scale climate signals manifest at regional and local scales. […] combining reanalysis, observations and kilometer-scale atmospheric modelling over Kilimanjaro. […] improved understanding of rainfall variability in Equatorial East Africa and refine the understanding of the climate proxy offered by the glaciers.
PI: Dr. Emily Collier, Humboldt-Universität zu Berlin
Target system: Fritz

ATMOS: Numerical atmospheric modeling for the attribution of climate change and for model improvement (08/2022–06/2025)
[...] aims to explore a novel climatic indicator, namely crustose coralline algae that grow in shallow ocean waters, for the purpose of improved global climate model evaluation. [...] improvement potential with regard to sea surface temperatures in the Southern Ocean and the effect of these ocean conditions [...]
PI: Prof. Dr. Thomas Mölg, FAU
Target system: Fritz

Geophysics and Geodesy

UrbanMorphology: A Geolingual Analysis to Global Urban Morphology (04/2024–04/2025; NHR STARTER)
[…] utilizes social media data as a tool to investigate the relationship between urban form and residents' opinions and emotions. […] reveals the potential impacts of physical environments on residents' opinions. This research not only enriches the scope of traditional urban morphology studies but also offers new perspectives and data support for urban planning and environmental policies.
PI: Dr. Richard Lemoine Rodriguez, Julius-Maximilians-Universität Würzburg
Target systems: Fritz & Alex

Theoretical Chemistry

ELTRANS: Electron transfer in organic and inorganic light-converting systems (10/2022–09/2026)
[...] design of new electrodes for photoelectrochemical water oxidation by studying the underlying electronic processes. [...] By simulating electron dynamics in

real-time and on a real-space grid, the project aims at unravelling charge-transport pathways in complex, interface-governed materials. [...]
PI: Prof. Dr. Stephan Kümmel, Universität Bayreuth
Target system: Fritz

Engineering Sciences

Mechanics and Constructive Mechanical Engineering

AkESoFlug: Acoustically and energetically self-optimising aircraft (09/2024–10/2025)
[...] By combining these simulations with experimental investigations, a clear separation of the different mechanisms in sound generation and their complex interactions will yield insights of high general validity, not yet available in the literature for drone propellers. The findings will enable conclusions to be drawn about which part of the system (propeller flow, blade structure, etc.) influences the emitted sound under various parameters. This will lead to a targeted approach to addressing acoustic issues in the development process. [...]
PI: apl. Prof. Dr. Stefan Becker, FAU
Target system: Fritz

CEEC-LSTM: EuroHPC Center of Excellence for Exascale CFD (07/2024–06/2027)
[…] enhance the precision, parallel efficiency, and energy efficiency of CFD simulations. […] improve energy efficiency contributing to sustainable computing practices. Using the developed algorithms, six different lighthouse cases of physical and engineering interest, ranging from aeronautical to atmospheric flows will be simulated. […] simulate the flow around a model merchant ship's hull […]
PI: Prof. Dr. Philipp Schlatter, FAU
Target system: Fritz & Alex

FRASCAL-FE: Computational continuum mechanics simulations at LTM for FRASCAL (11/2022–12/2026)
[...] Specifically, project P8 ("Fracture in Polymer Composites: Meso to Macro") aims to study the influence of different mesoscopic parameters, including microstructure morphology, on the macroscopic fracture properties of nano-particle reinforced polymers.
PI: Prof. Dr. Julia Mergheim, FAU
Target system: Fritz

FFRASCAL-MD: Particle-based computing at LTM for FRASCAL (09/2022–09/2027)
[...] In particular, sub-project P6 ("Fracture in Thermoplastic Polymers: Discrete-to-Continuum Coupling") provides a link between the level of atoms and the continuum with specific interest in the multiscale modelling and simulation of polymer fracture.
PI: PD Dr. Sebastian Pfaller, FAU
Target systems: Fritz & Alex

AkuRad: Fluid-Structure-Acoustic Interaction of Enclosed Radial Fans (09/2022–08/2025)
[...] investigate the multiphysical interrelationships of flow-related sound radiation of radial fans in volute casings using a combined, experimental, simulation-based approach. [...] tool that allows the flow-induced sound generation and its propagation in radial impellers to be analyzed [...]
PI: apl. Prof. Dr. Stefan Becker, FAU
Target system: Fritz

