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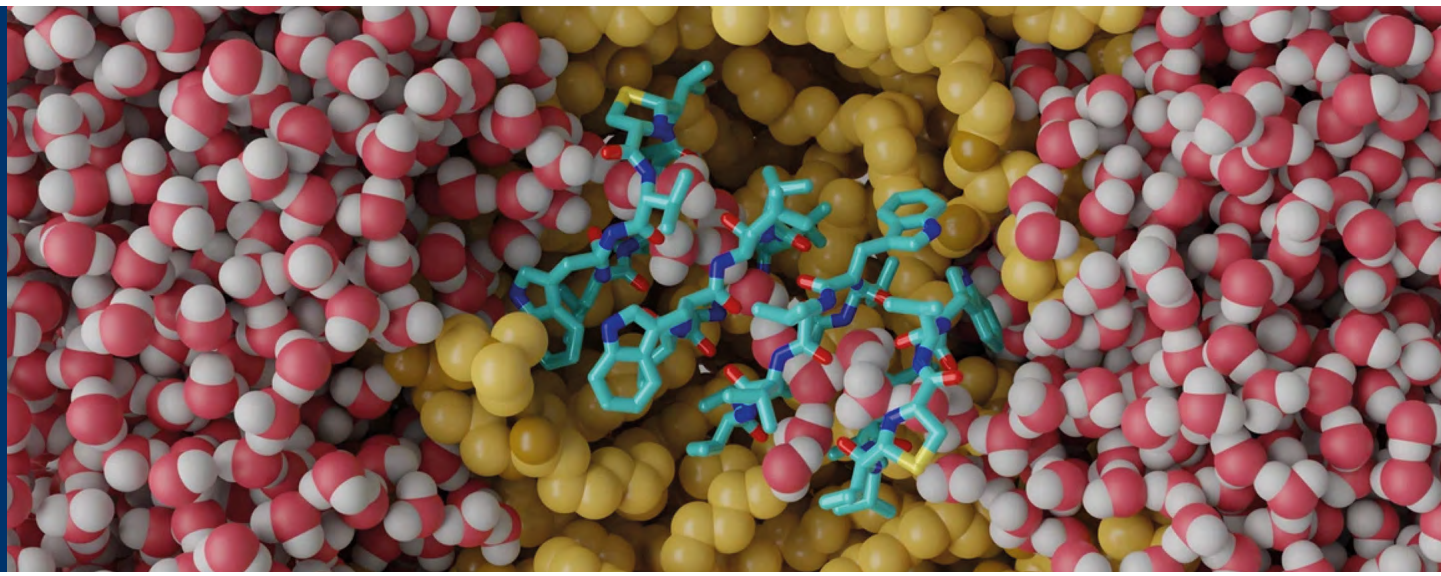

Erlangen National High Performance Computing Center (NHR@FAU)

Annual Report 2023

NHR FAU

ANNUAL REPORT 2023

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

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NHR@FAU Executive Board

Funding

The NHR services of NHR@FAU are funded by the Federal Ministry of Education and Research (Bundesministerium für Bildung und Forschung – BMBF) and the Free State of Bavaria participating in accordance with the resolutions of the Joint Science Conference (Gemeinsame Wissenschaftskonferenz – GWK) for the national high-performance computing at universities and the FAU.

Bundesministerium für Bildung und Forschung

HIGHTECH Agenda Bavaria

Gemeinsame Wissenschaftskonferenz GWK

The Tier3 services of NHR@FAU for the FAU and the region are funded by the German Research Foundation (Deutsche Forschungsgemeinschaft – DFG, in particular through grant 440719683), the Free State of Bavaria, and the Friedrich-Alexander-Universität Erlangen-Nürnberg (FAU).

DFG Deutsche Forschungsgemeinschaft

FAU Friedrich-Alexander-Universität Erlangen-Nürnberg

Erlangen National High Performance Computing Center (NHR@FAU)

Annual Report 2023

PREFACE

Prof. Dr. Gerhard Wellein, NHR@FAU Director

Dear Reader,

I am pleased to present the 2023 annual report of Erlangen National High Performance Computing Center. We are one out of nine national HPC centers at German universities (NHR centers) and also provide services to FAU's and northern Bavarian universities' researchers. As an NHR center, our offerings are open to scientists from all German universities and we are a member of the NHR Alliance (Verein für Nationales Hochleistungsrechnen e.V.).

In the first three years of operation we significantly improved the research environment for many areas of numerical simulation as well as artificial intelligence and machine learning at national and regional levels. We received affirmative feedback from the scientific community during our first reporting workshop in March 2023 and were ranked highly in the NHR-wide user survey in summer 2023.

I am also delighted about the support for our work, of which we have been assured in March 2023 during our NHR anniversary event from the City of Erlangen and the Free State of Bavaria. A core component of this support is the decision of the Free State of Bavaria in May 2023 to fund the construction of a "Northern Bavarian High-Performance Computing Center" at FAU with up to € 260 million. This will be the corner-stone of a modern, sustainable, and energy-efficient infrastructure for the entire northern Bavarian region. I would like to thank the Bayerisches Staatsministerium für Wissenschaft und Kunst (STMWK) for their trust and all those who have prepared this decision over the last few years and ultimately made it possible. A great deal of preparatory work has already been carried out "behind the scenes," particularly in terms of infrastructure and building layout, which can now be further refined and substantiated. My thanks go to the colleagues from the FAU administration, the construction office, and the RRZE/NHR@FAU, and especially the Leibniz Supercomputing Centre (LRZ).

Looking back into 2023, our Annual Report provides a comprehensive picture of all our activities but I would like to briefly present some highlights upfront from our four divisions: Systems & Services, Training & Support, Software & Tools, and Research.

Our Systems & Services division has achieved a robust and reliable operation of the systems, which have encountered strong user demands. The major productions systems Fritz (CPU) and Alex (GPU) are still listed among the fastest systems in the world and among the top ten academic systems in Germany. We had several extensions and upgrades; most notably we put 64 large-memory nodes with 1 TByte and 2 TByte of RAM as part of Fritz into operation, addressing the needs of projects mainly from quantum chemistry. As part of our investment strategy the division led the procurement of new systems to be installed in 2024/25. After an open procurement we selected an offer from MEGWARE to install more than 100,000 CPU cores along with a GPU part comprising almost 400 NVIDIA H100 GPUs. Parts of the investment have been paid by the State of Bavaria within its Hightech Agenda Bayern (HTA) and by new regional partners such as the University of Technology Nürnberg (UTN) and Hof University of Applied Sciences.

The Training & Support division has added newly developed courses along the focus topics of our center to its well-accepted and internationally renowned training program: Core-Level Performance Engineering, Performance Engineering of Linear Solvers (in collaboration with TU Delft and the University of Tennessee), and a full-day online tutorial on our flagship tool suite LIKWID. Further we extended our NVIDIA Deep Learning Institute training certifications towards multi-GPU programming. We are happy to see that there is also a tendency back towards on-site training; our first in-person Node-Level Performance Engineering (NLPE) tutorial at FAU was conducted in October. As a joint effort with the Systems & Services and Software & Tools divisions, we have enabled easy access to Fritz and Alex for course participants via Jupyterhub. This approach is also used in a growing number of lectures to do programming exercises on our hardware. Our support team has continued its user consulting efforts, helping many researchers to get their work done. This includes the enormously successful optimization of the EoCoE flagship code Alya, which resulted in a joint paper at IPDPS 2024.

The Software & Tools division develops, maintains, and supports tools and software for HPC. The most prominent product is our popular LIKWID tool suite, which is continuously being adapted to new architectures extended with new features. Within the NHR Alliance, we also focus on the joint development of cluster-wide and job-specific monitoring solutions. Our ClusterCockpit framework has made it into operational use on Fritz and Alex and is also installed at other HPC centers in Germany. Furthermore, our tools are a pivotal component of the project Energy-Efficient HPC (EE-HPC), which is funded through the BMBF GreenHPC initiative from 2022 to 2025 and is led by NHR@FAU. The EE-HPC project was presented at ISC 2023 in Hamburg as part of the “Powerstack” Birds of a Feather session, and with a research poster at SC23 in Denver. In 2023 our HPC Portal, which allows easy management and supervision of HPC projects and their assigned resources, was deployed for all NHR and new Tier-3 accounts. The migration of existing Tier-3 institutions is ongoing and will be finished in early 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 investigates the use of reduced precision and data compression in plasma simulation, while StroemungsRaum addresses the challenges of advanced solvers and parallel-in-time methods for CFD applications on Exascale machines. On top of many scientific contributions, our PhD students received several awards, including the Best Short Paper Award of the renowned PMBS workshop at SC23.

I am pleased to report that my NHR@FAU colleagues have continued to provide excellent services and training for scientists from all over Germany and have also further developed their own skills and research expertise. These activities are well received by the academic community, which is reflected by record numbers of almost 100 NHR projects and more than 150 local and regional projects. NHR@FAU thus continues to pave the way for new scientific discoveries. At the same time, we train the researchers of the future: In 2023, several hundred students used our clusters for their lecture homework and thesis work, exploring the power of HPC.

However, time does not stand still. I am looking forward to new challenges and opportunities in 2024, and I expect that the AI/ML wave will hit us with full force. Rest assured that we are well prepared.

Gerhard Wellein
on behalf of the NHR@FAU Executive Board

NHR@FAU AT A GLANCE

Organization

High performance computing (HPC) is 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 2021, these efforts have enabled FAU to 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 and the other NHR centers jointly operate the *NHR Alliance* (NHR-Verein). Besides fostering coordination and collaboration of the centers, the NHR Alliance also supports the scientific computing and HPC-related research, e.g., by running the *NHR Graduate School.*

NATIONALES HOCHLEISTUNGS RECHNEN

GRADUATE SCHOOL

Complementing its national duties, NHR@FAU is also responsible for FAU's local HPC infrastructure and HPC services. 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. Reflecting its national (Tier-2) and local (Tier-3) HPC service activities, NHR@FAU receives annual funding from both the NHR program and the FAU.

Regionales Rechenzentrum Erlangen
Der IT-Dienstleister der FAU

NHR@FAU is also a pillar of the HPC activities in the Free State of Bavaria. It complements the Tier-0/1 compute offerings and support services of the *Leibniz Supercomputing Centre* (LRZ) of the Bavarian Academy of Sciences and hosts one of the two offices of *KONWIHR*, the Competence Network for Scientific High Performance Computing in Bavaria. Within KONWIHR, NHR@FAU and LRZ collaborate with scientists at Bavarian universities to exploit the potential of the massive computational power available.

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.

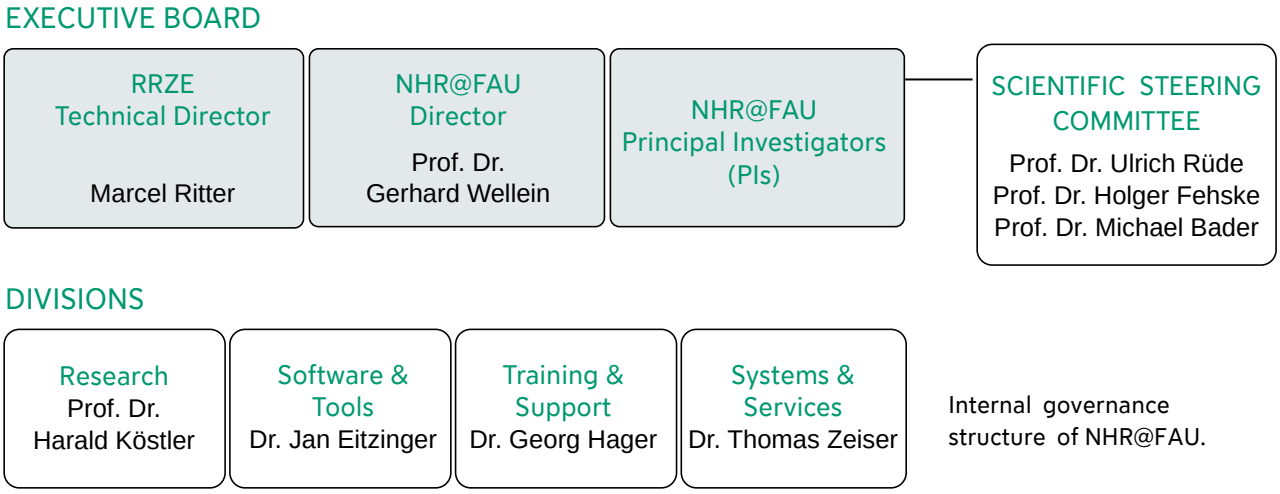
Executive board, divisions and steering committee

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 below), 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 Scientific Steering Committee* oversees the peer-review-based resource application and allocation process. It is supported by the NHR@FAU administrative office and closely coordinates with the executive board, systems administration, and support activities.

Services

The main application topics covered by NHR@FAU are in the areas of atomistic simulations of chemical processes, biomolecular structures, and material properties that are investigated with classical and quantum-mechanical methods. FAU's unique computational chemistry, biology, and materials science community can provide comprehensive, application-specific competence and support for the full spectrum of classical and quantum-mechanical atomistic simulation methods and the most popular



Internal governance structure of NHR@FAU.

application codes. User consulting and expert support within NHR@FAU is provided for the full range of electronic structure techniques for static calculations in chemistry, catalysis, and materials science.

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 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, and 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.

The first NHR conference

In September 2023 *the first NHR conference* took place at the Zuse Institute Berlin (ZIB). Almost 200 domain scientists, HPC consultants, decision makers, and administrative staff interacted at a vibrant event, which not only served to reflect the current state of the NHR effort but also sparked new collaborations for the years to come. The aim of the event was the exchange among researchers from the fields of Atomistic Simulation, Life Science, and Agent-based Simulation in their disciplines and with the HPC user community. In retrospect, it did exactly what it was meant to do: bring everyone together in a relaxed setting to foster exchange and collaboration.

Participants of the First NHR Conference in Berlin.

Invited speakers of the Celebratory Colloquium on March 15.

Attendees of the Results Symposium on March 16.

Celebrating two years of national HPC service in Erlangen

On March 15, a *Celebratory Colloquium* looked back on the last two years, featuring welcome addresses, scientific talks, and a guided tour to the Fritz cluster. NHR@FAU celebrated its two-year anniversary with representatives from politics, science, and administration and gave revealing insights into future-oriented interdisciplinary research fields and high-performance computing systems. In several welcome addresses and talks they illustrated that computing power, storage capacity, comprehensive technical support, and designated expertise as provided by the NHR@FAU have become an indispensable element of science.

After the lectures, the guests were invited to join a guided tour to the supercomputer Fritz, which is located in the chiller plant at FAU's south campus. The following day, in a *Results Symposium* more than 20 researchers showcased pioneering insights that have been achieved with the two new supercomputers *Alex* and *Fritz*. This event proved impressively that the efforts that were put into ramping up the center's operations over the past two years have been worthwhile.

SCIENTIFIC STEERING COMMITTEE

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

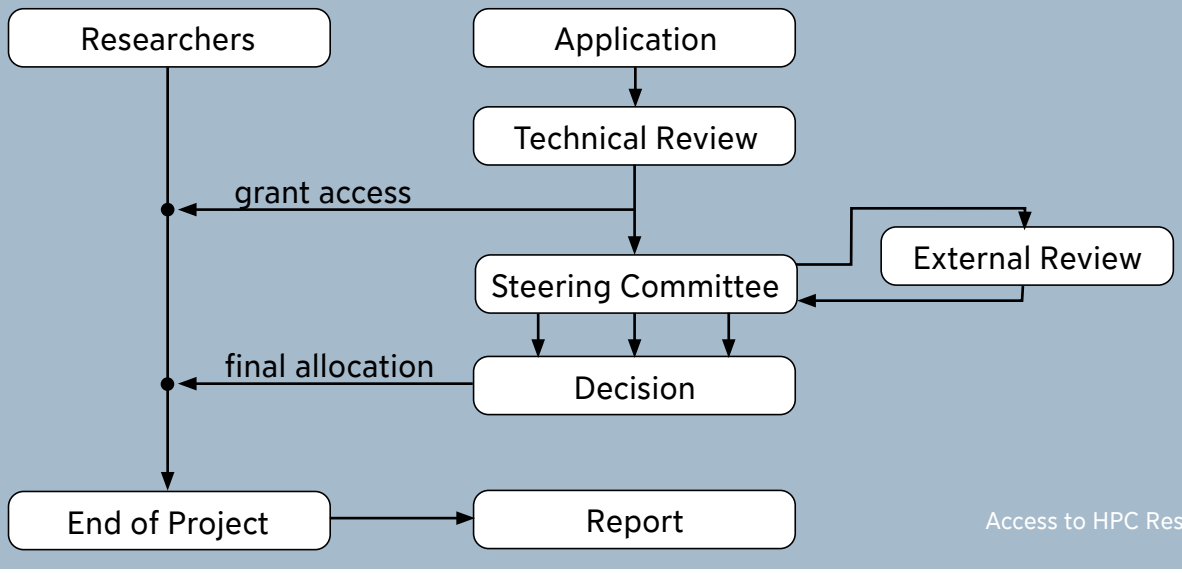
The steering committee of NHR@FAU comprises supercomputing experts from within and outside of FAU. The committee advises the NHR@FAU management and is responsible for important decisions concerning the compute time application process. This includes setting guidelines for the allocation of resources,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

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

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. For test and normal projects, applications for compute time are handled via a local, template-based process where the application form is directly sent to NHR@FAU. Starting with call Q3/2024, the applications for large-scale projects will be managed by the *JARDS* (Joint Application, Review and Dispatch Service) platform.



