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NEWS

Digitalisation of research and education

Super and quantum computing, artificial intelligence and visualisation: [Markus Blume](#), Bavarian Minister for Arts and Science, and [Judith Gerlach](#), Minister for Digital Affairs, came to the Leibniz Supercomputing Centre (LRZ) to find out about the state of the art in information technologies and the digitalisation of research and education. "This is where the IT heart of Germany beats: the



Leibniz Supercomputing Centre makes knowledge and advancement visible," Blume wrote on his [Instagram account](#). The new Minister of Science (left with Prof. Dieter Kranzlmüller) was accompanied by Prof. Dr. Thomas O. Höllmann, President of the [Bavarian Academy of Sciences and Humanities \(BADW\)](#), and Prof. Dr. Rudolf Gross, Director of the [Walther Meissner Institute](#), among others. In addition to the SuperMUC-NG, they discussed in particular the plans to embed a quantum processor in supercomputers, which should provide researchers with more computing power for modelling. In the Visualization Centre (V2C), Blume was also able to get an idea of research projects, such as the model of the Earth of the geophysicist

Prof. Dr. Hand-Peter Bunge or how the state of glaciers evolves. "With one of the most powerful high-performance computers in Europe, top international research is being conducted under the roof of the Bavarian Academy of Sciences and Humanities," Blume summed up his visit. "Big data for all disciplines - from the humanities to quantum research!"

The Minister of Digital Affairs, Gerlach, also visited the LRZ to find out about the infrastructures needed to digitise research and teaching. Prof. Dr. Dieter Kranzlmüller, Director of the LRZ, explained how scientists can process big data, using the example of the high-performance platform [terabyte](#) for earth observation data, which the computing centre operates with the German Aerospace Centre (DLR). In the V2C the project ["Learning with Digital Contemporary Witnesses" \(LediZ\)](#) impressed. The holograms of Abba Naor and Eva Umlauf told Gerlach about the (survival) lives of Jewish fellow citizens during the Nazi era.

Evaluation of Big Data at LRZ

Classifying images, identifying defined objects in Big Data, searching for recurring patterns or analysing language: Artificial intelligence (AI) methods are being used more and more in research. "The demand for graphics processing units or GPU is constantly increasing," reports Nicolay Hammer, PhD astrophysicist and head of the Big Data Artificial Intelligence team (BDAl) at the Leibniz Supercomputing Centre (LRZ). The computing centre has therefore expanded the [LRZ Artificial Intelligence Systems \(LAI\)](#). [DGX units](#) from NVIDIA with A100, Tesla V100 or P100 graphics cards are available for complex machine and deep learning, as well as additional systems with a total of 12 GPU. They offer between 16 and 80 gigabytes of GPU memory and 256 to 2000 gigabytes of main memory. "The systems primarily supports statistical data analysis, machine learning and deep learning methods, for example for pattern and image recognition" Hammer explains, and: "Overall, the systems offers a computing power of almost one petaflop per second." The LAI processes a quadrillion floating-point calculations per second, but in contrast to supercomputers, AI does not always have to work with the highest precision of 64 bits, consequently the performance can be increased to more than 25 petaflops.



Currently, the LAI are mainly used for speech and image recognition methods. The team advises researchers on the selection of systems, but above all on the processing of data. "It is often underestimated that data should be processed, unified and standardised for artificial intelligence methods and that data analysis generally requires enormous computing capacities," observes Hammer. Anyone who wants to [access the LAI](#) needs an LRZ-Identity for the Linux cluster. With a request to the LRZ Servicedesk, the LAI are released for use. After logging in, researchers can expect a clear frontend based on the open source software OpenOnDemand, with pull-down menus leading to a wide variety of functions, tools and the first AI applications for data analysis. The LAI can be started online by [interactive web servers](#) and will be further expanded. "As a service provider, we firstly want to support excellent research technically and with our experience," says Hammer, "and as an academic computing centre, we secondly are researching how we can further accelerate AI applications and workflows with the help of supercomputers."

A portal for the analysis of water

Clean water is essential for life. This makes it all the more important to find out what water contains. Industry is always experimenting with new materials and chemicals, agriculture with fertilisers and pesticides, and nature also regularly produces new bio substances. But how to detect the unknown? Laboratories and water suppliers rely on a combination of so-called target



and non-target screenings - and on the help of artificial intelligence. ["K21 - Collective and Artificial Intelligence in Trace Substance Tracking in Surface Water"](#) is the name of a research project of the Bundesministerium für Bildung und Forschung (BMBF, funding 02WDG1593 A-D) that is now moving from conceptual to practical work: The Leibniz Supercomputing Centre (LRZ) is building databases and a portal together with the [Technology Centre for Water \(TZW\)](#), the Langenau [State Water Supply](#), the [Technical University of Munich \(TUM\)](#) and laboratories. Its will collect and store analytics data on all aspects of water. Because the evaluation of the whole data is too much for individual companies, the plan is to research it with the help of artificial intelligence methods. You can read how this works and the challenges the team faces in the [report on the LRZ website](#).