Heat Energy Technology, Thermal Machines, Fluid Mechanics

AOTTP-DFG18-1: Characterization of molecular diffusion in electrolyte systems (08/2022–07/2025)
Electrolytes conduct electric current by the movement of ions while blocking the free movement of electrons. For applications of electrolytes as working fluids, the transport of ions is important and can be subdivided into diffusion, convection, and, in the presence of an electric field, migration. [...]
PI: Prof. Dr. Andreas Paul Fröba, FAU
Target systems: Fritz & Alex

Materials Science

MeMabyDe: Active learning for Memristive Materials by Design (06/2024–04/2025)
Future neuromorphic devices promise to yield computational performances superior to contemporary ar-

tificial neural network […] while consuming a fraction of the energy. […] explores disorder engineering in off-stoichiometric perovskites and their solid solutions to design critical properties of memristive devices, by combining […] Metalorganic vapour-phase epitaxy with novel AI-based active learning strategies.
PI: Prof. Dr. Luca Ghiringhelli, FAU
Target system: Alex

Materials4.0—AITDB: Ab initio thermodynamic database development (10/2022–04/2025)
[...] focus will be on phase stabilities of various phases, including dynamically unstable ones. Having acquired such a database, the phase stabilities can be put into practice by re-parametrizing binary phase diagrams and studying the implications on multicomponent phase diagrams.
PI: Prof. Dr. Blazej Grabowski, University of Stuttgart
Target system: Fritz

Systems Engineering

RoughOpt: High Fidelity Simulations to resolve homogeneous and heterogenous roughness using highly scalable Spectral Codes NEK5000 and NEKO (05/2024–04/2025)
[…] compare the accuracy and performance of high-order methods for resolving roughness due to square riblet in a turbulent channel flow using four different approaches, AMR, conformal, IBM, and overlapping at Rebulk=10000. Further, we expand this study to simulation of heterogeneous roughness in pipe flows using Nek5000, a spectral code for a better accuracy at Rebulk=11700.
PI: Venkatesh Pulletikurthi, Ph.D., FAU
Target system: Fritz

Voxray: Quantenrekonstruktion für industrielle Computertomographie (07/2023–09/2024)
[...] Wir entwickeln aktuell die neuartige Quanten-Rekonstruktionstechnik (QRT), die den Rekonstruktionsschritt in der Industrie-CT revolutioniert. [...] [Damit] wird die Ausbreitung der einzelnen Röntgenphotonen (der Quanten) simuliert und anschließend invertiert. [...]
PI: Dr. Darius Rückert, FAU
Target system: Alex

Electrical Engineering and Information Technology

IRIS-EIT: Leveraging Reasoning AI for solving Electrical Impedance Tomography inverse problem (08/2024–07/2025)
[…] leveraging advanced Reasoning AI techniques to address the inverse problem of reconstructing conductivity distributions from boundary electrical measurements. […] developing specialized neural networks tailored to specific EIT setups, addressing issues such as shape variations, uneven electrode distributions, electronic inconsistencies, and random noise. […]
PI: Dr. Ayman Abdelwahab Ameen Ahmed, FAU
Target system: Alex

SMoReM: Small Models as Role Models (04/2024–08/2025)
The project aims to investigate the potential of hyperparameter optimization in Large Language Models (LLMs) by using substantially smaller models in the optimization process. […] If confirmed, it would open an avenue for a significant reduction of computational resources and energy consumption in LLM training and, in this way, increase the sustainability of LLM design and application.
PI: Prof. Dr. Emanuël Habets, FAU
Target system: Alex

MultilingualTTS: Multilingual Text-to-Speech Synthesis (03/2024–05/2025)
[…] these systems were inherently mono-lingual […] Enabling such systems to synthesize text in multiple languages requires modifications to the acoustic model of the TTS pipeline, i.e., the module that converts text inputs to speech features. […] extend the parallel TTS architecture ForwardTacotron to enable multi-lingual speech synthesis. We perform various experiments to analyze the design of our model extension.
PI: Prof. Dr. Emanuël Habets, FAU
Target system: Alex

RTSD: Real-Time Speech Dereverberation (01/2024–04/2025)
Effective communication is crucial in dynamic settings […] develop an effective and efficient single-chan-

nel dereverberation model tailored for indoor environments, removing undesirable late reflections. We are exploring low-complexity models suitable for real-time applications and aim to extend our research to multi-channel dereverberation. […] promises substantial improvements in everyday communication scenarios.
PI: Prof. Dr. Emanuël Habets, FAU
Target system: Alex