The NHR@FAU steering committee decides on the assignment of expert consultants and on the final allocation of approved resources for all project types. 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 the above figure summarizes the general application workflow including the tasks of the steering committee.

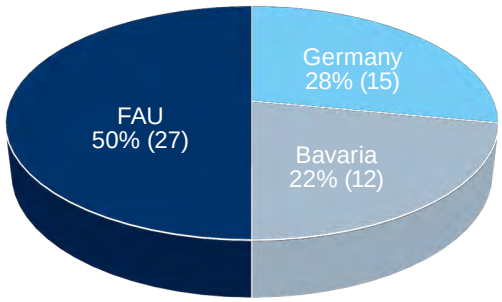
Applications for test and normal projects can be submitted at any time. Large-scale project applications are collected on a quarterly basis and are presented in four committee meetings to be decided upon. Test and normal projects are generally able to start using the compute resources within a fortnight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

Project statistics

Processing of NHR applications for computing time began in the second quarter of 2022. In the reporting year 2023, a total of 38 normal and 16 large-scale project applications were received and approved by the local steering committee. Of those 54, 39 came from Bavaria, which corresponds to a share of 72%. A total of 27 applications were received from FAU, as shown in the figure below. The remaining 15 applications were spread among six federal states.

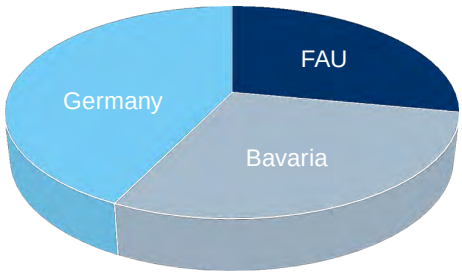
It is good to see that the awareness of the national service NHR@FAU is not concentrated in Bavaria, but also increasingly reaches the other federal states of Germany.



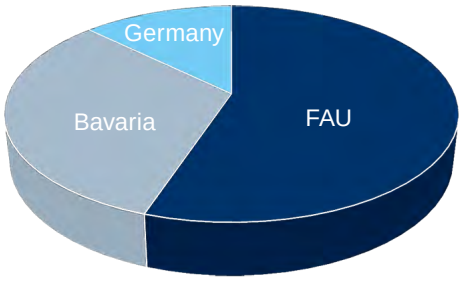
Origin of NHR@FAU 2023 approved projects: Geographical distribution of the 54 normal and large-scale NHR compute time projects.

The picture changes when looking at the awarded CPU core hours and GPGPU hours as shown in the figures on the right, respectively. A total of 600 million CPU core hours and 2.8 million GPGPU hours were awarded, which represents an increase compared to 2022 of approximately 100% in CPU allocations and 80% for GPU resources. The CPU allocations include several large-scale (non-FAU) proposals from our application focus topics in physics and life sciences with a combined volume of 230 million core hours. The GPGPUs projects are dominated by proposals from Bavaria—FAU researchers have been granted four large-scale projects (in the fields of atomistic simulations and medical image analysis) representing almost 25% of the overall allocations.

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, 29 working groups made use of this option.



Geographical distribution of the CPU core hours awarded to NHR projects in 2023.



Geographical distribution of the GPGPU hours awarded to NHR projects in 2023.

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.

The table below presents an overview of available resources for NHR projects at NHR@FAU and their actual utilization in 2023. Overall system availability was high, achieving values beyond 90%. Note that in Q3/2023 the Sapphire Rapids nodes with large main memory entered production. The CPU utilization was remarkably high throughout the year. Because of high NHR demands, Tier-3 capacities

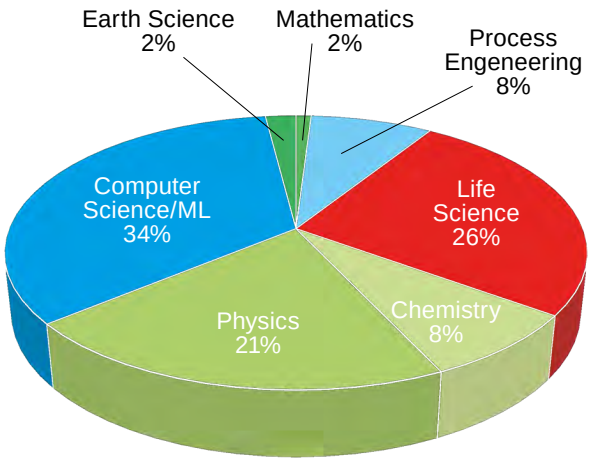
2023	CPU CLUSTER FRITZ [MILLION H]				GPU CLUSTER ALEX [MILLION H]			
	compute nodes	core hours		%	GPUs	GPU hours		%
		available	used	usage		available	used	usage
Q1	756	109	81	75	385	0.77	0.49	64
Q2	756	109	116	106	462	0.92	0.42	46
Q3	812	120	133	111	462	0.92	0.51	55
Q4	812	120	122	101	462	0.92	0.44	48
total		458	452			3.53	1.86	

Overview of available and used resources for NHR projects at NHR@FAU in 2023.

were used temporarily by NHR projects, leading to NHR utilizations beyond 100% in some quarters. On the other hand, GPU utilization in Q4 fell below 50% as some large-scale projects were completed in Q3 2023 and several newly accepted large-scale projects will only start in 2024 together with many new normal projects accepted in Q3/4 2023.

The figure on the right, shows the usage of NHR@FAU's systems in 2023, 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 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 number of projects applying machine learning techniques, which attests to the current attractiveness of AI-related topics such as image classification, segmentation, and deep learning.



Distribution of project research areas of NHR@FAU systems among scientific disciplines in 2023.

Projects active at NHR@FAU in 2023

A list of projects that were actively using the NHR@FAU resources in 2023 is provided in the Appendix (see page 63).

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 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. By the end of 2023, the next step has been initiated: together with LRZ, NHR@FAU will start to provide basic AI infrastructure for members of all Bavarian universities and Bavarian Universities of Applied Sciences.

An overview of HPC compute systems, the available architectures, and some notable highlights are shown in the table on page 16.

In 2023, operation of *Alex* (GPGPU cluster) and *Fritz* (parallel computer) and all the other systems was stable with only minor shortcomings in the storage area. 64 new high-memory nodes with 1 or 2 TB of main memory have been added to Fritz, and a few more nodes of the well-known types have been added to Alex. Some new architectures (in particular ARM-based and new GPGPUs) have also been added to the *Testcluster*.

The main activities took place in the background: The next procurement round has been started in spring 2023. The next HPC system will consist of a CPU-only parallel computer as well as a GPU-enabled parallel section—both with direct warm water-based cooling. After two dialog rounds with the vendors in summer, the contract for the HPC system to be delivered end of 2024 or early 2025 was signed before the end of the year 2023. The long delivery time is due to the

long lead time of some components and the fact that NHR@FAU will wait for the next CPU generation. Money from NHR, FAU, the new University of Technology in Nuremberg (UTN), two other universities (HS-Hof, KU-Eichstätt), and the Bavarian state government (for "BayernKI") have been combined in this effort. In Erlangen, HPC customers are traditionally closely involved in the design of the HPC hardware strategy and in all steps of the procurement process including early testing of the new systems. This time, we had scientists from Würzburg and Bamberg involved in the procurement and decision process.

With the award of the contract, the next phase of the procurement began: Various infrastructure tasks have to be addressed. The new system will be located next to Fritz in the technology center of the Faculty of Natural Sciences. In particular, the power infrastructure has to be extended significantly to support the new system which—with a possible extension—can draw more than 1 MW of electrical power.

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.

2023

SYSTEM	ARCHITECTURE	RESOURCE	ACCESS	HIGHLIGHT
Fritz	Intel Ice Lake & Sapphire Rapids HDR 100-IB	≈ 78,000 cores	NHR FAU	Top500 11/2023 #212
Alex	NVIDIA A40/A100/ HDR-IB (A100)	656 GPGPUs	NHR FAU	Top500 11/2023 #186 Green500 11/2023 #40
Meggie	Intel Broadwell OmniPath100	> 14,000 cores	FAU	major workhorse for FAU/region
Woody	mostly Intel Ice Lake/ throughput	> 2,500 cores	FAU	partially financed by users
TinyFAT	mostly AMD Rome/large memory	> 2,400 cores	FAU	all financed by users
TinyGPU	diverse NVIDIA GPUs/ various generations	> 150 GPGPUs	FAU	all financed by users; growing since 2009
Testcluster	various CPU architectures/generations (x86_64, ARM); various accelerators (NVIDIA, AMD, NEC)		NHR FAU	partially early-access hardware provided by vendors

Compute resources

Fritz parallel computer

NHR & Tier-3

Full operation since mid-2022

hpc.fau.de/systems-services/documentation-instructions/clusters/fritz-cluster/

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 November/December 2021 with additional extensions in fall 2022 and spring/summer 2023. The configuration of Fritz at the end of 2023 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) with 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) with a base frequency of 2.0 GHz, 105 MB shared L3 cache per chip, and 1,024 GB of DDR5-RAM.

Fritz parallel computer

- 16 compute nodes with direct liquid cooling (DLC), each with two Intel Xeon Platinum 8470 Sapphire Rapids CPUs (52 cores per chip) with 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; islands with 64 nodes (i.e. 4,608 cores); the blocking factor between islands is 1:4.
- The Red Hat Linux Enterprise (RHLE) clone AlmaLinux 8 is installed as operating system and user jobs are automatically scheduled via the 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%.

Alex GPGPU cluster

NHR & Tier 3

Full operation since mid of 2022

`hpc.fau.de/systems-services/documentation-instructions/clusters/alex-cluster/`

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 fall 2021, several extensions have been integrated during 2022 and 2023. The configuration of Alex at the end of 2023 is as follows:

- 2 front-end nodes, each with 2 AMD EPYC 7713 *Milan* CPUs (64 cores per chip) with a base frequency of 2.0 GHz with 256 MB hared 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 2 AMD EPYC 7713 Milan CPUs (64 cores per chip) with a base frequency of 2.0 GHz with 256 MB shared L3 cache per chip, 1,024 GB of DDR4-RAM, 8 NVIDIA A100 (each 40 GB HBM2-RAM at 1,555 GB/s; HGX board with NVLink; 9.7 TFlop/s in FP64 or 19.5 TFlop/s in FP32), 2 HDR200 InfiniBand HCAs, 25 GbE, and 14 TB of local NVMe SSDs.
- 18 GPGPU nodes, each with 2 AMD EPYC 7713 Milan CPUs (64 cores per chip) with a base frequency of 2.0 GHz with 256 MB shared L3 cache per chip, 2,048 GB of DDR4-RAM, 8 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), 2 HDR200 InfiniBand HCAs, 25 GbE, and 14 TB on local NVMe SSDs; 7 of these nodes belong to HS Coburg and one to FAU Audiolabs/FHG-IIS.
- 42 GPGPU nodes, each with 2 AMD EPYC 7713 Milan CPUs (64 cores per chip) with a base frequency of 2.0 GHz with 256 MB shared L3 cache per chip, 512 GB of DDR4-RAM, 8 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.
- The Alex cluster has native access to the Lustre-based parallel file system of Fritz through a 25/100 GbE connection and a dedicated central NVMe storage is available with an overall capacity of 1 PB. The RHLE clone AlmaLinux 8 is installed as operating system and user jobs are automatilly scheduled via the batch system Slurm.

Alex GPGPU cluster

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.

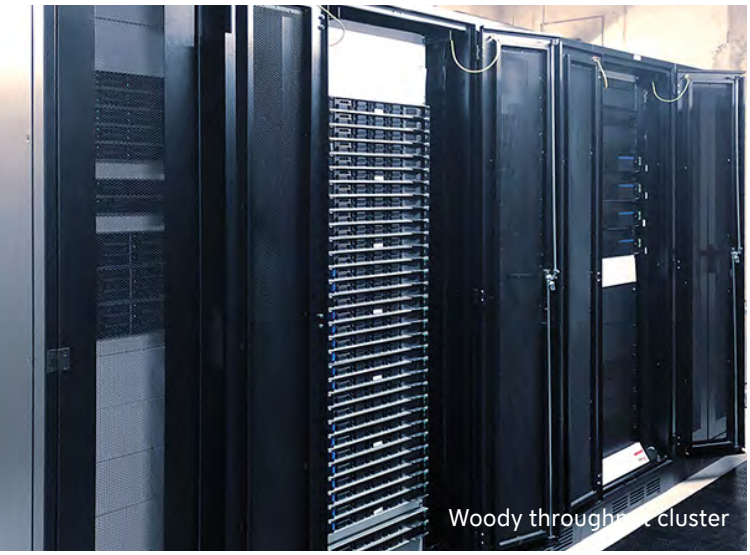
Meggie parallel cluster

Meggie parallel cluster

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) with a base frequency of 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. The systems and services team manages the active node count depending on demand in order to save energy.


Woody throughput cluster

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 (1) 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 (2) dual-socket nodes from 2022 with Intel Ice Lake pro-cessors. 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 turned on during high-demand phases.

TinyFAT cluster

Tier 3, 2016/2020

TinyFAT is a cluster dedicated to jobs with large memory demands. It consists of almost 50 dual-sock-et Intel Broadwell or AMD Rome nodes with 256 or 512 GB of main memory and local SSD storage.

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. But they are still to valuable to throw them away. They are now mainly used for teaching purpose and interactive development work through a Jupyterhub web-based service.

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.

System availability and usage 2023

There were no major outages in the year 2023. Table 3.2 shows an overview of core and GPU hours used. Although many FAU scientists submit NHR applications, the Tier-3 consumption is considerable especially on the GPU-enabeld systems!

SYSTEM	NHR	TIER3
Fritz	452 million core-h	50 million core-h
Meggie	–	58 million core-h
Woody	–	13 million core-h
TinyFAT	–	19 million core-h
Alex	1.86 million GPU-h	0.7 million GPU-h
TinyGPU	–	0.7 million GPU-h

Resources used by NHR and Tier-3 on the different systems in 2023.

TRAINING & SUPPORT

Division head:
Dr. Georg Hager

The *Training & Support* division at NHR@FAU is responsible for the HPC training program and all support activities beyond level two. 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. In the course of the year 2023, the training program was extended further with a full-day tutorial on the LIKWID tool suite and a new full-day tutorial on *Core-Level Performance Engineering*. Furthermore, Liaison Scientist Sebastian Kuckuk was certified as an NVIDIA DLI Ambassador for multi-GPU programming courses to be held in 2023. And finally, a new tutorial on *Performance Engineering for Linear Solvers* was developed in collaboration with TU Delft and the Innovative Computing Lab at the University of Tennessee. It will be presented for the first time at the ISC High Performance conference in May 2024.

In order to ease the entry barrier for inexperienced users and to streamline the workflow, a new access method to NHR@FAU systems was introduced in 2023. Course attendees can now log in at NHR@FAU clusters via a JupyterHub interface, which, among several other advantages, eliminates the need for dealing with SSH connections and the SLURM batch system. Although not appropriate for all courses, most online and on-site training events have been migrated to the new login method in the course of the year.

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.

Training activities

Courses and tutorials

In the following, we list courses and tutorials that were conducted in 2023 and were either organized by NHR@FAU, held by others with substantial contributions from NHR@FAU, or performed on invitation by NHR@FAU. 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, conveying 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.

Introduction to Hybrid Programming

This tutorial is conducted by Georg Hager in close collaboration with Rolf Rabenseifner from High-Performance Computing Center Stuttgart (HLRS) and Claudia Blaas-Schenner from TU Wien. Most HPC systems are clusters of shared memory nodes. To use such systems efficiently both memory consumption and communication time has to be optimized. Therefore, hybrid programming may combine the distributed memory parallelization on the node interconnect (e.g., with MPI) with the shared memory parallelization inside of 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

The three-day introduction to HPC 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 & Fundamentals of Accelerated Computing 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

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 above) since it covers the use of NVIDIA performance tools for the analysis of GPU programs written in CUDA C/C++, OpenACC, or OpenMP.

Courses and tutorials in 2023; if not stated otherwise, courses were held online.