Ideas for exascale and quantum computers

Meeting place for High Performance Computing (HPC): On 29 May, the [International Supercomputing ISC](#) will start in Hamburg, the first international HPC conference and trade fair that will once again take place in presence. The specialists from the Leibniz Supercomputing Centre (LRZ) are looking forward to meeting colleagues from all over the world. Technologies and software solutions for supercomputing will be presented until 2 June, and the [Top500 list](#) of the world's fastest supercomputers, which takes into account performance data from the first exascale systems, is eagerly awaited: How do they perform? And how can they be operated in an energy-efficient way? These are the questions this year, loosely based on the ISC motto "Transforming the Future". The LRZ will present its work together with the [High Performance Computing Centre Stuttgart \(HLRS\)](#) and the [Jülich Supercomputing Centre \(JSC\)](#) on the stand of the [Gauss Centre for Supercomputing \(GCS\)](#). Naturally, the talks here also revolve around [quantum computing](#): HPC brings this into research practice and, conversely, can be accelerated by quantum processors. On top, visitors can experience [the visualisation of the blood circulation in the human forearm](#) that will be on display at the booth. It illustrates how data from medicine can be visualised with graphical programmes. In addition, the GCS centres will present practical solutions with which scientists can create fascinating images of their research on the supercomputers. You can also meet LRZ specialists in the conference programme: Here is a selection of workshops and discussion panels where they will share their ideas and experiences:

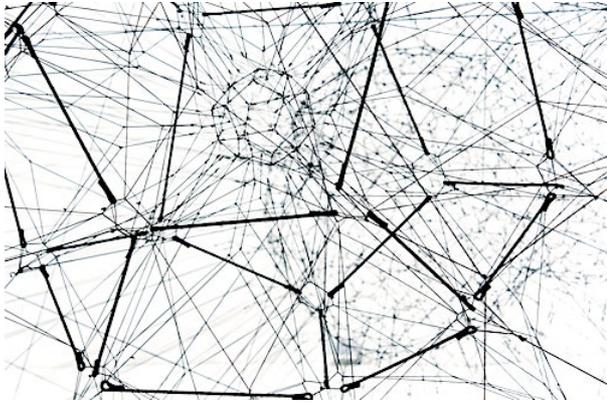


- **30 May 2022, from 4 pm:** [Open HPC](#). Together with Arian Reber from Red Hat and Christopher Simmons from the University of Texas, HPC expert David Brayford from the LRZ will show how container and cloud solutions make supercomputers around the world more accessible to researchers and what benefits this brings.
- **31 May 2022, from 11:30:** The [International Association of Supercomputing Centers \(IASCC\)](#) introduces itself. The newly formed organisation represents international supercomputing centres, promotes their networking and further development, deals with management strategies and the challenges for the future. Laura Schulz, who develops strategies for the LRZ and heads the department for quantum computing and technologies, will be lead this discussion.
- **31 May 2022, from 1 p.m.:** Volker Weinberg, responsible at the LRZ for the HPC education programme, will inform about how scientists can [make a career in supercomputing](#) and can further their education together with colleagues from other supercomputing centres and representatives of the Partnership for Advanced Computing in Europe (PRACE).
- **31 May 2022, from 14.30:** The [Message Passing Interface](#), or MPI for short, is a programming scheme for adapting processors. It is mainly used in the construction of supercomputers, also because it improves the networking of computing nodes. MPI is constantly being further developed by the users; in autumn, the last master version was published for the time being. LRZ Director Prof. Dr. Martin Schulz shows changes and further developments of MPI, also with respect to the integration of accelerators.
- **1 June 2022, from 10:45:** [Quantum Computing meets HPC](#) - what now: LRZ specialists Laura Schulz and Prof. Dr. Martin Schulz discuss with Prof. Dr. Sven Karlsson from the Danish Technical University (DTU) in Lyngby how both future technologies can cooperate and be advanced together. DTU and LRZ cooperate on integration issues and have jointly launched the HPCQC.org initiative together with the Technical University of Munich and the Ludwig-Maximilians-Universität München.
- **2 June 2022, from 9 am:** [Quantum and Hybrid Quantum/Classical Computing](#). Supercomputing centres bring quantum computing to practice. In a workshop, Prof. Dr. Dieter Kranzlmüller, Director of the LRZ, Prof. Dr. Vassil Alexandrov, Head of Research at the Hartree Centre STFC, Luke Mason, Head of HPC at the Hartree Centre STFC, and Dr. Ivano Tavernelli from the IBM Research Centre Switzerland show how hybrid computing can work.
- **2 June 2022, from 9 a.m.:** [Monitoring operational data MODA22](#). Smart control could also push supercomputers in terms of

energy efficiency. In a workshop, LRZ expert Dr. Michael Ott will present the LRZ's own monitoring tool DCDB and initial plans for processing operational data - the basics for training AI.