ALLMT: Acceleration of Large Language Model Training (01/2024–12/2024)
[…] accelerate training and convergence of large language models (LLMs) using novel optimizers such as Sophia and Lion. We train 3-billion parameter models, focusing on efficient optimizer configurations through an ablation study. […] evaluates training speed and quality, aiming to minimize the required computing resources. […] identify the most effective optimizer, […] offering a sustainable path for AI research.
PI: Prof. Dr. Emanuël Habets, FAU
Target systems: Alex & Fritz

DDRGI: Data-Driven Room Geometry Inference (01/2024–12/2024)
Knowing the room geometry may benefit many audio applications, including sound reproduction, audio rendering, acoustic scene analysis, and sound source localization. […] infer the room geometry using available room impulse responses from these types of devices. […] develop data-driven models that are robust to noise and to infer the room geometry faster and more accurately compared to classical methods.
PI: Prof. Dr. Emanuël Habets, FAU
Target system: Alex

GenSE: Generative AI for Real-time Speech Enhancement (12/2023–02/2025)
In today's fast-paced world, clear and effective com[…] focusing on generative rather than discriminative learning to design real-time speech enhancement solutions. […] pose the problem of speech enhancement as a resynthesis task rather than simply reducing the noise(s). […] resynthesize only the input speech signal at the output, thereby eliminating the other acoustic disturbances. […] advances the technical field of speech and acoustic signal processing […]
PI: Prof. Dr. Emanuël Habets, FAU
Target system: Alex

RTSE: Enhancing Speech Communication Using Real-Time Target Speaker Extraction (12/2023–11/2024)
[...] developing an advanced algorithm that not only distinguishes the target speaker from others but also actively suppresses background noise, resulting in a clearer and more intelligible audio output. [...] more effective communication in diverse and noisy environments [...]
PI: Prof. Dr. Emanuël Habets, FAU
Target system: Alex

Computer Science

ITEM: User's Choice of Images and Text to Express Emotions in Twitter and Reddit (12/2024–04/2027)
[…] contribute to multimodal emotion analysis and ensure that emotion-related information is not missed or misinterpreted in social media communication because computational models do, so far, not have access to the complete picture. […] answer research questions about how users of social media communicate their emotions, what influences their choices of modality and what the relation between the modalities is.
PI: Prof. Dr. Roman Klinger, Otto-Friedrich-University Bamberg
Target system: Alex

CEAT: Computational Event Evaluation based on Appraisal Theories for Emotion Analysis (12/2024–12/2025)
[…] create two approaches to assign these appraisal dimensions to textual event descriptions, firstly by building on top of semantic parsing and secondly in a deep learning setting. Based on these dimensions, we then predict the emotion associated with the textual fragment. This will lead to models that can automatically assign an emotion to an event description, even if no emotion words or self reports of feeling are available.
PI: Prof. Dr. Roman Klinger, Otto-Friedrich-University Bamberg
Target system: Alex

SVBRDF-Morphing: Generative Morphing of SVBRDF-based Material description (11/2024–10/2025; NHR STARTER)

[…] investigating novel methods to leverage deep generative techniques, such as diffusion models, for controlling material creation and editing within the latent space of these models. […] fine-tuning these models using publicly available datasets. Ultimately, our goal is to enable users to synthesize high-quality materials, allowing them to turn their imagination into reality.

PI: Prof. Dr. Tim Weyrich, FAU
Target system: Alex

DeepSmall: Meta-learning for regularizing deep networks under small data regimes (10/2024–09/2027)

[…] advance the capabilities of deep learning models to perform effectively on small tabular datasets. Handling small datasets such as in biomedical applications presents unique challenges […] develop robust and effective foundation models that perform well even in a small data regime. […] develop novel hyperparameter optimization methods tailored for large-scale deep-learning pipelines.

PI: Prof. Josif Grabocka, University of Technology Nuremberg
Target system: Alex & Fritz

ELMOD: Efficient language models for on-device deployment (10/2024–09/2025)

[…] understanding and developing strategies to train efficient multilingual models suitable for local and on-device deployment. […] data pre-processing and filtering to obtain high-quality training data, architectural design for efficient model inference, training of actual models, quantization of model parameters, and the evaluation of different model variants on established benchmark tasks.