EVENT	DATE(S)	PLACE	ATT.	TEACHER(S)
Node-Level Performance Engineering	May 11	ISC23, Hamburg	15	G. Hager
	Jun 27–30	HLRS	30	G. Hager, J. Eitzinger, B. Wesarg
	Oct 4–6	NHR@FAU, in person	12	G. Hager, T. Gruber, G. Wellein
	Nov 12–17	SC23, Denver	12	G. Hager, T. Gruber, G. Wellein
	Dec 4–6	LRZ	30	G. Hager, T. Gruber, G. Wellein
Introduction to C++ for beginners	Sep 14/15, 21/22, and 28/29	NHR@FAU	24	S. Dimitrovic*
Modern C++ Software Design	Oct 11–13	NHR@FAU	26	K. Iglberger*
Parallel Programming of High Performance Systems (PPHPS23)	Mar 7–9	NHR@FAU	20	A. Afzal, M. Wittmann, G. Hager, LRZ
Introduction to parallel programming with OpenMP	Mar 21/28	NHR@FAU	12	M. Wittmann
	Sep 20/27	NHR@FAU	12	
Roofline Modeling and Performance Engeneering	Nov 28–30	NHR@FAU	15	G. Hager
Fundamentals of Accelerated Computing with CUDA C/C++	Mar 8–9	NHR@FAU	15	S. Kuckuk, EUMaster4HPC*
Fundamentals of Accelerated Computing with CUDA Python	Mar 16	NHR@FAU, in person	19	S. Kuckuk
	Sep 18	NHR@FAU, in person	14	
Core-Level Performance Engineering	Apr 15–19	ICPE 2023, Coimbra, PT	7	J. Laukemann, G. Hager
	Oct 12	NHR@FAU	25	
	Oct 21–25	PACT 2023, Vienna, AT	7	
Performance Analysis on GPUs with NVIDIA tools	Apr 4	NHR@FAU	29	D. Ernst
	Jul 9–14	IHPCSS, Atlanta, GA	25	
	Oct 10	NHR@FAU	26	
Introduction to the LIKWID Tool Suite	Jul 24	NHR@FAU	16	T. Gruber, G. Hager
GROMACS	Oct 10–12	FAU	12	R. Böckmann, M. Trollmann

* denotes an invited teacher from outside FAU

Introduction to C++ for beginners

The one-week course with a focus on essential language features and the syntax of C++, is held by Slobodan Dmitrovic. Additionally, it introduced many C++ software development principles, concepts, idioms, and best practices, 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 gives insight into the different aspects of C++ (object-oriented programming, functional programming, generic programming) and teaches guidelines to develop mature, robust, maintainable, and efficient C++ code.

Introduction to Parallel Programming with OpenMP

This two-day course with hands-on exercises is designed and conducted by Markus Wittmann. It introduces OpenMP from the ground up for developers who have no prior experience with parallel programming. The first day focuses on CPUs only, while the advanced second day covers performance issues and accelerator programming.

Tutorial on the GROMACS molecular dynamics package

The five-day hands-on course conducted by the group of Rainer Böckmann, Professorship of Computational Biology covered an introduction into the molecular dynamics engine GROMACS, including fundamental commands and applications. Participants learned how to prepare and run simulations of biomolecular systems including membranes and proteins at an atomistic and coarse-grained level of resolution. Post-processing and analysis of simulation trajectories were a large part of the tutorial. The course is usually embedded in the Bachelor programs of Biology and Integrated Life Sciences but had five places available for people from NHR. The course was held in person and took place in the CIP of the Biology Department.

Roofline Modeling and Performance Engineering

The invited lecture series at the AQTIVATE Training Workshop on Exascale Computing and Scalable Algorithms is given by Georg Hager. The lectures covered the basics of the Roofline model, case studies, and model-based code optimization and performance engineering.

LIKWID

The popular LIKWID tool suite was presented by Thomas Gruber as part of several courses at other sites in 2023. LIKWID (see page 32) is in wide use at many computing centers worldwide for affinity control, performance analysis, and monitoring. It contributes significantly to the visibility and reputation of NHR@FAU within the HPC community. The success of LIKWID has led to the development of a dedicated full-day online tutorial, which was conducted for the first time by Thomas Gruber and Georg Hager in 2023.

Python for HPC

This course, which is organized by the Max Planck Compute and Data Facility (MPCDF), teaches approaches to using Python efficiently and reasonably in an HPC environment. In addition, topics more related to software engineering such as packaging, publishing, testing, and the semi-automated generation of documentation were covered. Finally, basic visualization tasks using matplotlib and similar packages were discussed. Participants from FAU were invited to attend.

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.

HPC in a nutshell

Each month a two-hour online introduction into NHR@FAU systems, access formalities, and basic usage was provided by Katrin Nusser and Markus Wittmann. This well-received format aims at reducing the entry barrier for new and inexperienced users. The content is continuously being updated to reflect recent changes in NHR@FAU systems and access rules.

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 2023, 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 (`fau.tv/course/id/1146`) and/or the NHR@FAU YouTube channel (`youtube.com/NHRFAU`). A complete list with all events and links to slides and video recordings can be found at `hpc.fau.de/systems-services/support/hpc-cafe/`.

The following focus topics have been covered in 2023:

NHR@FAU hardware development 2024/25 by Gerhard Wellein, December 19.

Vienna Ab-Initio Simulation Package (VASP) Benchmarks by Alireza Ghasemi, November 21.

GPU Top Trumps! by Dominik Ernst, October 24.

Software installation for users—containers, conda, SPACK by Markus Wittmann, Katrin Nusser, and Thomas Gruber, September 12.

Using the Jupyterhub service at NHR@FAU and PyTorch profiling at work by Johannes Veh, July 11.

Computer architecture 101 for scientists by Georg Hager, June 13.

Mid-term hardware strategy at NHR@FAU by Gerhard Wellein, and Thomas Zeiser, April 25.

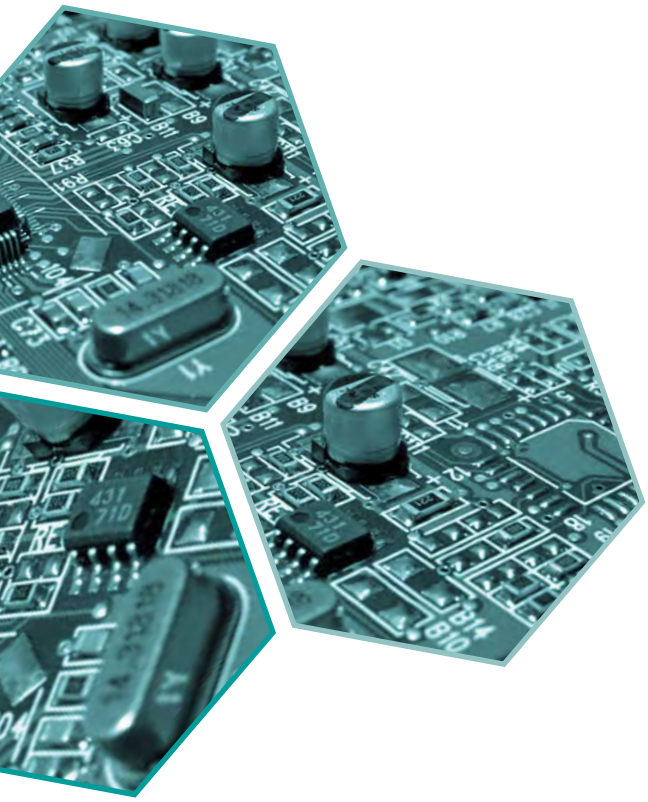
The missing Python introduction for scientists by Tamás Gál (ECAP), March 21.

The KONWIHR program—overview and funding opportunities—case studies by Gerhard Wellein, Hans-Joachim Bungartz (TUM), Katrin Nusser, Gerasimos Chourdakis, Nils Meyer, Martin Kronbichler, and Georg Hager, February 14.

Introduction to the NHR@FAU HPC Portal and the ClusterCockpit monitoring system by Jan Eitzinger, January 10.

NHR PerfLab Seminar series

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 `hpc.fau.de/research/nhr-perflab-seminar-series/`.



The following talks have been given in 2023:

Mixed-precision computing: An overview by Théo Mary, Sorbonne University and French National Center for Scientific Research (LIP6), Dec 12, 2023 (online).

A review of processor advances over the past thirty years—an outsider's perspective by Jan Eitzinger, NHR@FAU, Nov 7, 2023 (hybrid).

Facing challenges in computational fluid mechanics with Lattice Boltzmann methods, OpenLB and high performance computers by Mathias Krause, Karlsruhe Institute of Technology, Oct 17, 2023 (hybrid).

The linear algebra mapping problem and how programming languages solve it by Paolo Bientinesi, University of Umeå, Sep 12, 2023 (online).

DGEMM on integer tensor cores by Hiroyuki Ootomo, Tokyo Tech, Sep 5, 2023 (online).

Towards robust and efficient AI at scale by Charlotte Debus, Karlsruhe Institute of Technology, Jul 11, 2023 (online).

LLVM in HPC—enabling performance portability, interoperability, and novel features by Johannes Doerfert, Lawrence Livermore National Laboratory, May 30, 2023 (online).

The comedy club of HPC—low-rank matrix approximation takes the stage! by Hatem Ltaief, King Abdullah University of Science and Technology, May 16, 2023 (online).

Conquering noise with hardware counters on HPC systems by Ahmad Tarraf, Technical University of Darmstadt, Apr 18, 2023 (online).

Asynchronous MPI communication with OpenMP tasks—spawning task dependency graphs across nodes by Joachim Jenke (né Protze), RWTH Aachen University, Apr 4, 2023 (hybrid).

Configuration-aware performance analysis by Florian Sattler, Saarland University, Feb 14, 2023 (online).

Digital reality: from learned models via synthetic data to trusted-AI—and back! by Philipp Slusallek, German Research Center for Artificial Intelligence and Saarland University, Jan 31, 2023 (online).

Projects

The *EoCoE-II* project ended officially in 2021. Especially for the flagship code *Alya*, the optimizations developed for GPUs could be applied across many parts of the matrix assembly and led to acceleration factors of up to 40. A collaborative paper with the lead developer about the optimization strategies was accepted for publication at *IPDPS 2024*.

Furthermore, the continuation project *EoCoE-III* was accepted in 2023. NHR@FAU again participates with performance engineering activities in various flagship codes. See page 45 for details.

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 2023, KONWIHR granted the following scientific project applications:

Performance Optimization for the SYCL implementation of UTBEST, Prof. Aizinger, University of Bayreuth, small project.

Modernizing Checkpointing and Output in the Earthquake Simulation Software SeisSol, Prof. Bader, TU München, small project.

Development and optimisation of a program package for simulations of strained polymer networks—CHEMBREAK, Prof. Smith, FAU Erlangen-Nürnberg, small project.

Memory optimization and OpenMP acceleration of large-scale GW calculations, Prof. Wilhelm, University of Regensburg, small project.

Unbinned analysis framework for Gammapy, Prof. Funk, FAU Erlangen-Nürnberg, small project.

Performance-Optimierung und Parallelisierung eines Codes zur Lösung von partiellen Differentialgleichungen auf dünnen Gittern, Prof. Pflaum, FAU Erlangen-Nürnberg, small project.

NewWave: New Roads for Computational Wave Propagation, Prof. Igel, LMU München, large 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 2023-1, Oct 4, 2023.

KONWIHR workshop for projects from 2022-2, Apr 12, 2023.

NHR Graduate School

In 2023, the second cohort of students were admitted to the *NHR Graduate School*. Two students, Fabian Böhm and Daniel Bauer, received a PhD scholarship at NHR@FAU. They are hosted at the Chair for System Simulation (Prof. Rüde). Their research revolves around efficient and scalable numerical solvers. They started working on a code generator designed for node-level optimized, extreme-scalable, matrix-free finite element operators on hybrid tetrahedral grids. The memory access patterns and in-core execution are automatically optimized by leveraging the grid's local structure. The resulting generated code achieves up to a 58-fold speed-up compared to manual reference implementations.

Dissemination and Outreach

Dissemination of activities and results are an integral part of the NHR@FAU activities. Event and course announcements, success stories from the support (see on page 29), calls for compute time projects, talk recordings, etc., are disseminated via social media channels (YouTube, Twitter), our bi-monthly newsletter (see on page 29), 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.

New customer acquisition

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. Finally, the concept of the NHR Alliance and the resources at NHR@FAU were detailed in various online and on-site talks at Universities:

The National High Performance Computing Alliance and NHR@FAU: New structures and opportunities by G. Wellein, Jul 2023.

The National High Performance Computing Alliance and NHR@FAU: New structures and opportunities by G. Wellein at the 35th Molecular Modeling Workshop 2023, FAU, May 15, 2023.

News from NHR@FAU—Fritz, Alex, and Woody by J. Veh and G. Hager at the ECAP Seminar, FAU, Jan 19, 2023.

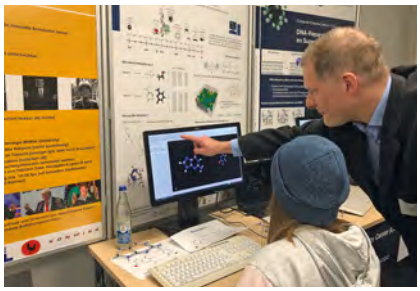
Long Night of Sciences

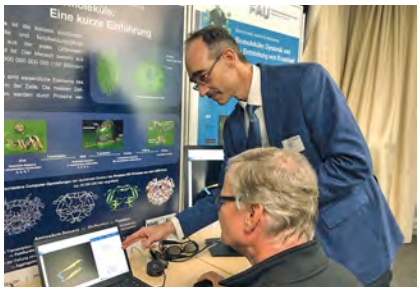
Every two years, the *Lange Nacht der Wissenschaften* (Long Night of Sciences) is conducted as a popular science event in the entire Nuremberg Metropolitan Area. In 2023, NHR@FAU presented itself again in an *HPC Village*: Teaming up with several high-profile customers, the technology and the exciting applications of supercomputers were showcased and visitors learned how various FAU institutions, such as medicine, geography, chemistry, and computational biology use simulations on high-performance computers for their research. This activity was met with considerable interest from the general public (see more on page 29).

Success stories from the support

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 `hpc.fau.de/about-us/success-stories/`.

Long Night of Sciences '23: Teaming up with several high-profile customers, the technology and the exciting applications of supercomputers were showcased and visitors learned how various FAU institutions, such as medicine, geography, chemistry, and computational biology use simulations on high-performance computers for their research.





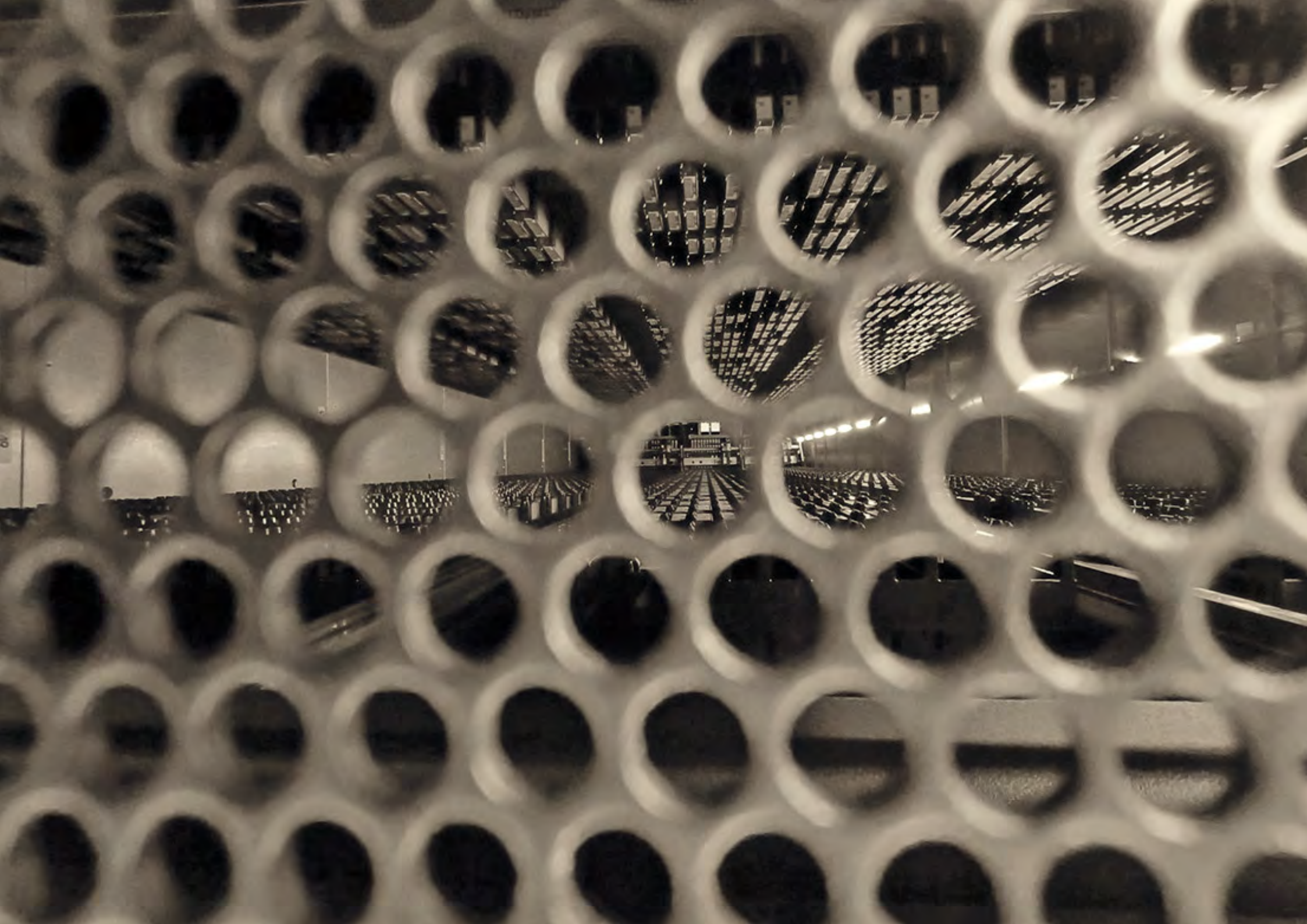
Social media

In order to widen its reach to potential customers and audiences, NHR@FAU leverages social media channels. Currently, we concentrate mostly on dissemination via recorded lectures, seminars, and tutorials, which are published either on the *NHR@FAU YouTube channel* (`www.youtube.com/@NHRFAU`) or the *FAU video portal* (`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.