The LRZ Advisory Board: Scientists advise the data centre

Supervision and suggestions - both come together in the [Advisory Board of the Leibniz Supercomputing Centre \(LRZ\)](#): 30 professors, mainly from Bavarian universities and research centers, form this committee. "Various interest groups are represented here," says Prof. Dr. Arndt Bode, one of the advisory board members, Director of the LRZ until 2017 and holder of the chair for



computer technology and organization at the Technical University of Munich (TUM). "The representatives of the Bavarian Academy of Sciences are more likely to take on supervisory duties, the others advise the board of directors on aspects of use and all about services." This year, the LRZ, the IT service provider for universities and research institutes in Bavaria, supercomputing centre and an institute of the Bavarian Academy of Sciences (BADW), is celebrating, its 60th birthday: an opportunity to take a look behind the scenes and present its [boards and committees](#) and above all its [history](#). The Advisory Board is still a relatively young group, but it already refers to the technical developments of the scientific compute centre. Read on the [LRZ website](#) how the Advisory Board came into being and who is part of it and why.

Figures of the Month

When it comes to computer technology, the Leibniz Supercomputing Centre (LRZ) has a lot to offer to scientists. A small inventory of nodes and services: SuperMUC-NG consists of a total of **6336 nodes** with **304,128 computing cores**. They can perform **26,300 quadrillions** floating-point calculations or **26,300 petaflops** per second. **144 nodes** are Intel Skylakes, which alone contribute **600 petaflops** to the performance. The system is also complemented by **64 compute nodes** with **3072 cores** from Intel and NVIDIA for cloud computing. In addition to the high-performance computer, the LRZ also offers the CoolMUC systems, each with **812** or **148 computing nodes**, which achieve **946** and **394 teraflops** per second. They also feature Intel processors (Haswell EP and Knights Landing) and are networked via Infiniband. While the SuperMUC and CoolMUC systems are primarily used for modelling and simulation, systems also are available for the statistical evaluation of data, which are particularly suitable for artificial intelligence methods: **2 DGX-1** systems, each with **80 compute processing units (CPU)** and **8 graphics processing units (GPU)** from NVIDIA, as well as **12 more GPU** add its performance to near **1 petaflop** per second. And last but not least, researchers can compute with quantum technologies: The Quantum Learning Machine from Atos and the simulator from Intel each work with **42 qubits**.



WORKSHOPS & EVENTS

Quantum Computing – Technology and fields for application

Until tomorrow, 29 April 2022, the new [World of Quantum](#) conference will be held at the Munich Exhibition Centre. The LRZ will be there in Hall A4 at the Munich Quantum Valley (MQV) stand. The Munich Centre for Quantum Science and Technology (MQST) and the Institute for Lifelong Learning of the TUM will also be present. Visitors will be able to see posters explaining the LRZ's plans and tasks in research projects on future technology, learn about education and qualification opportunities, and find out about research activities in Munich. And they can contact the qCREW@LRZ personally, because it has exciting opportunities for people who want to actively shape the future and IT.

Programming GPU for deep learning

Graphic Processing Units (GPU) are also made for artificial intelligence (AI) and machine deep learning applications. From **10 to 13 May 2022**, researchers can learn how to prepare and programme these new processors for their own tasks in an online course organised by the Partnership for Advanced Computing in Europe (PRACE). Experienced instructors from European supercomputing centres will introduce the programming models on OpenACC and CUDA, show how to use GPUs and how neural networks can be trained with them. [Information and registration](#)

Introduction to the HPC systems at LRZ

Using computational fluid dynamics (CFD) as an example, you will get to know the Linux cluster of the LRZ: In the crash course on **May 11., 2022**, learn how to log in, set up a user environment, load files and folders into the system, and plan applications using SLURM. The practical exercises will focus on the programs ANSYS CFX as well as StarCCM+, with which especially computations of fluid mechanics are possible. [Information & registration](#)

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Pushing the limits of computing

In presence and online, the [International Association for Computing Machinery \(ACM\) conference](#) will take place in Turin from **17 to 19 May 2022**. "Computing Frontiers" explores the limits of computing and data processing and how they can be overcome. Super- and quantum and hybrid computing will be discussed, as well as problems of energy consumption. LRZ experts Dr Josef Weidendorfer, Dr Martin Ruefenacht, Dr Michael Ott and Dr Amir Raoofy will present solutions for integrating quantum processors into supercomputers, for smart control of applications and computers and for limiting energy consumption.