PI: Prof. Dr. Emanuël Habets, FAU
Target systems: Alex & Fritz

HAnS: Adapting ASR Systems, Combining with LLMs, LipReading (08/2024–07/2025)

The KIZ, Institute for Artificial Intelligence at the Technische Hochschule Nuremberg focuses with projects on automatic speech and image processing. A strong focus lies in the development of ASR-related systems for medical & health applications, as well as generative system in the speech and vision domain.

PI: Prof. Dr. Tobias Bocklet, Technische Hochschule Nürnberg Georg Simon Ohm
Target system: Alex

INTELICECT: Intelligent systems with visual and linguistic comprehension for Continuous reasoning (08/2024–07/2025)

[…] integrating visual and linguistic comprehension within intelligent systems to enable continuous reasoning. […] reliance of contemporary systems on natural language processing for reasoning, underscoring the need to enhance these capabilities with robust visual reasoning. […] recalibrating processing pipelines across visual and linguistic domains to redefine the frontiers of intelligent systems. […]

PI: Prof. Dr. Thomas Seidl, Ludwig-Maximilians-Universität München
Target system: Alex

MeshGPTRLHF: MeshGPT with RLHF: Generating Triangle Meshes with Human Preference for Decoder Only Transformers (08/2024–07/2025)

[…] leverage the synergy between the Text-to-Text Transfer Transformer (T5) for processing natural language inputs and apply RLHF for aligning these language inputs with geometric outputs. […] make the generation more controllable by incorporating natural languages, where the application of reinforcement learning techniques play the key role, specifically RLHF and Decoupled Policy Optimization […]

PI: Prof. Dr. Matthias Schubert, Ludwig-Maximilians-Universität München
Target system: Alex

DBS-M4: Multi-modal Model Merging (07/2024–06/2025)

The integration of multiple generative models across disparate modalities presents a promising avenue for advancing multimodal AI. However, achieving seamless fusion while preserving the integrity of individual modal representations remains a formidable challenge. […] leverages cross-attention mechanisms to compose multimodal generative models from independently pre-trained unimodal decoders.

PI: Prof. Dr. Volker Tresp, Ludwig-Maximilians-Universität München
Target system: Alex

TA-Wikip-LLM: Time-Aware Wikipedia Specialist LLM (07/2024–01/2025; NHR STARTER)
[…] pre-training an LLM on annual Wikipedia dumps spanning the last decade in two different languages: English and German. […] accurately retrieve and generate knowledge reflective of the state of Wikipedia at any given year within the specified range. […] the model should be capable of providing historical context-sensitive responses by leveraging Wikipedia data from various years.
PI: Prof. Dr. Alan Akbik, Humboldt-Universität zu Berlin
Target systems: Alex & Fritz

NumESC: Numerical Algorithms, Frameworks, and Scalable Technologies for Extreme-Scale Computing (06/2024–12/2026)
[…] developing scientific computing algorithms and optimized mathematical software libraries that are suited for efficiently handling the vast quantities of newly arising data. We develop the scalable Bayesian inference library INLA_DIST whose computational bottleneck operations are matrix decomposition, solving linear systems and selected inversion of sparse matrices. […]
PI: Prof. Dr. Matthias Bollhöfer, Technische Universität Braunschweig
Target system: Fritz & Alex

ULM: Unifont Language Models—Causal multilingual open-vocabulary character language models with bitmaps (05/2024–04/2025; NHR STARTER)
[…] rely on bitmaps of GNU Unifont that encodes almost the entire Unicode set into 16 by 16 pixels as an input to train networks that equitably model any input language to address the above-mentioned shortcomings. […] evaluate our models […] in various downstream tasks like sequence classification or question answering, in a highly multilingual and cross-lingual context. […]
PI: Prof. Dr. Goran Glavaš, Julius-Maximilians-Universität Würzburg
Target system: Alex

SelPredMultiMod: Analysis of Selective Prediction on Multimodal Models (05/2024–04/2025; NHR STARTER)
[…] advance the idea of selective prediction to improve and develop new, especially multimodal, models. […] benchmark existing models and improve their capability by investigating novel approaches that improve the inherent trade-off between coverage (portion of questions answered) and risk (error on that portion). We will evaluate our novel approaches on a set of diverse multimodal tasks to understand their generalizability.
PI: Prof. Dr. Marcus Rohrbach, Technical University of Darmstadt
Target system: Alex