NHR@FAU newsletter

The bi-monthly NHR@FAU newsletter is a publication that summarizes recent and upcoming events at NHR@FAU and the NHR association. 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. In 2023, six newsletters were published. All newsletters are available at `hpc.fau.de/nhrfau-newsletters/`.

A mailing list has been set up to alert about the publication of a new issue. It is open for everyone to subscribe at: `lists.fau.de/cgi-bin/listinfo/nhr-newsletter`.



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 (`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*, and *MachineState.* The *ClusterCockpit* Monitoring Framework can be found at `github.com/CC`.

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). 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* (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).

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.

Performance tool suite

LIKWID (`github.com/RRZE-HPC/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 Super Computer Center in Guangzhou, the Vienna Scientific Cluster (VSC), or the Barcelona Supercomputing Center (BSC).

Moreover, 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 2023, support for the AWS Graviton 3 and the HiSilicon TaiShan v110 chips was added in LIKWID. Moreover, in 2020 Apple released the M1, its first ARM chip; after the Asahi Linux team ported Linux to the Apple M1, support for these chips was added to LIKWID as well. To ensure software functionality during development, LIKWID was integrated in the CI/CD infrastructure of NHR@FAU. Furthermore, the CI/CD infrastructure creates software packages for different Linux-based operating systems. The Julia team (mainly Carsten Bauer from NHR center PC2) created a Julia interface to LIKWID (`github.com/JuliaPerf/LIKWID.jl`).

Open Source Architecture Code Analyzer

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 and available at `github.com/RRZE-HPC/OSACA`.

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 at `godbolt.org`, which allows using OSACA from a browser without any installation.

In 2023 we enhanced the supported micro-architectures by the Apple M1 Firestorm to further increase our pallet of ARM processors and enabled a machine-readable YAML output to provide a generic API for other tools. Furthermore, we continued our successful core-level performance engineering (CLPE) tutorial that uses OSACA as the main analysis tool and held the tutorial at the *ICPE 23* conference (`icpe2023.spec.org/`), the *PACT 23* conference (`pact2023.github.io/`), and at a course for the NHR customers.

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.

By employing 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 this 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 currently search for funding and a new maintainer for further development of Kerncraft. Please reach out to Thomas Gruber and Jan Laukemann for any questions or requests regarding Kerncraft.

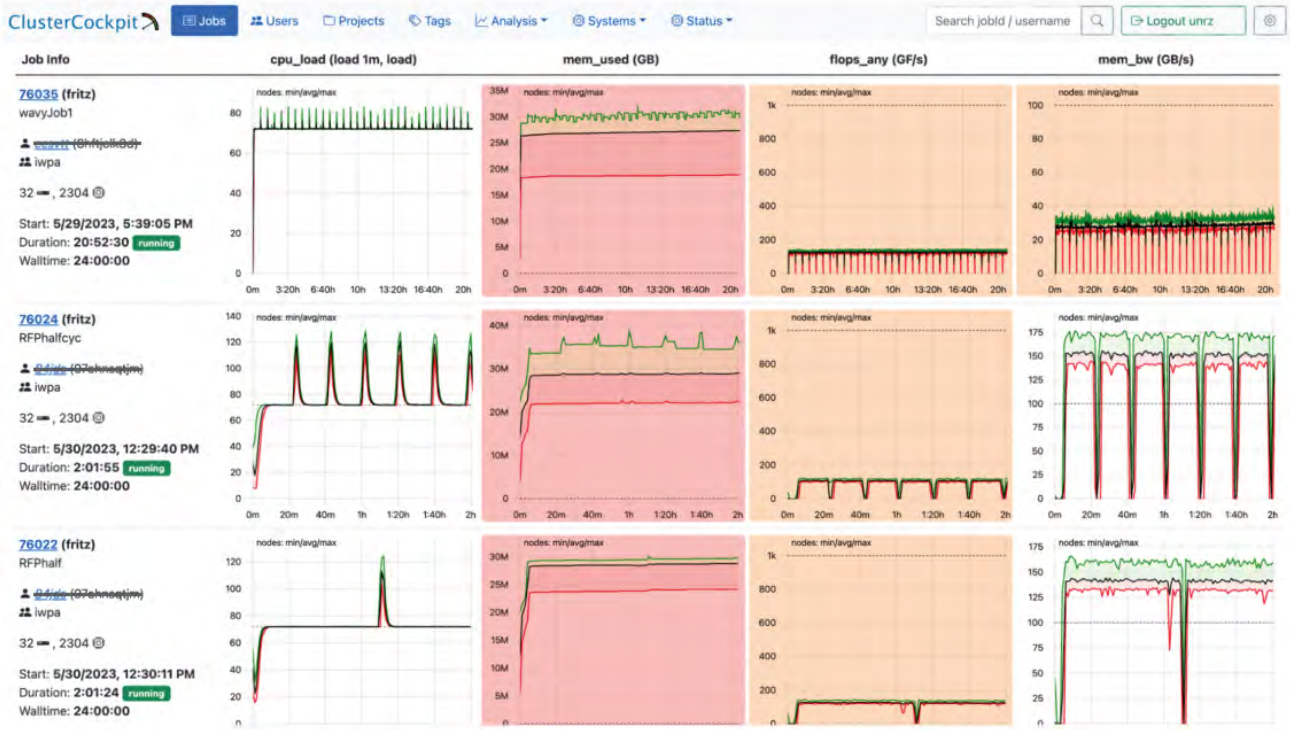
MachineState

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 and available at `github.com/RRZE-HPC/MachineState`.

Monitoring framework

ClusterCockpit (`clustercockpit.org`) is a full-stack framework for job-specific performance monitoring 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 tailor-made software stack for job-specific performance monitoring.

ClusterCockpit currently comprises `cc-backend` (web API backend), `cc-frontend` (web-based user 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. Four members of the team (Jan Eitzinger, Thomas Gruber, Christoph Kluge, and Rafael Ravedutti) contributed to the development of ClusterCockpit in 2023, focusing on



Screenshots of the ClusterCockpit web interface. Left: job list of running jobs; right: single-job view showing the resource utilization in a polar plot and diagnostic Roofline plot.

stability and ease of installation and maintenance. ClusterCockpit is in production use at NHR@FAU, PC2 Paderborn, DKRZ Hamburg, and the University Bonn. It is funded as part of the BMBF EE-HPC project (`eehpc.clustercockpit.org`), which started in fall 2022 (see page 45). Our aim is to establish ClusterCockpit as an attractive open-source offering for job-specific performance monitoring in academic HPC centers.

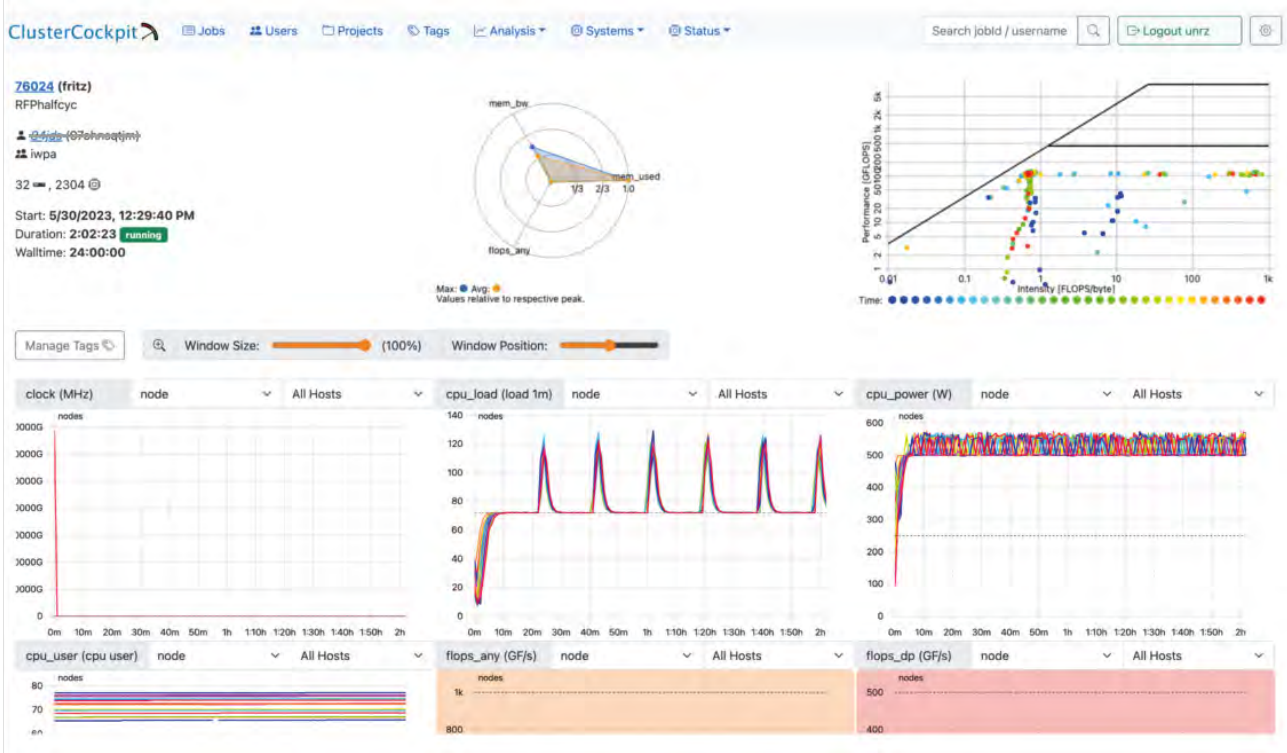
MD-Bench

MD-Bench (`github.com/RRZE-HPC/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 2023 in Gdansk, Poland, where it won the Best Paper Award. MD-Bench is maintained by Rafael Ravedutti.

The Bandwidth Benchmark

The *Bandwidth Benchmark* (`github.com/RRZE-HPC/TheBandwidthBenchmark`) 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 (`github.com/RRZE-HPC/TheBandwidthBenchmark/wiki`) feature results for many processor architectures. The Bandwidth Benchmark is maintained by Jan Eitzinger.



SERVICES

HPC Portal

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. It is in production use (`portal.hpc.fau.de`) and the default user management solution for external users and teaching accounts. It is planned to transfer existing Tier-3 groups to the HPC Portal and make it the only supported management solution by the end of 2023. The HPC Portal is maintained by Christoph Kluge.

NHR Moodle learning platform

Since 2021, we have been hosting and administrating a *Moodle* server for general use within the NHR Alliance (`moodle.nhr.fau.de/`). Login is enabled through DFN-AAI Single-Sign-On authentication. 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.

NHR@FAU ClusterCockpit service

For usage within the FAU, we administer a central *ClusterCockpit* monitoring server that can be reached at `monitoring.nhr.fau.de`. 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 access the ClusterCockpit monitoring service through the *HPC Portal.* This service is jointly maintained by Katrin Nusser from Systems & Services and Jan Eitzinger, Thomas Gruber, Christoph Kluge from Software & Tools.

URL short-link service

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

Services for internal use

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

- A LimeSurvey instance for online surveys
  `survey.nhr.fau.de`
- A Discourse forum software instance for documentation and knowledge transfer
  `community.nhr.fau.de`
- A Hedgedoc collaborative Markdown editor
  `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.

Talks

G. Hager and J. Eitzinger: ***Resources for High Performance Computing at FAU.*** Talk at the FAU Graduate Centre, Feb 16, 2023.

G. Hager and J. Eitzinger: ***Resources for High Performance Computing at FAU***. Talk at the FAU Graduate Centre, Sep 14, 2023.

T. Gruber: ***Pinning, Hardware Counting, and Microbenchmarking with LIKWID***. Invited guest lecture in the CSE 6230—"High Performance Parallel Computing" lecture, Georgia Institute of Technology, March 9, 2023.

RESEARCH

Division head:
Prof. Dr. Harald Köstler

The overarching goal of the *Research* division's 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.

Performance modeling and performance engineering

People

Dominik Ernst, Ayesha Afzal

GPU performance modeling

The paper ***Alya towards Exascale: Optimal OpenACC Performance of the Navier-Stokes Finite Element Assembly on GPUs*** was accepted at the *International Parallel and Distributed Processing Symposium* [12]. It presents the work being done in the context of the EoCoE-II project, where opportunities for large speed-ups in the OpenACC GPU port of the Navier-Stokes matrix assembly routine of the finite element code *Alya* where found. A thorough analysis and performance counter based measurements explain the mechanisms behind the performance improvements.

NHR@FAU also contributed to the *International HPC Summer School* (IHPCSS) that has been held in Atlanta, USA in 2023 with a tutorial by Dominik Ernst about ***GPU Performance Analysis*** (for details on this tutorial, please see page 22). The IHPCSS is jointly organized by HPC institutions from the USA, Canada, Europe, Japan, and Australia.

Together with the Chair for Hardware Architecture at the Department of Computer Science at FAU, NHR@FAU co-hosted a student team that prepared for a participation in the *Student Cluster Competition* at the *Supercomputing Conference 2023*. NHR@FAU supported the team with access to their complete hardware arsenal, system administration and application expertise, vendor contacts, and most importantly, with their team advisor Dominik Ernst.

Performance of Memory-bound Applications

We have previously published our work on developing and validating the analytic performance model for the propagation speed of idle waves, which emerge when a delay on a specific process propagates throughout the parallel program and thus "ripples" through the system. To incorporate noise effects into this model, using a range of HPC platforms and benchmarking scenarios, we investigated how these idle waves interact nonlinearly within a parallel code on a cluster and decay due to system noise, system topology, and application load imbalance. Further, we analyzed how memory-bandwidth bottlenecks affected the propagation of idle waves, which suggested that the subsequent desynchronization and automatic asynchronous communication for a variety of application properties and parameters, including saturation point, matrix structures, domain decomposition, and communication concurrency, might speed up code execution. This research has been further expanded upon in numerous directions, which model how various compute kernels share memory bandwidth in a ccNUMA contention domain and explain how the utility of using principal component analysis, clustering techniques, correlation functions, and a novel phase space plot can help identify, classify, and characterize the dynamics of large-scale MPI parallel programs.

In 2023, three papers authored by Afzal et al. were published, and one of them has been awarded the *Best Short Paper Award*. The specifics of these publications can be found below in chronological order.

In June 2023, our article ***Making Applications Faster by Asynchronous Execution: Slowing Down Processes or Relaxing MPI Collectives*** was published in a special issue of the *Future Generation Computer Systems (FGCS)* Journal and released with open access [1]. This manuscript was submitted on an invitation from the *International Conference on Parallel Processing and Applied Mathematics (PPAM'22)* for an expanded version of our earlier paper. This research work was started in April 2022 during the visit of professor Stefano Markidis from *KTH Royal Institute of Technology* in Stockholm to NHR@FAU. Funding from the *HPC- Europa3 Transnational Access* program made his visit possible, enabling European researchers to collaborate on HPC projects and have access to the most cutting-edge HPC systems. The findings published in the extended paper [1] expanded the utility of phase-space graphs as a new tool to visualize parallel program dynamics and investigated five microbenchmarks and applications on different supercomputer platforms. It sheds light on the fact that noise, independent of its source, is not always detrimental and how it can be leveraged for performance improvements if certain conditions are met.

In November 2023, our research article ***SPEChpc 2021 Benchmarks on Ice Lake and Sapphire Rapids Infiniband Clusters: A Performance and Energy Case Study*** was published at the 14th Workshop on *Performance Modeling, Benchmarking, and Simulation of High Performance Computer Systems (PMBS)*, which was held in conjunction with the *ACM/IEEE Supercomputing Conference* in Denver, CO. This study assesses the performance, power, and energy characteristics of the SPEChpc 2021 benchmark suite on Intel Ice Lake and Sapphire Rapids CPUs. It identifies common patterns like memory bandwidth limitation, communication overhead, MPI serialization, superlinear scaling, and alignment issues. Power dissipation and energy measurements show Intel server CPUs have high idle power levels, making race-to-idle strategies crucial. The paper was released with open access [2].