Learn C++ and programme with it

The C++ programming model is made for planning workflows in a logical, structured way. C++ contains language features and paradigms for precondition-oriented or object-oriented programming. As with many other programming languages, when coding, you must decide which language features to use and how. How to use C++ skillfully you will learn in the 3-day course from **May 18 to 20, 2022**. Your own projects would be helpful for learning, but you will also learn about application examples. [Information & registration](#)

Programming for parallel systems

HPC systems usually consist of clusters with shared memory nodes. For efficient use of these systems, usage of memory and communication time should be optimized. Programming schemes such as MPI or Open-MP help to do this; they can be used to parallelize memory capacities on the node link as well as memory within each node. In this 3-day PRACE course **from June 22 to 24, 2022**, different parallel programming models will be explained and strategies using the described programming schemes will be discussed. [Information & registration](#)

Optimise HPC codes

Algorithms for supercomputing and HPC should run faster and more smoothly because they can save electricity. In a three-day PRACE course from **27 to 29 June 2022**, participants will learn how to optimise their codes and adapt them to the characteristics of various European supercomputers. [Information & registration.](#)

Programming GPU with Open ACC

Big Data in research can be efficiently analysed with the help of artificial intelligence: In this three-day classroom course at the High Performance Computing Centre Stuttgart (HLRS) from **12 to 14 July 2022**, researchers will learn how to accelerate applications using the open source programming scheme Open ACC, how to use and train neural networks with data. Another topic on the agenda: how multilayer networks can be parallelised. Participants can expect a mix of lectures and practical exercises - good if they already have their own ideas for data evaluation with artificial intelligence. [Information & registration](#)

ANSYS Fluent for Computational Fluid Dynamics

Consisting of 13 lectures and about 6 practical exercises, this seminar, which runs from **October 27 to December 8, 2022**, introduces the use of the fluid dynamics software package ANSYS Fluent. This supports computations and simulations of computational fluid dynamics in particular. Participants will learn about typical CFD workflows for ANSYS and application examples. In addition, they learn how ANSYS works and is integrated on the LRZ Linux cluster. For this they will receive the Linux Primer. Participants should know the basics and numerical methods of fluid mechanics and have completed first calculations. [Information & Registration](#)

USED THINGS FOR FURTHER SERVICE

The LRZ is always getting rid of used hardware and furniture - a constantly updated list of things we want to give away can be found [online](#). Here you can also read where to direct your interest. The equipment and furniture are free of charge for institutes, chairs and other research institutions.

JOB OFFERS

You will find an international and diverse team in Garching, which is constantly growing. If you don't find a suitable job profile below, please visit the [career page](#) of the Leibniz Supercomputing Centre or send an [unsolicited application](#). We are LRZ - and curious about you!

[Manager](#) for the CRM system

[IT specialist](#) for support of MAC- and mobile devices

[IT spezialist](#) for expansion of hosting-environments

[HPC engineer](#) for evaluation of new technology and for co-design of hard- and software

[Expert HPC and parallel computing](#) for tasks of chemistry and life sciences

[HPC software engineer](#) for the quantum software stack

[Computer scientist](#) for development and support of AI and data driven applications

[IT spezialist/System consult](#) for the multiple authentication

[Software developer](#) for the research data management

[Expert for HPC](#) and parallel computing for development for HPC-Application accelerated by GPU

[Clark for licences](#)

[Student Assistant](#) for PR and Content

[Student Assistant](#) for ITSM software development

[Student Assistant](#) for video services

[Student Assistant](#) for service desk

MORE TO READ

Here you will find links to latest information from the german-european supercomputing community and our cooperation partners

- The [newsletter](#) of the Bavarian Academy for Science and Humanities
 - [Publications](#) of the Gauss Centre for Supercomputing (GCS): GCS-News und Inside
 - [Infoletters](#) of the Gauß-Alliance
 - Publications of PRACE: [PRACE Digest, Jahresbericht](#)
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- The LRZ Newsletter is published in German and English. You can find the latest and former editions on the [LRZ-Website](#).
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- You can subscribe or unsubscribe the LRZ-Newsletter via our [website](#).
- Current information about the LRZ and about courses and events can also be found on [Twitter](#) and [LinkedIn](#).

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Photos: Fotos: Alina Grubnya/Unsplash, Anderson Rian Klwak/Unsplash, Alex König/STMKW, Th. Obermeier/LRZ, Nejk Soklic/Unsplash