MoMaSJ: Learning hierarchical behavior for mobile manipulation towards human assistance (04/2024–06/2025)
[…] assistive robots will need to autonomously accomplish household tasks and naturally interact with humans. […] still limited to specific installations and specialized to single tasks. […] advance beyond the current ad-hoc solutions by conducting research […] developing methods for robot learning of mobile manipulation for intelligent assistance.
PI: Prof.'in Georgia Chalvatzaki, Ph.D., Technical University of Darmstadt
Target system: Alex

DeepNephro: Deep learning and pathomics augmented nephropathology (03/2024–09/2025)
[…] hochmoderne virtuelle Pathologieplattform […] umfassende Analysen in Form von Pathomics durchführen, um unser Verständnis der Histopathologie der Niere zu vertiefen. […] Ansätze für Deep Learning und Pathomics zu entwickeln und anzuwenden, um den Übergang zu einen innovativen quantitativen Pathologiediagnostik bzw. bis hin zu einer personalisierten präzisions Pathologie zu erleichtern.
PI: Prof. Dr. Dorit Merhof, University of Regensburg
Target system: Alex

MULTILARGELM: Exploring Finetuning of Large Language Models on Multi-Node Clusters (03/2024–05/2025)
[…] optimizing pretrained Large Language Models (LLMs) […] focusing on energy efficiency and do-

main-specific performance. […] analyzing LLMs' power consumption […]; developing benchmarks to assess LLMs in specific domains; training baseline models […] balancing performance with resource use; enhancing dataset quality using LLMs; and improving information retrieval through LLM-supervised fine-tuning. […]
PI: Prof. Dr. Andreas Maier, FAU
Target system: Alex

SysGART: Systematic Generalization for Abstract Reasoning Tasks (03/2024–02/2025; NHR STARTER)
[…] leveraging insights from recent findings on systematic generalization. […] exploit the compositional nature of ARC tasks. […] develop an algorithm capable of systematic generalization, extrapolating from specific examples to novel test scenarios. […] enhance the performance of AI systems on the ARC benchmark, […] contribute to the broader understanding of abstract reasoning in artificial intelligence.
PI: Prof. Dr. Barbara Plank, Ludwig-Maximilians-Universität München
Target system: Alex

FastDiffRend: Echtzeit Verbesserung von Tiefenkarten und 3D-Geometry mittels differenzierbaren Rendering (02/2024–12/2025)
[…] enhance neural image-based rendering approaches for the online generation of novel views while the scene is still being captured. […] develop and integrate a novel differential rendering method that fulfills real-time requirements and thus, will be highly beneficial for the visualization quality by refining depth maps and camera poses. […]
PI: Prof. Dr. Marc Stamminger, FAU
Target system: Alex

DeepNeuro: Exploring novel deep learning approaches for the analysis of diffusion imaging data (02/2024–04/2025)
Diffusion imaging (DI) has rapidly become one of the most important non-invasive tools for clinical brain research in recent years. […] a framework is developed that determines important diffusion characteristics and statistics and uses this information to synthesize individual diffusion data or a complete data set. […] significantly reduce the measurement times for diffusion sequences in clinical studies […]
PI: Prof. Dr. Dorit Merhof, University of Regensburg
Target system: Alex

VideoLLM: Multimodal Foundation Model for Long Video Understanding (02/2024–01/2025)
In the realm of multimodal AI, comprehending lengthy videos presents a formidable challenge, given the rising demand for automated processing of such content. Videos, rich in both text and images posing difficulties for existing AI models like the Transformer. […] Our research employs visual encoders and pretrained large language model, such as LLaMA, to address this challenge.
PI: Prof. Dr. Volker Tresp, Ludwig-Maximilians-Universität München
Target system: Alex

InvRadarSim: Inverse Radar Simulation and Rendering for Scene Parameter Reconstruction using Gradient Descent (01/2024–12/2026)
[…] transfer concepts from inverse rendering to radar simulation and reconstruction, thereby bridging the gap between recent research from the fields of computer graphics and millimeter-wave multiple-input-multiple-output (MIMO) imaging radar. […] match the scene parameters of a radar simulation to observations of a real radar and derive shape or material properties to improve simulation and reconstruction fidelity. […]
PI: Prof. Dr. Marc Stamminger, FAU
Target system: Alex