In November 2023, our research paper ***Physical Oscillator Model for Supercomputing*** was published at the 14th Workshop on *Performance Modeling, Benchmarking, and Simulation of High Performance Computer Systems (PMBS)*, which was held in conjunction with the *ACM/IEEE Supercom-*

puting Conference in Denver, CO. This paper proposed a physical oscillator model to describe the dynamics of interacting parallel processes, inspired by the Kuramoto Model. The model uses a sparse topology matrix and two interaction potentials for resource-scalable and resource-bottlenecked applications. It mimics the propagation of delays and the synchronizing and desynchronizing behavior of scalable and bottlenecked parallel programs. The paper has been awarded the *Best Short Paper Award* and was released with open access [3].

In 2023, our poster entitled ***Making Applications Run Faster by Slowing Down Processes?***, authored by Ayesha Afzal, Georg Hager, and Gerhard Wellein, was presented at the *ISC High Performance Conference*, which took place in Hamburg, Germany [4]. The contribution of this poster sparked significant interest and discussions among attendees of the poster reception at ISC.

Performance tools

Our developments and research in the field of performance related tools is bundled in the Software & Tools division (for details see page 31), which collaborates closely with the Research division.

People

Thomas Gruber (LIKWID, ClusterCockpit and MachineState), Jan Eitzinger and Christoph Kluge (ClusterCockpit), Jan Laukemann (OSACA), Julian Hammer (Kerncraft)

LIKWID

We have maintained and extended the *LIKWID* tool suite in 2023 with new architectures and new features. On the CPU side, the current Intel microarchitecture *SapphireRapids* and AMD microarchitecture *Zen4* were added. The company HPE developed a backend for AMD GPUs and extended the backend for Nvidia GPUs. In order to increase the flexibility for all GPU backends, the new “application daemon” hooks into the target application for better measurement control. For the *EE-HPC project (BMBF)*, a new interface to manipulate system settings has been added. All these changes were released on time in version 5.3.0 for the *Supercomputing Conference 2023*. The rather new communication channels with the users (Matrix chats) are well received by the community.

MachineState

The *MachineState* tool uses a structured approach to gather as much information as possible about the system and the user application. This information can be used solely to document the system state but allow the comparison of old and future system states. In 2023, the tool was extended to include AMD GPUs and the related ROCm library.

ClusterCockpit

ClusterCockpit is a framework with job-specific monitoring for HPC systems. It consists of multiple components for data acquisition, storage and visualization.

`cc-metric-collector`

The `cc-metric-collector` runs on each compute node to periodically collect & receive metrics, process them and send them to a data storage facility. The `cc-metric-collector` is developed collaboratively with the *NHR@KIT* (NHR center at Karlsruhe Institute of Technology). It consists of many metric collectors covering various aspects of compute nodes (OS, CPU, GPU, network, file systems). No Golang interface existed for the AMD GPU-related ROCm SMI library, thus an interface was generated to integrate it into the collector (*go-rocm-smi*). Furthermore, metrics can be received asynchronously from remote locations like remote management cards or even other `cc-metric-collector` instances. After processing the metrics (renaming, unit conversation with `cc-units` package, etc.), they can be sent out a big set of data storage facilities like data bases or message busses. In the year 2023, the main work went into bug fixes in the rather young codebase to stabilize its execution on the compute nodes and to reduce overheads.

cc-node-controller

The `cc-node-controller` component allows the manipulation of system settings at runtime. The development started after the new LIKWID "sysfeatures" module was released in November 2023. It was developed as part of the EE-HPC project and plays together with the `cc-energy-manager` that constantly monitors the energy usage of the compute node. It waits for signals sent by the `cc-energy-manager` and manipulates system settings like CPU frequencies or power limits.

cc-event-store

In contrast to the `cc-metric-store`, `cc-event-store` stores events sent out by the `cc-node-controller` and other components. It consists of HTTP and NATS receivers, a SQLite database and a HTTP API for querying. The development is in early state but it allows to keep track of system changes performed by the `cc-node-controller`. In the end, these events should be shown integrated into the metric plots in the web-based visualization component cc-backend.

Building blocks for sparse linear algebra and stencil solvers

People

Christie Alappat, Jan Laukemann, Dane Lacey

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

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. To address the irregular sparsity of time-evolving, multi-dimensional data, we developed a new dynamic streaming tensor factorization (STF) framework that efficiently linearizes and dynamically time slices (DTS) streaming sparse tensors on-the-fly and, thus, significantly improves data reuse and memory throughput. By accelerating real-life sparse streaming tensor algorithms in such manner, we could observe a speedup of up to an order of magnitude over state-of-the-art algorithms with a various number of sparse tensors on modern Intel CPUs [soh2023ALTOstream].

Lightweight MPI+X-parallel sparse matrix-vector multiplication library

We've published the first release of a lightweight and user-friendly C++ library specifically designed to optimize the performance of the sparse matrix-vector multiplication (SpMV) operation. This operation is widely used in numerous applications and often becomes the primary performance bottleneck. The implementation is based on a hardware-efficient data storage format called SELL-C-σ, which is proven to deliver excellent performance on CPUs, GPUs, and wide-SIMD manycore accelerators. The library employees hybrid MPI+X parallelization, enabling efficient distribution of computational tasks across multiple nodes or processors. Furthermore, it provides advanced features such as communication hiding and domain partitioning, further optimizing the overall performance and usability of the SpMV operation. One may use the library as a stand-alone benchmark to assess SpMV optimization strategies on a given architecture, or as a simple "header-only" library for use in applications. Modern adaptive-precision methods on CPUs and GPUs are currently under development for the next release.

Software engineering for HPC and data analytics

The research presented in this area is a joint work of NHR@FAU and the *Lehrstuhl für Systemsimulation* (LSS), where mainly the group of Prof. Köstler is involved.

People

Rafael Ravedutti, Sebastian Kuckuk, Kajol Kulkarni, Shubham Kavane

Performance engineering and code generation for molecular dynamics and particle simulations

We worked on the development of MD-Bench (`github.com/RRZE-HPC/MD-Bench`), a performance-focused prototyping harness to evaluate the performance of molecular dynamics (MD) kernels with several strategies and configurations on different machines. It contains state-of-the-art implementations for both the Verlet Lists and Cluster Pair algorithm from LAMMPS and GROMACS, respectively, and it focuses on providing simple and clean implementations from major community codes to enable in-depth performance engineering of such kernels. During the past year, efforts were made to provide support for distributed-memory parallelism using MPI, covering different domain partitioning (and workload balance) strategies available in the community packages. The super-cluster variant for improving the efficiency of the Cluster Pair algorithm on GPUs was also discussed and a preliminary version implemented. Apart from this, performance and energy evaluation studies were done as part of an introductory course on performance engineering, which is particularly important as one of the goals of MD-Bench is to be used for teaching activities.

MD-Bench's first paper entitled ***MD-Bench: A generic proxy-app toolbox for state-of-the-art molecular dynamics algorithms*** was published in the *14th International Conference on Parallel Processing and Applied Mathematics*, in Gdansk, Poland, and received the Best Paper Award (`hpc.fau.de/2022/09/14/md-bench-best-paper-award/`), an extended version of the paper entitled ***MD-Bench: A performance-focused prototyping harness for state-of-the-art short-range molecular dynamics algorithms*** was published in the *Special Issue of the Future Generation Computer Systems* (FGCS) journal (`doi.org/10.1016/j.future.2023.06.023`), which provides significant performance insights for such kernels in distinct CPU targets through measurements done with hardware performance counters and static analysis tools such as the *Intel Architecture Code Analyzer* (IACA) and the *Open Source Architecture Code Analyzer* (OSACA).

Finally, Rafael also develops *P4IRS* (`github.com/rafaelravedutti/pairs`), a framework for the code generation of particle simulation kernels in C++, targeting multi-CPU and multi-GPU clusters using OpenMP, MPI, and CUDA. The framework uses a simple symbolic description in Python to setup the simulation and to describe the potentials and/or force fields, and then generates optimal code for the chosen hardware using domain knowledge from such simulations achieved in MD-Bench experimentation and performance studies. A manuscript entitled ***P4IRS: An Intermediate Representation and Compiler for Parallel and Performance-Portable Particle Simulations*** (`doi.org/10.2139/ssrn.4714072`) was submitted to the *Computer Physics Communications* journal, which demonstrates the capabilities and performance for the code generated by *P4IRS* to solve MD and DEM simulations in the Fritz and JUWELS-Booster supercomputers.

Surrogate models for computational fluid dynamics

The analysis of flow fields using the Navier-Stokes equation is both computationally expensive and complex. There is currently a lack of a generalized 3D dataset that can serve as a common reference. This study aims to generate a generalized fluid dynamic dataset for 3D artificial single and multiple geometries and to develop an efficient and complex surrogate model capable of predicting high Reynolds number and complex geometry flows. Supervised training is performed using a CNN-based (U-Net) surrogate model to infer average velocity components. The generated dataset can be used as a benchmark for evaluating the performance and comparing the results of different algorithms or models, with the trained weights also being useful for pre-training.

The WaLBerla Framework was employed to produce a total of 10,000 random single and multiple geometres simulations up to a Reynolds number of 15,000, with objects positioned at various locations in the domain using a Python-based automation script.

Several tests were conducted to validate the obtained dataset. Additionally, various standardization methods were utilized to make the training data (input geometries and WaLBerla simulations) more suitable for efficient training. Two prominent methods used were Min-Max Normalization and Standardization (Z-Score normalization). It was found that model performance was better with standardization compared to Min-Max normalization.

The study involved predicting average fluid velocity components by training the deep-learning model with the generated dataset. An advanced surrogate model (U-Net), consisting of over 500 million parameters, was developed to predict the average velocity flow field in high Reynolds number and complex geometry setups. Considering the model's complexity and the difficulty in fitting it into a single GPU memory, different strategies were employed, including data and model parallelism. Microsoft's DeepSpeed Zero strategies were implemented using PyTorch Lightning modules.

The focus was on evaluating the model's capacity to perform in high Reynolds number, multi-geometry complex flow scenarios. Various methods were used to analyze the model's performance, including capacity evaluation using a small dataset of 16 training samples, with the aim of overfitting the model until the training loss was reduced to zero. The final training loss for the overfitting experiment was recorded to be 0.12. The model was also trained on a dataset of 1,000 samples using four NVIDIA A100 GPUs, with the training and validation loss recorded at 0.21 and 0.19, respectively. Future work aims to improve model performance further by training on a larger dataset of around 10,000 samples.

A comparative study of the energy measurements for training the large-scale model was also performed. It was concluded that simply using the maximum number of GPUs available for training is not always the best strategy. The optimal GPU selection depends on finding the right balance between energy consumption, computational load on each GPU, and the time required to complete the training.

Projects

The Research division of NHR@FAU led and participated in several research projects in 2023. Funding sources were the *NHR Alliance*, the *DFG*, and the *EU Horizon 2020* program.

NHR Alliance central projects with NHR@FAU partners

Portable and Efficient Pinning for Hybrid HPC

(PI: Thomas Gruber)

Controlling the process and thread affinity of HPC applications is crucial in achieving consistent performance behavior of applications. With the increasing topological complexity of computing systems nowadays, the performance-critical task of properly pinning the application to nodes, hardware threads inside the node, as well as coprocessors becomes tedious, requires deep knowledge of the runtime-specific affinity mechanisms, and is still error-prone due to the different behavior exhibited by MPI libraries as well as the configurations of the compute clusters. The goal of this project is to develop a pinning wrapper for MPI-distributed applications that provides consistent, portable, and easy-to-use affinity control on NHR cluster systems. By including intranode parallelism and a variety of co-processors types in the feature set, the pinning wrapper is applicable for a wide range of current and future cluster systems. This helps the users of NHRswitch clusters and run their applications with the expected performance independent of the configuration of the system.

Automatic Detection of Pathological Jobs for HPC User Support

(PI: Jan Eitzinger)

This project will develop an automated rule-based detection system for pathological HPC jobs. Examples for pathological jobs are over-parallelization, software pipelines with a decreasing degree of parallelism, or a lack of process binding. Detection of pathological jobs will be defined by parametrizable rules, which can be extended and specified by HPC experts. The

detection system will support “action templates” that describe countermeasures for a specific pathological job category. The detection system will support automated actions, such as direct notification of HPC users and forwarding of completed action templates to assist in mitigating the detected issue.

Energy Efficiency and Performance of AI at Scale

(PI: Harald Köstler)

With the rise of artificial intelligence and the accompanying demand in compute resources, the energy efficiency of large-scale deep learning (DL) becomes increasingly important. In the first stage of this project, we measure and analyse energy consumption and computational performance of scientific DL workloads at scale with the aim to uncover the correlation between these two. Along these lines, wedevelop easy-to-use, low overhead tools for measuring energy consumption and performance. These tools can be incorporated by AI developers into their code for basic assessment of these metrics, fostering awareness for GreenAI and GreenHPC. Based on the insights from the first stage, we develop new approaches to increase energy efficiency of DL workloads through means of performances optimization in the second stage of the project.

DFG project

Dynamic HPC software packages: Seamless integration of existing software packages and code generation techniques

Complex phenomena in the natural and the engineering sciences are increasingly being studied with the help of simulation techniques. This is facilitated by a dramatic increase of the available computational power, and *Computational Science and Engineering* (CSE) is emerging as a third fundamental pillar of science.

CSE aims at designing, analyzing, and implementing new simulation methods on high-performance computing systems such that they can be employed in a robust, user-friendly, and reliable fashion to a wide variety of scientific and engineering problems. Considering the high cost of supercomputing, reaching the best possible computational efficiency becomes a primary criterion and is central to the research agenda of CSE. Furthermore, HPC software must support a range of increasingly complex applications on modern heterogeneous and volatile hardware platforms, where often many different algorithms are combined to model interacting physical processes. For that, HPC software often has to be modified extensively to make full use of the additional performance of newly released architectures. Our main goal is to provide a new class of dynamic software frameworks to the HPC users that combine existing and established HPC frameworks with current code generation technology to increase the productivity when introducing new applications or porting to new platforms. We will show the benefits of this approach for three real-world multi-physics applications:

(1) optimization of wind turbines and wind farms,
(2) formation and dynamics of dunes that occur in many environmental systems such as riverbeds, and
(3) simulation of charged particles in microfluidic flows.

BMBF projects

DAREXA-F: c 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 heterogenous 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 (`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. 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.

EE-HPC: Energy efficient HPC

The energy consumption of HPC data centers is a decisive factor in the procurement and operation of the systems. *EE-HPC* (`eehpc.clustercockpit.org/`) achieves 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 holisticapproach ensures flexible and broad use for a wide range of applications.

StroemungsRaum—Novel Exascale-Architectures with Heterogeneous Hardware Components for Computational Fluid Dynamics Simulations

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* (`gauss-allianz.de/de/project/title/StroemungsRaum`) 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 finer-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 efficiency, 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.

EU project 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 (`eocoe.eu`). After a first extension EoCoE-II the second extension EoCoE-III starts 2024.

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, among others, the organization of courses and tutorials but also “hackathons”, where project collaborators can apply advanced performance analysis techniques using their own simulation codes.

These codes include *waLBerla-wind* for simulating wind parks, *Alya* for simulating multi-physics problems, *GYSELA*, a code for simulating plasma turbulence in fusion reactors, and *EURAD-IM*, a program for predicting and analyzing air quality.

PhD defenses

Jonas Schmitt, ***Automating the Design of Multigrid Methods with Evolutionary Program Synthesis.***

Publications

[1] A. Afzal, G. Hager, S. Markidis, and G. Wellein: ***Making Applications Faster by Asynchronous Execution: Slowing Down Processes or Relaxing MPI Collectives***. In: Future Generation Computer Systems (2023), ISSN 0167-739X. DOI: 10.1016/j.future.2023.06.017

[2] A. Afzal, G. Hager, and G. Wellein: ***SPEChpc 2021 Benchmarks on Ice Lake and Sapphire Rapids Infiniband Clusters: A Performance and Energy Case Study.*** In: Proceedings of the SC '23 Workshops of The International Conference on High Performance Computing, Network, Storage, and Analysis, Nov 2023, p. 1245-1254. DOI: 10.1145/3624062.362419

[3] A. Afzal, G. Hager, and G. Wellein: ***Physical Oscillator Model for Supercomputing.*** In: Proceedings of the SC '23 Workshops of The International Conference on High Performance Computing, Network, Storage, and Analysis, Nov 2023, p. 1231-1235. DOI: 10.1145/3624062.362553

[4] A. Afzal, G. Hager, and G. Wellein: ***Making Applications Run Faster by Slowing Down Processes?*** Research Poster at ISC High Performance 2023. hpc.fau.de/files/2023/06/Poster-final.pdf

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[11] S. Faghih-Naini, V. Aizinger, S. Kuckuk, R. Angersbach, and H. Köstler (2023). ***p-adaptive discontinuous Galerkin method for the shallow water equations on heterogeneous computing architectures.*** arXiv:2311.11348

[12] 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. Accepted for publication at IPDPS 2024, the 38th IEEE International Parallel & Distributed Processing Symposium. Preprint: arXiv:2403.08777

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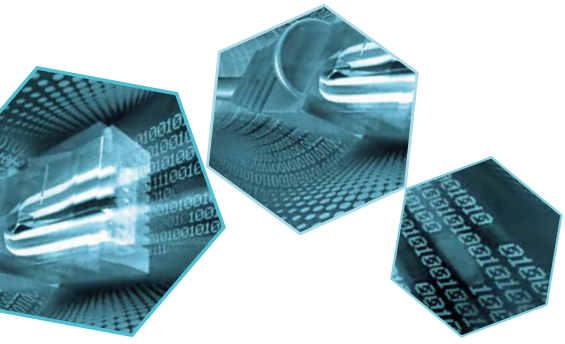

Talks

A. Afzal: ***Performance Modeling Challenges in Extreme Scale Computing***. Online talk at ICIAM 2023 Minisymposium *Progress and Challenges in Extreme Scale Computing and Big Data* [02458], Waseda University, Tokyo, Japan, Aug 22, 2023.