DeepVehicleVision: Simulating Sensors for Vehicle Vision in Virtual Environments (01/2024–03/2025)
Developing autonomous driving and advanced driver-assistance systems is getting more important for the automotive industry. […] Virtual testing environments can pose solutions if they reach the necessary realism. This project tries to achieve this by training neural networks on real sensor data and transferring the trained systems to the virtual driving simulation.
PI: Prof. Dr. Marc Stamminger, FAU
Target system: Alex

GMFM: Generative Multimodal Foundation Model Pretraining and Finetuning (01/2024–12/2024; NHR STARTER)
[…] propose a novel approach that utilizes a decoder-only architecture for direct alignment of pixel-level images and text in a generative framework. […] streamlines the process, improving efficiency and effectiveness in multimodal tasks, without incorporating additional large vision encoders. […] developing a state-of-the-art multimodal foundation model by leveraging a decoder-only architecture.
PI: Prof. Dr. Volker Tresp, Ludw.-Max.-Univ. München
Target system: Alex

DocTraSeg: Research on handwriting analysis, object tracking and segmentation based on machine learning (12/2023–01/2026)
[…] exploring the potential of Convolution Neural Networks (CNNs) and Vision Transformers (ViTs) in two fundamental tasks of computer vision, i.e., handwriting analysis, object tracking and segmentation. […] aims at continuously estimating the state of an object based on a given bounding box extracted by a simple rectangle/mask from the initial frame of a video sequence. […]
PI: Fei Wu, Ph.D., FAU
Target system: Alex

Opt-3D-SSO: Optimizing neural 3D reconstruction rendering quality for small-sized objects (12/2023–11/2025)
Neural radiance fields promise 3D reconstructions with higher photorealism. […] Starting from an initial available implementation, we aim to improve algorithms and hyper-parameters to increase achievable quality. At the same time, we want to optimize the representation format of the 3D information to allow for efficient real-time rendering of the obtained model.
PI: Dr. Joachim Keinert, FAU
Target system: Alex

Odeuropa Image Processing: Image Processing strand of the EU Horizon 2020 Odeuropa Project entailing the automated recognition of smell references in historical artworks (12/2023–03/2025)
[...] we explore and develop new uses of mixed methods and computing in the fields of digital art history and computer vision. Finally, we build an interactive notebook-based demonstrator to show how images can be retrieved by means of their olfactory references.
PI: Dr. Vincent Christlein, FAU
Target system: Alex

DiffSE: Diffusion models for Speech Enhancement (12/2023–12/2024)
[...] enhancing with diffusion models during inference is computationally expensive, therefore we aim at reducing the computational costs of diffusion models by reducing the architecture footprint and modifying the diffusion process itself.
PI: Prof. Dr. Timo Gerkmann, University of Hamburg
Target system: Alex

TriFORCE: Learning adaptive reusable skills for intelligent autonomous agents (11/2023–09/2025)
[...] we will show that these seemingly different problems have similarities and common causes, and we will address them by introducing a new unifying view that will guide our research for more efficient and practical Deep RL methods that can be used in everyday applications. [...]
PI: Prof. Dr. Carlo D'Eramo, Julius-Maximilians-Universität Würzburg
Target system: Alex

MAGNET4Cardiac7T: Physics-Informed Deep Learning Algorithms for Modeling Electro-Magnetic Fields in the Human Thorax (10/2023–09/2025)
[...] Physics Informed Neural Networks will be used to train neural networks based on Maxwell's equations, which will allow to calculate the energy deposition in the body within a few minutes. [...]
PI: Dr. Anna Krause, Julius-Maximilians-Universität Würzburg
Target system: Alex

OLMAP: Adapting LLMs to Align with User Preferences (11/2023–12/2024; NHR STARTER)
We are planning to develop and evaluate approaches for fine-tuning large language models with the goal of combining different learning objectives i.e. preference learning and language modeling.
PI: Dr. René Jäkel, Technical University of Dresden
Target system: Alex