C. L. Alappat: ***Accelerating Sparse Iterative Solvers and Preconditioners Using RACE.*** Talk at the SIAM CSE23 Minisymposium *Performance Engineering and Applications* (MS199), Amsterdam, The Netherlands, Mar 1, 2023.

R. Ravedutti Lucio Machado, J. Eitzinger, and H. Köstler. ***Optimizing Particle Simulations: Performance Analysis and Code Generation with MD-Bench and P4IRS.*** 9th International Conference on Discrete Element Methods (DEM9), Erlangen, Germany, Sep 17–21, 2023.

T. Gruber: ***Pinning, Hardware Counting, and Microbenchmarking with LIKWID***. Invited guest lecture in the CSE 6230—*High Performance Parallel Computing* lecture, Georgia Institute of Technology, March 9, 2023.

G. Hager: ***Physical Oscillator Model for Supercomputing.*** Short paper presentation at PMBS23, the 14th Workshop on Performance Modeling, Benchmarking and Simulation of High Performance Computer Systems, Denver, CO, Nov 13, 2023.

G. Hager: ***SPEChpc 2021 Benchmarks on Ice Lake and Sapphire Rapids Infiniband Clusters: A Performance and Energy Case Study.*** Paper presentation at PMBS23, the 14th Workshop on Performance Modeling, Benchmarking and Simulation of High Performance Computer Systems, Denver, CO, Nov 13, 2023.

G. Hager: ***Application Knowledge Required: Performance Modeling for Fun and Profit.*** Keynote at ICPE 2023, the 14th International Conference on Performance Engineering, Coimbra, Portugal, Apr 19, 2023.

G. Hager: ***Performance Engineering in CSE: A Bird's-Eye View.*** Talk at the SIAM CSE23 Minisymposium *Performance Engineering and Applications* (MS167), Amsterdam, The Netherlands, Mar 1, 2023.

G. Hager: ***Performance Modeling and Performance Engineering***. Invited lecture series at the AQTIVATE Training Workshop on Exacale Computing and Scalable Algorithms, Stockholm, Sweden, Nov 27–Dec 14, 2023.

J. Laukemann: ***OSACA – A Multi-Platform Static Code Analyzer for In-core Performance Prediction***. Talk at Scalable Tools Workshop 2023, Lake Tahoe, California, USA, Jun 19, 2023.

NHR@FAU APPLICATION FOCUS

Liaison Scientists:
Dr. Frank Beierlein, PD Dr. Anselm Horn,
Dr. Sebastian Kuckuk, Rafael Ravedutti,
Marius Trollmann, Dr. Egor Trushin

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 crossfertilization of materials and life sciences, which often use the same or very similar simulation techniques.

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.

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.

Activities of Liaison Scientists

Dr. Frank Beierlein

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

NHR activities, projects, and support

Frank was part of the organizing team for the 36th Molecular Modelling Workshop, which took place as a hybrid event in Erlangen from Mar 13–15, 2023. Together with Petra Imhof, Frank organized the Computational Chemistry part of the *Tag der offenen Labortür*, which took place on Apr 4, 2023. Together with the other NHR@FAU team members and Petra Imhof, Frank presented Computational Chemistry and NHR@FAU at the *HPC Village of the Lange Nacht der Wissenschaften 2023*. 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 NHR@FAU support staff is further ensured by regularly attending the HPC Café.

As one of the two Liaison Scientists (LS) responsible for Amber, Frank provides support for Amber customers of NHR@FAU, together with Anselm Horn. Frank trained scientists for performing standard MD and thermodynamic integration free energy simulations with Amber on the NHR@FAU GPU cluster Alex. Jorge Amador Balderas from the Imhof group and and Raphael Desrues (in 2023 Erasmus student from Université Toulouse III, now Master student at Université Paris Cité) use Frank's scripts and protocol to investigate e.g. DNA-repair mechanisms, while Eduard Neu from the Gmeiner group investigates opioid receptor ligands, and compares the Amber results to Gromacs and FEP+. The Gmeiner group (NHR project ***Medchem-Dynamics***, Susanne Gleich, Nico Staffen, Eduard Neu) is 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). Watching the Amber list and the Amber literature ensures being up-to-date on what happens in the Amber community. Together with the NHR@FAU support staff, Frank continues optimizing the setup of Amber simulations for efficient use on the GPU cluster Alex.

Frank is an expert in parameterizing nonstandard residues and ligands for Amber. Together with Anselm Horn (Sticht group), Frank 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 submitted in December 2023 and accepted in January 2024.

In his current research on DNA repair mechanisms, Frank 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'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. Frank currently writes a proposal for an extension of this NHR project. Additionally, Frank supports Petra Imhof's NHR project ***b186dc*** (DNA-glycosylase—DNA base excision rpair) and Petra Imhof's DFG project on DNA repair (IM141/1-3).

In their teaching (see on the right) and research acitivites 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 and training

Frank 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 2023, ***ThC ab initio – PR, MM MAESTRO – UE***, ***Bio-Organic & Bio-Inorganic Chemistry – LAB BioIOC-LAB***, and ***Drug Discovery – LAB DD-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***. In: RSC Med. Chem. 2024, 15, 1189–1197. DOI: 10.1039/D3MD00609C (submitted in 2023, accepted in Jan 2024).

Frank Beierlein, Anselm H. C. Horn, Heinrich Sticht, Andriy Mokhir, Petra Imhof: ***In Silico Study of Binding of Camptothecin-Based Pro-Drugs to Human Carboxylesterase 2***. In: Biomolecules 2024, 14, 153. DOI: 10.3390/biom14020153 (submitted in 2023, accepted in Jan 2024).

Talks

Frank Beierlein, Senta Volkenandt, Petra Imhof, DNA-Repair Mechanisms: ***Molecular Simulations and Computational Alchemy***, 35th Molecular Modeling Workshop, Erlangen, Mar 13–15, 2023.

Posters

Frank Beierlein, Senta Volkenandt, Petra Imhof, ***DNA-Repair Mechanisms: Molecular Simulations and Computational Alchemy***, 35th Molecular Modeling Workshop, Erlangen, Mar 13–15, 2023.

Jorge Antonio Amador-Balderas, Frank Beierlein Senta Volkenandt, Petra Imhof, ***Effect of N140D and T197A mutations on DNA repair enzyme Thymine DNA Glycosylase***, 35th Molecular Modeling Workshop, Erlangen, Mar 13–15, 2023.

Frank Beierlein, Senta Volkenandt, Petra Imhof, ***DNA-Repair Mechanisms: Molecular Simulations and Computational Alchemy***, Hybrid Workshop on Computer Simulation and Theory of Macromolecules, Hünfeld, Apr 28–29, 2023.

Frank Beierlein, Senta Volkenandt, Petra Imhof, ***DNA-Repair Mechanisms: Molecular Simulations and Computational Alchemy***, NHR Conference ’23, Berlin, Sep 18–20, 2023.

NHR@FAU, Computer-Chemie-Centrum/AK Imhof, ***DNA-Reparatur im Supercomputer***, Lange Nacht der Wissenschaften, Erlangen, Oct 21, 2023.

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 Mar 13–15, 2023. Frank is an active member of this society and supports the managing board as helping hand and cash auditor (“Kassenprüfer”). He also contributed scientifically by giving a talk and presenting posters; at this opportunity, the excellent computing facilities and support of NHR@FAU were emphasized, in addition to the scientific results. Together with Petra Imhof and the HPC staff, Frank explained computational chemistry and NHR@FAU at the Lange Nacht der Wissenschaften in Oct 2023. At the *Tag der offenen Labortür* on Apr 4, 2023, the Imhof group presented the field of computational chemistry to potential new FAU students. At the “Workshop on Computer Simulation and Theory of Macromolecules”, Frank presented a poster on DNA repair mechanisms, acknowledging NHR@FAU.

Collaboration with other Liaison Scientists and HPC staff

Together with Anselm Horn, Frank is the responsible Liaison Scientist for Amber. Frank 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 Jan 2024. Together with the NHR@FAU support staff, the Amber performance is optimized on the NHR@FAU HPC systems. The Gmeiner group was supported in collaboration with Anna Kahler, Harald Lanig and

Thomas Zeiser. Together with Petra Imhof and the HPC staff, Frank presented NHR@FAU at the Lange Nacht der Wissenschaften 2023. Together with Petra Imhof, the other LS and Harald Lanig, Frank is part of the organizing team of the annual Molecular Modeling Workshop.

PD Dr. Anselm Horn

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

NHR activities, projects, and support

Anselm used his long-standing expertise in the generation of force field parameters to support two projects by the creation of missing parameters, which were crucial in pursuing the research question. First, histamine parameters in different protonation states were created to investigate the potential influence of tautomerism upon histamine binding to the H1R receptor [1]. Next, a post-translationally modified version of the amino acid tyrosine, sulfo-tyrosine, was parameterized to study the binding properties of the HIV1-neutralizing antibody PG16 with the aim of designing pharmacologically active peptides derived from that antibody [2]. The results of this study were also presented at the Molecular Modelling Workshop (MMWS) in Erlangen [3] as well as at the NHR conference in Berlin [4], and the parameters are now publicly available to the scientific community.

Since the AI-driven folding software AlphaFold has been gaining increased attention, Anselm downloaded, installed and tested a stand-alone version LocalColabFold to make protein folding prediction available at NHR@FAU at large-scale instead of using the web version with limited runtime. In the meantime, a user-friendly module installation is available at NHR@FAU. This has attracted the workgroup of Prof. Dr. Martin Eilers (University Würzburg), who is currently running a test project in preparation of a large-scale proposal.

Performance tests

The AMBER program suite provides a standardized benchmark set, which enables tuning of code and compilation as well as comparison of different hardware architectures. Anselm performed this benchmark set analysis to provide potential users with NHR@FAU-specific performance results for the GPU cards A40 and A100 installed on Alex. Furthermore, the performance of AMBER on Alex for molecular systems with a systematically increased size was discussed with Dr. Plamen Dobrev and other scientists from the LRZ (Munich).

To gain experience in the AMBER-specific coarse-grained force field Sirah, Anselm performed several molecular dynamics calculations for test systems. Sirah may be regarded an alternative method compared to the widely used MARTINI force field within the Gromacs molecular dynamics package.

Teaching and training

Anselm continued to work on an extension of the Tips&Tricks for AMBER to provide a first help for new users. His experiences from the projects have been shared within other groups in Erlangen. He was especially involved into the training of the new PhD student Olena Denysenko, who joined the GRK2504 “Novel antiviral approaches” in March 2023. First results were presented at the NHR conference in Berlin [5], supported by an NHR travel grant to Ms Denysenko.

An introductory course to MD with AMBER following the inverted-classroom approach was tested with an intern at the Bioinformatics (Marie Sieger). The experiences might allow an upscaling of this kind of teaching to a NHR@FAU course offered for a larger cohort of users.

Outreach

Anselm was part of the organisational committee of the MMWS 2023 in Erlangen that provided a special HPC section (“HPC meets Molecular Modelling”) [6]. He presented a poster about the NHR@FAU computational facilities informing potential users about the procedure for application. Additionally, he advertised “free” small-scale test project access to the NHR@FAU clusters: a low-threshold service where no full proposal had to be

written, but users could test the suitability of the cluster hardware for their own research problems. At the "NHR-Festkolloquium" (Mar 15) [7] and the NHR Results Symposium (Mar 16) [8] he took the opportunity for discussion and exchange with other participants.

He further continued support on the AMBER Mailing List supporting national and international users to overcome problems, especially in the area of parameter generation. He thus tried to increase the visibility of NHR@FAU both, as a local brand and as part of the NHR initiative [9].

For the public event *Long night of the sciences* (Lange Nacht der Wissenschaften 2023) on Oct 25, 2023 Anselm prepared two posters. From the late afternoon until midnight, he informed the interested public about the NHR@FAU cluster and his work as Liaison Scientist. An on-site demonstration of molecular visualization complemented his part at the "HPC village" [10].

The October NHR-Newsletter provided a spotlight article about Anselm. His research interests as well as his work for NHR@FAU were presented therein to the user community [11].

Exchange and collaboration with other Liaison Scientists

Anselm is engaged in a collaboration project with Dr. Frank Beierlein applying his expertise in force field parameter generation. The project resulted in a joint publication of two NHR@FAU PI research groups Imhof and Sticht [12].

A regular, yet mostly informal exchange between the Liaison Scientists was the weekly online meeting. Organized by Dr. Harald Lanig, the NHR@FAU executive secretary, this Zoom meeting every Wednesday provided a platform for mutual exchange about many topics, organisational, technical, and scientific, with the focus of the later on atomistic simulations.

An important opportunity for the exchange with other Liaison Scientists and NHR@FAU people was the monthly HPC Café. Especially during the coffee session right before the scientific or technical talk given by experts in their field fruitful discussions stimulated various ideas.

Administrative tasks

Anselm acted as scientific and technical reviewer for NHR@FAU proposals and as advisor in NHR@FAU projects. Moreover, he joined the users committee ("Nutzerausschuss") and participated in meetings about further grants for the extension of the HPC clusters at NHR and the FAU.

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[4] MMWS 2023, Erlangen. Poster P07. *Book of Abstracts MMWS2023*

[5] NHR Conference 2023, Berlin. PosterID P-LS-06. *Book of Abstracts NHR Conference 2023*

[6] MMWS 2023, Erlangen. mmws2023.mgms-ds.de/index.php?m=125

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Dr. Sebastian Kuckuk

Chair of Computer Science 10 (System Simulation) and NHR@FAU

NHR activities, projects, and support

Sebastian played an important role in advising the NHR pathfinder project titled ***Energy Efficiency and Performance of AI at Scale***, conducted in collaboration with Charlotte Debus and colleagues from NHR@KIT. A notable outcome of this collaboration was the master thesis authored by Amritanshu Verma, titled ***Performance Engineering of Transformer on GPU vs CPU***. The thesis made a significant contribution through the custom implementation of deep learning pipelines, specifically based on the transformer architecture. This approach allowed for a comprehensive study of the performance and energy consumption characteristics of different code components.

In addition to his involvement in the aforementioned project, Sebastian provided valuable input for other master theses. One of them was ***Computational Investigation of Charged Particles in Fluid Flow*** by Ravi Somayajula. Furthermore, he continues to contribute to the ongoing thesis of Mohammad Shanur Rahman, which focuses on accelerating deep neural network (DNN) inference with Winograd convolutions on edge GPUs.

Sebastian continued to offer consultation for Vadym Aizinger's group at the University of Bayreuth, focusing on numerical solvers, computations on block-structured grids, and optimizing GPU usage. This collaboration involved several meetings and a joint workshop between the University of Bayreuth and NHR@FAU, where recent research findings were discussed, and ideas for future research directions were exchanged. The outcomes of this collaboration included the publication of a joint paper titled ***Discontinuous Galerkin method for the shallow water equations on complex domains using masked block-structured grids*** in Advances in Water Resources, as well as a joint preprint covering ***p-adaptive discontinuous Galerkin method for the shallow water equations on heterogeneous computing architectures***.

Additionally, Sebastian contributed his expertise to the KONWIHR project ***Continuous Benchmarking for the GHODDESS framework***. In this context, he provided input for extending an existing continuous integration pipeline, which checks new code versions for correctness of produced results. The extension involved the incorporation of a continuous benchmarking pipeline, tracking the performance behavior of each new code version.

Lastly, Sebastian undertook the implementation of a benchmark application for a collaborative research activity between NHR@FAU and the University of Basel, comprising two distinct components. The first involves the synthesis of a series of images through ray-tracing, while the second entails image processing by calculating optical flow between different images within the series. The image processing component employs a geometric multigrid solver.

The application has been designed to strike a balance between regions constrained by computational performance and those limited by main memory bandwidth. Additionally, its distributed memory parallelization makes it particularly well-suited for investigating the impacts of load imbalance and exploring balancing techniques, along with studying idle waves in highly parallel programs.

Teaching and training

Sebastian, a certified NVIDIA Deep Learning Institute (DLI) university ambassador with the "Accelerated Computing" specialization, possesses the expertise to instruct introductory courses on GPU programming with C++ and Python, as well as advanced courses covering techniques for multi-GPU and multi-node applications.