Gerthia: Training and Evaluating Domainspecific German Foundational Language Models (07/2023–04/2025)
This project aims to identify existing shortcomings in the German NLP/LLM landscape, by training a large German language model from scratch in a controlled setting, finetuning it on several different domains, and finally evaluating its performance on domainspecific, but also broad and general downstream tasks. We will make the models, code, results and findings public and accessible for the German NLP community.
PI: Prof. Dr. Andreas Hotho, Julius-Maximilians-Universität Würzburg
Target system: Alex

EmpkinSA01: Multimodal Bodyshell Camera (05/2023–10/2025)
[...] novel, multimodal sensor concept for high-precision, non-contact detection of the envelope of the human body and the velocity vector of each point on this envelope. [...] leveraging Deep Learning approaches, which operate on the previously-mentioned sensor data [...]
PI: Prof. Dr. Marc Stamminger, FAU
Target system: Alex

digiOnko: Mit digitaler Medizin gegen Brustkrebs, AP5—Histopathologie (12/2022–09/2025)
[...] improving the screening, early detection, diagnosis, treatment and aftercare for women with breast cancer. [...] Deep learning methods will be used to analyze digital Whole Slide Images (WSI), in particular to automatically calculate scores and improve treatment decisions.
PI: Prof. Dr. Andreas Maier, FAU
Target system: Alex

DeepPano: Erzeugung von Panoramabildern aus 3D-Laser-Punktewolken und Kamerabildern (12/2022–09/2025)
[...] data obtained by the 3D-indoor-scanning systems [...] who can deliver high-quality 3D point clouds and registered input images. [...] focus on novel neural rendering techniques [...], on the generation of panoramic images, and [...] to achieve free-viewpoint video, based on this data, in real-time.
PI: Prof. Dr. Marc Stamminger, FAU
Target system: Alex

IRRW: Scaling Inverse Rendering to the Real World (08/2022–07/2025)
How do we best represent objects and their variations for inverse rendering? Can a combination of classical and novel techniques increase photorealism whilst retaining a low dimensional and interpretable representation? And given such object models: How do we efficiently infer the scene graph [...]
PI: Prof. Dr. Bernhard Egger, FAU
Target system: Alex

ICETHICKNESS: Machine learning-based retrieval of ice thickness/internal structures from radargrams (07/2022–06/2026)
[...] we aim at using and modifying machine learning techniques from medical imaging as well as natural language processing and apply those to glaciological radargrams to extract information on ice thickness and internal structures of ice bodies.
PI: Dr. Vincent Christlein, FAU
Target system: Alex

Construction Engineering & Architecture

CEEC-LSS: Center of Excellence for Exascale CFD (07/2024–12/2026)
[…] Computational Fluid Dynamics (CFD) is one of the most prominent areas that clearly requires, and even motivate exascale computing to be part of the engineering and academic workflows. […] CFD has the potential of reaching exascale performance, as one of the few application areas. […] Emphasis is furthermore given to new or improved algorithms that are needed to exploit upcoming exascale architectures. […]
PI: Prof. Dr. Harald Köstler, FAU
Target system: Alex

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J.-Y. Verhaeghe. Exploring advanced visualization of MPI-parallel programs. Master thesis (front and back cover)
FAU/Georg Pöhlein (p. 5)
Marius FW Trollmann and Rainer A Böckmann. mRNA lipid nanoparticle phase transition. In: Biophys. J. 121.20 (Oct 2022), pp. 3927–3939. DOI: https://doi.org/10.1016/j.bpj.2022.08.037 (p. 15, 60)
p101ae | GPCRSCOMPEVO: Computational models of structure, dynamics and evolution of GPCRs. Peter W. Hildebrand, Universität Leipzig (p. 15)
a103bc | CosmosTNG: galaxy formation and evolution with constrained cosmological magnetohydrodynamical simulations at cosmic noon. Chris Byrohl, Heidelberg University (p. 15)
b144dc | HEISSRISSE: Massively Parallel Simulation of the Melt Pool Area during Laser Beam Welding using the Lattice Boltzmann Method. Harald Köstler, FAU (p. 15)
b106dc | DNARepairTDG—DNA Repair by Thymine DNA Glycosylase. Frank Beierlein, FAU (p. 15)
c104fa | EEA_TC: The Influence of Tropical Cyclones on Kilimanjaro’s Glaciers. Emily Collier, Humboldt-Universität zu Berlin (p. 15)
FAU | Giulia Iannicelli (p. 20)
MEGWARE Computer Vertrieb und Service GmbH (p. 21, 22, 36)
TF FAU | FATHER&SUN (p. 8, 18, 26)
FAU | Harald Sippel (p. 28)
NHR-Verein e.V./Monique Drees (p. 28)
Canva (p. 30, 32, 35, 36)
kjpargeter | freepik (p. 54)

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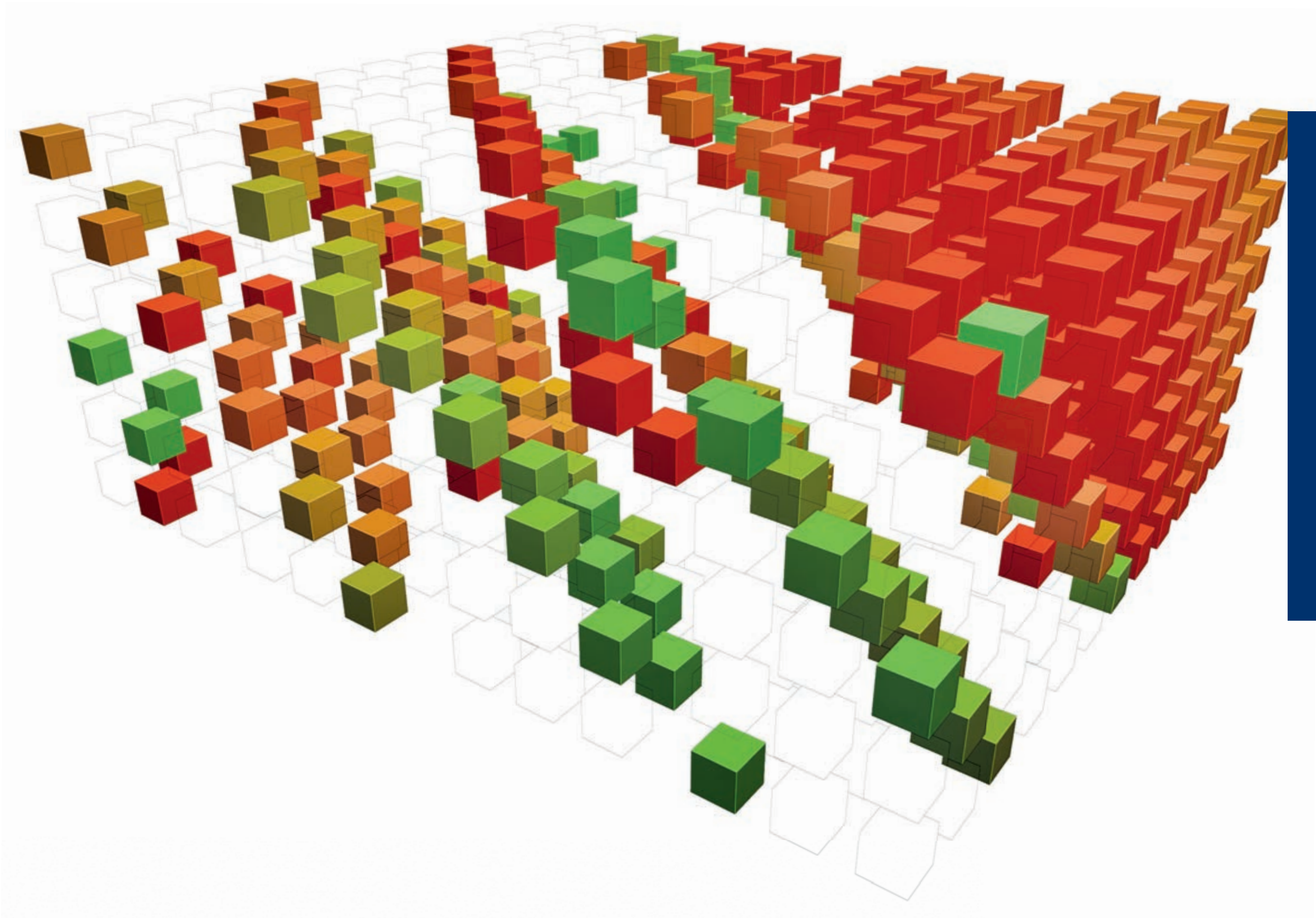

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