In 2023, he conducted a total of five courses at the NHR@FAU. One of these sessions was a special edition tailored for EUMaster4HPC students. Another course took place independently of the DLI, given a temporary pause on the DLI's side. This session utilized NHR@FAU's local supercomputer, Alex, yielding highly satisfactory results. 80% of the workshops were delivered in-person, attracting a total of 62 participants (from 70 registrations). The attendees highly

recommended the courses to their colleagues, providing an average score of 4.7 out of 5 based on 28 total votes.

In addition to these introductory courses, preparations for delivering multi-GPU courses, specifically ***Accelerating CUDA C++ Applications with Multiple GPUs and Scaling CUDA C++ Applications to Multiple Nodes***, were done in 2023. These efforts culminated in a successful test run in February 2024, following the DLI's resumption of support for course deliveries. The test run received an impressive recommendation score of 4.7 out of 5, based on feedback from 15 participants.

Sebastian actively contributed his expertise to support the ***High-End Simulation in Practice (HESP)*** lecture, taking charge of exercise classes. The practical exercises and mini-project were specifically designed to delve into GPU programming, GPU performance engineering, and technologies relevant to simulating particulate systems. In total, 25 students successfully participated, benefiting from the hands-on experience facilitated by Sebastian.

Meetings, travel, and community outreach

Presentation on ***Code Generation for the Simulation of Ocean Flows on Block-Structured Grids*** at SIAM Conference on Computational Science and Engineering (CSE), Amsterdam, Netherlands, Feb 26–Mar 03, 2023.

Joint workshop between University Bayreuth and NHR@FAU, Bayreuth, May 5, 2023.

Publications

Richard Angersbach, Sebastian Kuckuk, and Harald Köstler. ***Generating Coupling Interfaces for Multiphysics Simulations with ExaStencils and waLBerla*** in 2023, IEEE International Parallel and Distributed Processing Symposium Workshops (IPDPSW). 2023, p. 651–661. DOI: 10.1109/IPDPSW59300.2023.00112

Sara Faghih-Naini, Sebastian Kuckuk, Daniel Zint, Samuel Kemmler, Harald Köstler, and Vadym Aizinger. ***Discontinuous Galerkin method for the shallow water equations on complex domains using masked block-structured grids***. Advances in Water Resources, 2023, 182, 104584.
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Sara Faghih-Naini, Vadym Aizinger, Sebastian Kuckuk, Richard Angersbach, and Harald Köstler. ***p-adaptive discontinuous Galerkin method for the shallow water equations on heterogeneous computing architectures***. arXiv:2311.11348

Rafael Ravedutti

Chair of Computer Science 10 (System Simulation) and NHR@FAU

NHR activities, projects, and support

Rafael worked as a Liaison Scientist until 03/2023 and changed full-time to the BMBF EE-HPC project afterwards. Rafael was a Liaison Scientist in the field of molecular dynamics (MD) simulations with a special focus on software and performance engineering. He worked on the performance-oriented prototyping harness MD-Bench1, which helps to build in-depth knowledge about the performance characteristics of short-range molecular dynamics applications. His second focus was on domain specific languages for particle simulations in general. Rafael was involved in support for several third party funded projects, e.g. benchmarking GROMACS for EE-HPC, and software engineering support for the DFG project Dynamic HPC software packages.

Teaching and training

Rafael was closely involved in teaching MD and HPC related courses for the FAU students. These were MD-Bench and HPC related projects at the MuCoSim Seminar, the MPI lecture PAMPI, and the lecture High End Simulation in Practice.

Collaboration with other Liaison Scientists

Rafael collaborated with other Liaison Scientists to define new test cases in MD-Bench. Marius Trollmann provided input files for an Argon test case originating from GROMACS.

Publications

R. Ravedutti Lucio Machado, J. Eitzinger, H. Köstler, and G. Wellein: ***MD-Bench: A generic proxy-app toolbox for state-of-the-art molecular dynamics algorithms.*** In: Wyrzykowski, R., Dongarra, J., Deelman, E., Karczewski, K. (eds) Parallel Processing and Applied Mathematics. PPAM 2022. Lecture Notes in Computer Science, vol 13826. Springer, Cham. PPAM 2022 Best Paper Award.
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Marius Trollmann

Department of Biology (Professorship for Computational Biology) and NHR@FAU

NHR activities, projects, and support

Marius 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 GPGPUs and CPUs. In his role, Marius has provided support to NHR-funded projects, ensuring optimal utilization of available resources. In a notable contribution, he conducted benchmark calculations for a large-scale computing project (*Project ID: b174dc*) during the application phase, estimating the required computing times. Additionally, he played a role in two NHR project applications (*Project ID: b188dc, c102fd*) by contributing to the technical reviews of the proposals.

Scientific results

As a PhD-student, Marius applies and enhances his expertise by utilizing available resources in his own research projects. Notably, he contributed significantly to two recent studies published in the journal ***Nature Communications***. The projects provided novel insights into the (highly-debated) non-universal effect of cholesterol [1] on the bending elasticity of lipid bilayers and elucidate the molecular mechanism of the cyclic antimicrobial peptide lugdunin [2] (see figure on the right).

Outreach

Marius Trollmann participated at the first NHR conference in Berlin and presented a poster about his actual research. A list of his further outreach activities can be found below.

Teaching and training

Marius actively contributes to the education and training of both new and existing users of HPC systems. He prepared and carried out an online tutorial for the MD package GROMACS with participants across Germany (Oct 10–12, 2023). Leveraging a Jupyterhub instance, participants accessed and utilized local HPC resources, fostering a hands-on learning experience. The tutorial received high acclaim, with an evaluation score of 4.8 out of 5 possible points (Result of an anonymized survey sent to the participants after the tutorial: “How would you rate the overall quality of the GROMACS tutorial? Please rate from 1 (poor) to 5 (excellent).”). The success of the online tutorial prompted the integration of HPC resources into the on-site GROMACS tutorial for the module ***Strukturbiologie*** within the Bachelor Biologie/Integrated Life Sciences program. Consequently, undergraduate students came in touch with the NHR, and learnt how to apply highly optimized software on HPC systems early in their academic journey. The knowledge and experience acquired during these tutorials were subsequently shared with other groups to facilitate the organization of similar hands-on tutorials. Moreover, Marius is currently planning online tutorials focusing on more advanced topics, along with transitioning additional on-site tutorials to HPC systems in 2024.

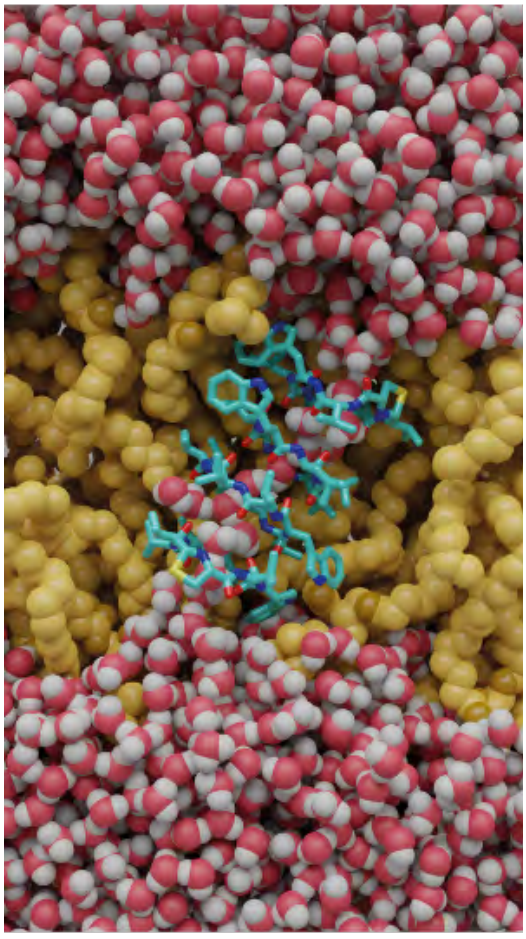
Orientierungsmodul ***Strukturbiologie I***, Master Zell- und Molekularbiologie/Integrated Life Sciences

Orientierungsmodul ***Strukturbiologie II***, Master Zell- und Molekularbiologie/Integrated Life Sciences

Python for Bioinformatics and Data Analysis, Master Zell- und Molekularbiologie/Integrated Life Sciences/Integrated Immunology

Fachmodul ***Strukturbiologie***, Bachelor Biologie/Integrated Life Sciences

In the Orientierungsmodul Strukturbiologie I and Orientierungsmodul Strukturbiologie II courses, students are given the opportunity to prepare and conduct their own molecular dynamics (MD) simulations to work on a realistic research hypothesis. The course Python for Bioinformatics and Data Analysis offers an introduction to the popular programming language Python, highlighting its applications in the natural sciences.



Stack of four lugdunin molecules (atoms colored in cyan (C), red (O), blue (N) and yellow (S) in a lipid bilayer (atoms colored in beige). Water molecules (atoms colored in red (O) and white (H) diffused spontaneously into the channel during the MD simulation [2].

Meetings, travel, and community outreach

Weekly virtual NHR@FAU Liaison Scientist meeting

35th Molecular Modelling Workshop 2023, Mar 13–15, 2023 Erlangen (contributed talk).

Meeting between NHR@FAU and the LRZ Biolab, Mar 03, 2023 (online).

NHR@FAU-Festkolloquium, Mar 03, 2023, Erlangen.

NHR@FAU Results Symposium, Mar 16, 2023, Erlangen.

European Biophysical Societies' Association (EBSA) Congress Jul 31–Aug 04, 2023, Stockholm (poster presentation).

NHR Conference '23, Sep 18–20, 2023, Berlin (poster presentation).

Lange Nacht der Wissenschaften (public event), Oct 21, 2023, Erlangen.

Publications

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Dr. Egor Trushin

Chair of Theoretical Chemistry and NHR@FAU

NHR activities, projects, and support

Egor Trushin has been involved in the development and implementation of quantum chemistry and density functional methods in a number of computational quantum chemistry packages.

The main contribution has been made to the Molpro Quantum Chemistry Software [1]. Egor Trushin contributed computational methods to Molpro, in the development of which he has been involved for several years:

- A random phase approximation and σ-functional program [2, 3], which allows for an accurate calculation of various chemical properties such as, e.g., reaction energies and barrier heights of chemical reactions or the determination of geometries and vibrational properties of molecules.
- A numerically stable optimized effective potential (OEP) exact-exchange (EXX) program [4], which makes numerically stable OEP-EXX calculations feasible even with basis sets from standard basis set libraries, which was mostly impossible before.
- A Kohn-Sham inversion program [5], which solves the fundamental problem of Kohn-Sham density functional theory to construct Kohn-Sham exchange-correlation potentials corresponding to given electron densities.

These programs are already available or will be available to users in the next Molpro releases.

σ-functional [2, 3] calculations are also available in the latest version of the ADF [6] package, to which Egor Trushin contributed part of the code.

As an expert in scientific programming and quantum chemical method development, in his current research Egor Trushin continues to contribute to various community codes, such as Molpro, PySCF [7], PySCFAD [8], and ORCA [9], as well as in the development of new computational methods.

Teaching and training

Egor is involved in teaching and supporting young researchers in scientific programming and use of modern quantum chemistry codes. He has also created a series of tutorials in the form of Jupyter notebooks on the use of quantum chemistry methods developed in the Theoretical Chemistry Department at FAU.

Publications

E. Trushin, A. Görling. ***Avoiding spin contamination and spatial symmetry breaking by exact-exchange-only optimized-effective-potential methods within the symmetrized Kohn-Sham framework.*** In: J. Chem. Phys. 159 (2023) 244109.
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E. Trushin, J. Erhard, A. Görling. ***Violations of the v-representability condition underlying Kohn-Sham density-functional theory***. Accepted to Phys. Rev. A.

E. Trushin, S. Fauser, A. Mölkner, J. Erhard, A. Görling. ***Shedding light on the dark side of density-functional theory: accurate correlation potentials from the self-consistent random phase approximation***. Submitted.

Posters

E. Trushin, S. Fauser, J. Erhard, A. Görling. ***Chemical Accuracy at Low Computational Cost with σ- Functionals for the Kohn-Sham Correlation Energy***. NHR Conference ’23, Berlin, Sep 18–20, 2023.

APPENDIX

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Publications which used NHR@FAU resources

The following list contains the publications (mentioned to us) that used NHR@FAU resources.

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A. Afzal, G. Hager, S. Markidis, and G. Wellein: ***Making Applications Faster by Asynchronous Execution: Slowing Down Processes or Relaxing MPI Collectives***. In: Future Generation Computer Systems—the international journal of escience, 148:472–487, Nov 2023. DOI: 10.1016/j.future.2023.06.017

R. Angersbach, S. Kuckuk, H. Köstler: ***Generating Coupling Interfaces for Multiphysics Simulations with ExaStencils and waLBerla***. International Parallel and Distributed Processing Symposium (IPDPS), St. Petersburg, Florida USA, May 15–19, 2023, In: 2023 IEEE International Parallel and Distributed Processing Symposium Workshops (IPDPSW), Los Alamitos, CA, USA, 2023. DOI: 10.1109/IPDPSW59300.2023.00112

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Compute projects

In this section we list all compute projects that used NHR@FAU resources (parallel computer Fritz & GPGPU cluster Alex) in 2023, 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 PI. Abstracts are truncated as indicated by square brackets; full-length abstracts can be found at `hpc.fau.de/about-us/nhr-compute-time-projects/`.

Humanities and Social Sciences

Humanities

Pose22: Pose Estimation on Russian International News Media (Large Scale, 10/2022–12/2023)

[...] studying the mechanisms used for disinformation, in particular viewpoint manipulation, by Russian state-sponsored media. [...] create a dataset fully annotated with pose information of the English-language programs found on the now-banned YouTube presence of RT (Russia Today) [...]

University: FAU Erlangen-Nürnberg
Target systems: Fritz & Alex

ProtCTRL: A conditional transformer for à la carte protein sequence generation (07/2022–06/2023)

[...] protein design process relied on searching the global minima of multidimensional energy functions, [...] required significant computational times for each run. Recent advances in NLP have produced protein language models capable of generating fit protein sequences within seconds. [...]

University: University of Bayreuth
Target system: Alex

Life Sciences

Basic Research in Biology and Medicine

ChannelProtonation: Investigating the Influence of Protonation States on Cation Conductivity in Ion Channels through Molecular Dynamics Simulations (10/2023–12/2024)

[...] 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. [...]

University: Technical University of Berlin
Target system: Alex

ORmd: Systematic molecular dynamics simulations of the odorant receptor family (Large Scale, 10/2023–09/2024)

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 [...]

University: Technical University of Munich
Target system: Alex

AmPeL: Interaction of Antimicrobial Peptide Lugdunin with Membranes (Large Scale, 07/2023–06/2024)

[...] 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. [...]

University: FAU Erlangen-Nürnberg
Target systems: Fritz & Alex

AMPARGating: Investigation of cation gating and conduction mechanism of an AMPAR-type glutamate receptor (07/2023–06/2024)

[...] AMPAR with bound auxiliary proteins to reveal the mechanisms by which the cation gating and conduction is modulated. [...] subunit composition which is thought to represent a stabilized open state and a different subunit composition which has an influence on the polyamine block. [...]

University: Humboldt-Universität zu Berlin
Target system: Fritz

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.

University: FAU Erlangen-Nürnberg
Target system: Alex

Dynasome3: Exploring Protein Dynamics Space to Improve Protein Function Prediction (Large Scale, 10/2022–09/2024)

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. [...]

University: Georg-August-Universität Göttingen
Target system: Fritz

CoupledFoldBind: Conformational presentation switching processes studied by Molecular Simulations (07/2022–12/2024)

[...] 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. [...]

University: Technical University 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. [...]

University: University of Augsburg
Target systems: Fritz & Alex

GPCRSCOMPEVO: Computational models of structure, dynamics and evolution of GPCRs (Large Scale, 07/2022–12/2024)

[...] 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.

University: Leipzig University
Target systems: Fritz & Alex

DNARepairTDG—DNA Repair by Thymine DNA Glycosylase (06/2022–09/2023)

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.

University: FAU Erlangen-Nürnberg
Target system: Alex

Antivirals: Structure-based design and optimization of ligands for novel antiviral strategies (04/2022–06/2024)

[...] 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. [...]

University: FAU Erlangen-Nürnberg
Target system: Alex

GPCRSIM: Metadynamics simulations of ligand binding/unbinding and receptor activation/deactivation for G-protein coupled receptors (Large Scale, 04/2022–04/2024)

GPCRSIM uses classical (force-field) molecular dynamics simulations to determine binding sites, binding free energies and activation/deactivation free-energy profiles for predominantly class A G protein coupled receptors. [...] observe rare events such as binding or activation [...]

University: FAU Erlangen-Nürnberg
Target systems: Fritz & Alex

ImmunoDomains: Interplay of immune receptors and lipid environment in signaling (Large Scale, 04/2022–09/2023)

[...] immune receptors expressed on the surface of a variety of cells is typically characterized by the sensing of an external signal, followed by signal modulation and transmission into the cell. [...] affected by the composition, structure, and characteristics of the plasma membrane [...]

University: FAU Erlangen-Nürnberg
Target system: Alex

Plant Sciences

CEC: Convergent evolution of carnivorous plants (08/2022–09/2024)

[...] By comparison of the genetic and transcriptomic landscape between carnivorous and non-carnivorous plants, we may be able to identify the common genetic elements required for plant carnivory. This will not only grant us insights into plant carnivory, but into plant evolution as a whole.

University: University of Würzburg
Target system: Fritz

Medicine

MIA-NORMAL: Medical Image Analysis with Normative Machine Learning (Large Scale, 10/2023–09/2024)

[...] 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. [...]

University: FAU Erlangen-Nürnberg
Target system: Alex

Medchem-Dynamics: Molecular Dynamics and Docking Studies with Multifunctional Receptor-Ligand Complexes (Large Scale, 01/2023–03/2024)

[...] 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. [...]

University: FAU Erlangen-Nürnberg
Target system: Fritz

MASCARA: Molecular Assessment of Signatures ChAracterizing the Remission of Arthritis (12/2022–01/2024)

[...] we will investigate the generation of synthetic chest X-rays using latent diffusion models. This way, we will be able to generate large amount of data necessary to train chest X-ray classification networks while preventing leakage of patient identity.

University: FAU Erlangen-Nürnberg
Target system: Fritz

PatRo-MRI-2: Pathology-robust image reconstruction in Magnetic Resonance Imaging (10/2022–12/2026)

[...] 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.

University: FAU Erlangen-Nürnberg
Target system: Alex

GastroDigitalShirt: Development and test of deep neural network models for the automatic detection of body sounds to monitor digestion in control group and patients with intestinal disorders (09/2022–11/2023)

[...] develop an unobtrusive wearable technology for long-term digestion monitoring, termed GastroDigitalShirt. We investigate low-amplitude bowel sounds (BS) as indicators of digestive disorders, including chronic inflammatory bowel diseases (IBD). [...]

University: FAU Erlangen-Nürnberg
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. [...]

University: 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 [...]

University: Aalen UAS
Target systems: Fritz & Alex

Neurosciences

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 (08/2022–02/2025)

[...] 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 [...]

University: FAU Erlangen-Nürnberg
Target systems: Fritz & Alex

Natural Sciences

Physical and Theoretical Chemistry

AKES: Chemical Modelling of Processes in Pharmaceutical Chemistry (11/2022–02/2024)

Covalent inhibitors currently experience a renaissance in medicinal chemistry due to their various advantages, including prolonged residence times, lower sensitivity against pharmacokinetic aspects, and high efficacy. Our work addresses the reaction mechanisms of cysteine protease rhodesain with covalent inhibitors.[...]

University: Julius-Maximilians-Universität Würzburg
Target system: Alex

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. [...]

University: University of 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. [...]

University: FAU Erlangen-Nürnberg
Target systems: Fritz & Alex

Chemical Solid State and Surface Research

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 (Large Scale, 07/2022–12/2024)

[...] 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 [...]

University: FAU Erlangen-Nürnberg
Target system: Fritz

Molecular Chemistry

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).

University: 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 [...]
University: University of Stuttgart
Target systems: Fritz & Alex

Condensed Matter Physics

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.

University: 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.

University: FAU Erlangen-Nürnberg
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. [...]

University: FAU Erlangen-Nürnberg
Target system: Fritz & Alex

SELRIQS: Series expansions for long-range interacting quantum systems (06/2023–12/2024)

[...] 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.

University: FAU Erlangen-Nürnberg
Target system: Fritz

AHPO4TauID: Automatic hyperparameter optimization of Graph Neural Networks for tau neutrino identification in KM3NeT/ORCA (05/2023–07/2023)

[...] promising results achieved in first trainings will be further improved in this NHR project by conducting a systematic search for the optimal hyperparameters of the networks, a task known as automatic hyperparameter optimization.

University: FAU Erlangen-Nürnberg
Target system: Alex

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. [...]

University: University of Regensburg
Target system: Fritz

MultiDyn: Dynamics of complex networks of oscillators (Large Scale, 01/2023–12/2023)

This project is designed to provide a wide-ranging stability phase diagrams classifying the distribution of self-organized periodicities and complex motions of various sorts in families of coupled nonlinear oscillators when more than one control parameter is varied simultaneously.

University: FAU Erlangen-Nürnberg
Target system: Fritz

ALFQMCsim: Emergent and critical phenomena in correlated electron systems: Quantum Monte Carlo simulations (Large Scale, (10/2022–12/2024)

[...] 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. [...]

University: Julius-Maximilians-Universität Würzburg
Target system: Fritz

nqsQuMat: Neural quantum states for strongly correlated quantum matter (Large Scale, 12/2022–09/2024)

[...] 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.

University: University of Augsburg
Target system: Alex

DMFT2TBLG: DMFT study of a heavy-fermion model for twisted bilayer graphene (12/2022–03/2024)

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. [...]

University: Julius-Maximilians-Universität Würzburg
Target system: Fritz

FRG: Functional Renormalization Group calculations for material analysis (11/2022–12/2024)

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. [...]

University: RWTH Aachen
Target system: Fritz

CLSfiniteV: Finite volume study of 2 + 1f QCD from lattice simulations (Large Scale, 10/2022–09/2023)

[...] In this study we plan to investigate the systematic effects introduced by the finite volume of the system, which is important in particular for quantities like low energy constants, pseudoscalar masses and decay constants, or the axial charge of the nucleon.

University: University of Regensburg
Target system: Fritz

Astrophysics and Astronomy

HESSML: Advanced Machine Learning Analysis for the H.E.S.S. Telescopes (08/2022–01/2024)

[...] With this project, we aim to develop a variety of new analysis methods for H.E.S.S. data, including improved identification of muonic events, exploration of geometric deep learning techniques, fast simulation approaches and new data augmentation strategies.

University: FAU Erlangen-Nürnberg
Target system: Alex

ECOGAL_MW: Full disk modeling of the Milky Way (05/2023–04/2024)

[...] This project interweaves the unique expertise of four European research groups at the forefront of science in the four pillars of astronomy and astrophysics: observations, theoretical simulations, instrumentation and data analysis.

University: University of Heidelberg
Target system: Fritz

Transient3body: Transient formation in three-body encounters between stars and black holes (03/2023–05/2024)

[...] To investigate the impact and outcomes of dynamical interactions we perform hydrodynamics simulations of various types of three-body encounters using the moving-mesh magnetohydrodynamics code AREPO.

University: Ludwig Maximilian University of Munich
Target system: Fritz

CosmosTNG: galaxy formation and evolution with constrained cosmological magnetohydrodynamical simulations at cosmic noon (Large Scale, 07/2023–06/2024)

[...] (i) a direct comparison between simulations and observations in the COSMOS field, (ii) a new tool to explore galaxy formation in constrained environments, and (iii) a probe of the physics and distribution of gas in and around galaxies – from the circumgalactic to intergalactic medium – at cosmic noon.

University: University of Heidelberg
Target system: Fritz

Particles, Nuclei, and Fields

CLS3pt: Hadron structure observables on lattices at low pion masses (Large Scale, 10/2023–09/2024)

[...] 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.
University: FAU Erlangen-Nürnberg
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. [...]
University: University of Regensburg
Target system: Fritz

DPDa: Quark Double Parton Distributions of the Nucleon (Large Scale, 04/2023–06/2025)

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. [...]
University: University of Regensburg
Target system: Fritz

addlight: The spectrum of charmonium and glueballs: adding the light hadrons (Large Scale, 01/2023–04/2026)

[...] 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.
University: University of Wuppertal
Target system: Fritz

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

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. [...]
University: FAU Erlangen-Nürnberg
Target system: Fritz & Alex

Mathematics

Bio-FROSch: Modeling and simulation of pharmaco-mechanical FSI for an enhanced treatment of cardiovascular diseases and non-Newtonian micro-macro blood flow simulations (07/2023–06/2024)

[...] 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. [...]
University: Universität zu Köln
Target system: 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.
University: Technical University of Dortmund
Target system: Fritz & Alex

Atmospheric Science, Oceanography and Climate Research ATMOS: Numerical atmospheric modeling for the attribution of climate change and for model improvement (08/2022–03/2025)

[...] 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 [...]
University: FAU Erlangen-Nürnberg
Target system: Fritz

Statistical Physics, Soft Matter, Biological Physics, Nonlinear Dynamics

CLINT-M02: Multiscale modelling of SILP and SCILL catalysis (07/2023–06/2025)

[...] identify, characterise and enhance effects, occurring on a multitude of molecular time and length scales, which favourably affect the overall reaction's turn over. [...] devise a hybrid quantum mechanics/molecular mechanics approach to embed local quantum characterisation [...] into inhomogeneous IL films.

University: FAU Erlangen-Nürnberg
Target system: Alex

CRC1411D04: Design of Particulate Products: Modelling particle aggregation and assembly into optimal structures (03/2023–06/2024)

[...] develops and applies new methods to study not only the self-assembly process itself but also the properties of the self-assembled nanostructures. [...] closely interact with experimental work that is conducted in the framework of the Collaborative Research Centre Design of Particulate Products.

University: FAU Erlangen-Nürnberg
Target system: Fritz & Alex

EnSimTurb: Towards ensemble simulations of fully developed turbulence (12/2022–04/2026)

[...] 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.

University: University of Bayreuth
Target system: Fritz & Alex

Engineering Sciences

Mechanics and Constructive Mechanical Engineering

FLINSENOI: Flow induce self-noise (Large Scale, 01/2023–06/2024)

[...] Transient and scale-resolving simulations are needed to extract the quantities of interest, such as turbulent dissipation, anisotropy of turbulence, Reynolds stress, flow-acoustic source terms, velocity and pressure fluctuations as well as temporal spectra. [...]

University: FAU Erlangen-Nürnberg
Target system: Fritz

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.

University: FAU Erlangen-Nürnberg
Target system: Fritz

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 [...]

University: FAU Erlangen-Nürnberg
Target system: Fritz

FFRASCAL-MD: Particle-based computing at LTM for FRASCAL (09/2022–09/2024)

[...] 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.

University: FAU Erlangen-Nürnberg
Target systems: Fritz & Alex

Fluid Mechanics, Technical Thermodynamics and Thermal Energy Engineering

AOTTP-DFG18-1: Characterization of molecular diffusion in electrolyte systems (08/2022–07/2024)

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. [...]

University: FAU Erlangen-Nürnberg
Target systems: Fritz & Alex

Materials Science

ASiMENiS: Atomistic simulation of microstructure elements in Ni-based superalloys (01/2023–04/2024)

[...] The goal of this project is to understand dislocation mobility and the formation of local defect phases in the microstructure. The atomistic simulations involve high-throughput ab-initio calculations and large-scale molecular-dynamic simulations with machine-learning potentials based on the atomic cluster expansion.

University: Ruhr-Universität Bochum
Target systems: Fritz & Alex

Materials4.0—AITDB: Ab initio thermodynamic database development (10/2022–01/2025)

[...] 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.

University: University of Stuttgart
Target system: Fritz

Systems Engineering

Voxray: Quantenrekonstruktion für industrielle Computertomographie (07/2023–06/2024)

[...] 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. [...]

University: FAU Erlangen-Nürnberg
Target system: Alex

Electrical Engineering and Information Technology

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 [...]

University: FAU Erlangen-Nürnberg
Target system: Alex

MMSP: Multi-Microphone Speaker Separation (07/2023–06/2024)

[...] Our research focuses on separating speech sources in predefined spatial regions, for example, related to the seats in a car or the seats in a conference room. We employ deep neural networks for the separation process.

University: FAU Erlangen-Nürnberg
Target system: Fritz

Computer Science

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.

University: University of Hamburg
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 (12/2023–11/2024)

[...] 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.

University: FAU Erlangen-Nürnberg
Target system: Alex

OLMAP: Adapting LLMs to Align with User Preferences (NHR starter, 11/2023–10/2024)

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.

University: Technical University of Dresden
Target system: Alex

TriFORCE: Learning adaptive reusable skills for intelligent autonomous agents (11/2023–10/2024)

[...] 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.[...]

University: Julius-Maximilians-Universität Würzburg
Target system: Alex

MAGNET4Cardiac7T: Physics-Informed Deep Learning Algorithms for Modeling Electro-Magnetic Fields in the Human Thorax (10/2023–09/2024)

[...] 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. [...]

University: Julius-Maximilians-Universität Würzburg
Target system: Alex

XXL-CT-Segmentation: Instance segmentation of XXL-CT Volumes (06/2023–06/2024)

XXL-Computed Tomography [...] can contain multiple 10,000 of different entities of depicted objects with varying properties (shapes, densities, materials, compositions) which are hard to delineate. [...] develop deep learning based instance segmentation algorithms to delineate these entities [...]

University: FAU Erlangen-Nürnberg
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 [...]

University: FAU Erlangen-Nürnberg
Target system: Alex

digiOnko: Mit digitaler Medizin gegen Brustkrebs, AP5—Histopathologie (12/2022–09/2024)

[...] 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.

University: FAU Erlangen-Nürnberg
Target system: Alex

DeepPano: Erzeugung von Panoramabildern aus 3D-Laser-Punktewolken und Kamerabildern (12/2022–04/2024)

[...] 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.

University: FAU Erlangen-Nürnberg
Target system: Alex

HEISSRISSE: Massively Parallel Simulation of the Melt Pool Area during Laser Beam Welding using the Lattice Boltzmann Method (10/2022–11/2023)

Using abstraction layers and code generation concepts, software developed with waLBerla is sustainable [...] One of the significant aspects [...] lies in the validation of newly implemented models and algorithms, and in the interoperability with models from the partners in the research unit. [...]

University: FAU Erlangen-Nürnberg
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 [...]

University: FAU Erlangen-Nürnberg
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.

University: FAU Erlangen-Nürnberg
Target system: Alex


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D. Ruppelt, M.F.W. Trollmann,..., S. Grond, R.A. Böckmann, and C. Steinem, 2024. *The antimicrobial fibupeptide lugdunin forms water-filled channel structures in lipid membranes*. Nature Communications, 15(1), p.3521.
DOI: 10.1038/s41467-024-47803-6 (front and back cover, p. 55)
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kjpargeter, freepik (p. 47)

Editor:

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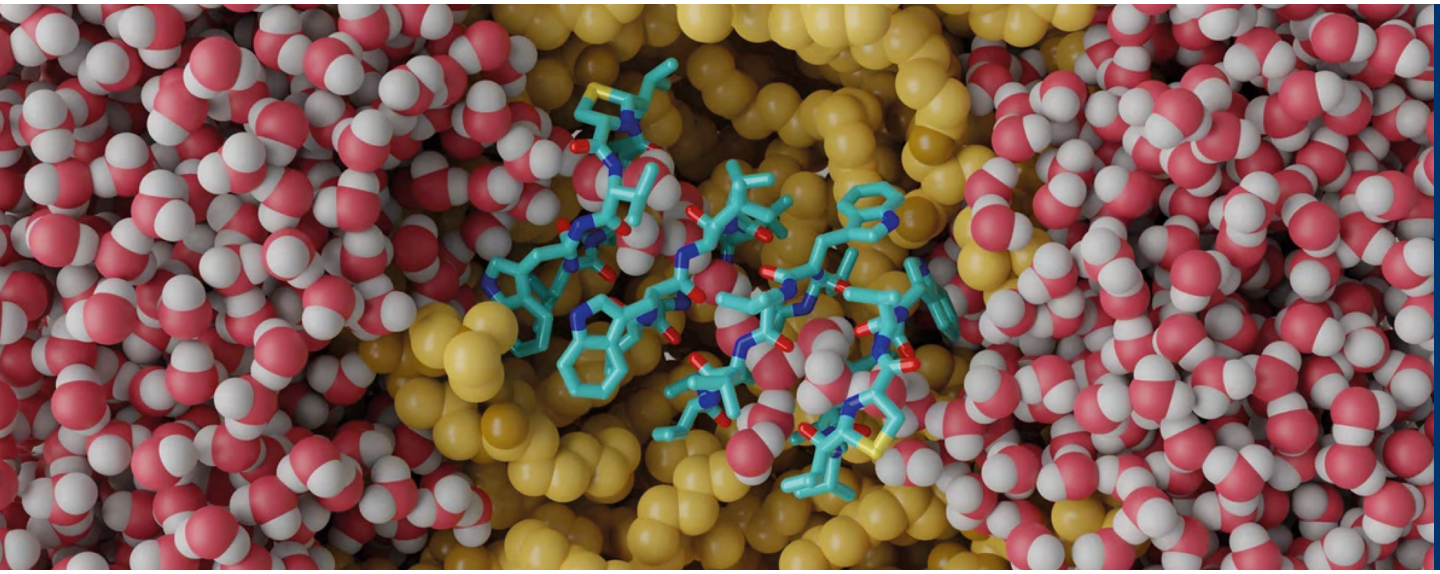
ISSN 2751-8647

Erlangen, August 2024



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