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INFORMATIONS & IMPRINT
The Free State of Bavaria is relying on the Leibniz Supercomputing Centre (LRZ) of the Bavarian Academy of Sciences and Humanities for its High-Tech Agenda: The new AI Agency, which supports the Bavarian AI Council appointed in December 2020, has been established at the leading Bavarian scientific computing center. 21 internationally renowned experts from universities, science and industry are driving forward research into artificial intelligence (AI) and its use in business and society. The board represents the network for AI Agency and advises it: "With the AI Agency, we are doing everything we can to implement AI made in Bavaria strategically and practically and to strengthen internationally Bavaria's appeal as a location for the development and research of AI," says Laura Schulz, Managing Director of the AI Agency and Head of Strategy at the LRZ.

The AI Agency promotes research projects around AI, machine learning and automation throughout the state. To advance AI initiatives and large-scale strategic projects, it will forge partnerships among research institutions and with companies and organizations. Through the resulting network, smart applications and technologies from research will be brought to widespread use. Another important concern of the AI agency is the training and qualification of specialists in the digitization and automation of economic and social processes. The new agency, which is currently forming and working on its program, is closely linked to the LRZ in terms of personnel: In addition to Laura Schulz, Prof. Dr. Dieter Kranzlmüller, Director of the LRZ, and Prof. Dr. Thomas Seidl, Member of the LRZ Board of Directors and Head of the Munich Center for Machine Learning, are represented on the AI Council, which is chaired by Prof. Dr. Saim Haddadin from the Technical University of Munich.

**Bavaria's quantum offensive**

On January 11, 2021, the Bavarian Academy of Sciences and Humanities (BAdW), the Fraunhofer-Gesellschaft, the Max Planck Society for the Advancement of Science, and the Munich universities, LMU and TUM, sealed their commitment to the Munich Quantum Valley (MQV). With the support of the Leibniz Supercomputing Centre (LRZ) and the Walter-Meißner-Institut, both institutes of BAdW, work will be carried out here on quantum technologies as well as on hardware and software for quantum computing: "This is an important step for Bavaria as a research location," comments Prof. Dr. Dieter Kranzlmüller, Director of the LRZ, about the high-tech offensive. "We are pleased to be able to play a part in this. Because here, science, research, founders and industry will find a stimulating environment, opportunities for cooperation and exchange in order to steadily develop quantum technologies and quantum computing and bring them to market."

In the MQV, science and industry will research quantum technology and develop it to market maturity. To this end, the participating institutions will recruit top researchers, establish a centre for quantum computing and quantum technologies, where the technical fundamentals will be explored and basic technologies will be developed. A technology park is also planned for the production and use of components. Universities and research institutions will qualify and train the scientists, engineers and computer specialists needed there. "At the LRZ, the topic of quantum computing has been a focus for quite some time," Kranzlmüller reports. "On the Super-MUC-NG, we already provide a quantum computing simulator with 42 qubits." Since 2019, the Bavarian Quantum Computing eXchange (BQCX) network has also been meeting every second Wednesday of the month, the next time on February 10, by the way (see below). First educational offers around quantum computing are on the LRZ program.

**Photo: Bavaria's Minister President Markus Söder (center) with the heads of the institutions that will be involved in Munich Quantum Valley. (STMWSUK)**
Improving the world with quantum

She already stands out: "Your work is on the cutting edge, and you are an example of the top-class minds in the Bavarian quantum ecosystem," said Laura Schulz, co-initiator of the Bavarian Quantum Computing eXchange-Network (BQCX) of the Leibniz Supercomputing Centre (LRZ) enthusiastically. In September 2020, Daniëlle Schuman presented the results of her Bachelor's thesis to the community of researchers and entrepreneurs during a digital meeting. In it, the 23-year-old computer scientist dealt with neural networks and showed that these applications for machine learning do not only run on conventional computers, but also on quantum annealers: "Great presentation of a highly topical subject," said Dr. Fabio Buffo, high-performance computing specialist at Amazon Web Service (AWS), in praise of her talk.

On the LRZ website, we introduce Daniëlle Schumann: the first portrait of a serie of young scientist, working on exciting topics and researching future technologies. We will present more of these persons to watch in future. "For my bachelor's thesis, I rewrote a library of neural networks, added to it and tested it on a quantum simulator, which worked great," Schuman says. "Hopefully, my work will gain relevance in computing practice." That's to be expected: Machine learning supports the processing of data. Annealers, in turn, are quantum computers, and the hopes of business and science rest on them to be able to evaluate huge amounts of data even faster. (vs)

Photo: Quantum annealer chip (D Wave Systems)

SuperMUC simulates the formation of stars

If you pour milk into it, the beverage does not immediately turn a uniform beige color. Instead, bright vapors and small eddies are initially distributed in it. In similar processes, turbulence, stars are formed in space, but instead of milk and coffee, interstellar gases, molecules and dust interact with each other at different speeds. What exactly happens in these vortices has now been traced by a research team with the help of supercomputers at the Leibniz Supercomputing Centre (LRZ) in Garching: Under the direction of Prof. Dr. Ralf Klessen from the Center for Astronomy at Heidelberg University and Prof. Dr. Christoph Federrath from the Australian National University Canberra, the largest simulation of interstellar turbulence was created in around 45 million computing hours on the SuperMUC. It can be used to demonstrate when and how stars form. The model also mapped the so-called sonic scale, the transition between supersonic and subsonic velocities in the motions of gas clouds. The team around Klessen and Federrath reports on their work in the scientific journal "Nature Astronomy", and the Gauss Centre for Supercomputing (GCS) and the Australian National University also dedicate an article to the unique and excellent work. (vs)

Figure on the right: Section of interstellar turbulence from Ch. Federrath, R. Klessen et al.
Satisfying users

The Leibniz Supercomputing Centre (LRZ) is working on its services and optimizing communication with its users. In the future, a cross-departmental team of eight will deal with complaints from dissatisfied users. "Complaints point to potential for optimization that we as a service provider may underestimate in our day-to-day work," explains Natalie Vogel, Team Leader Customer Relationship Management (CRM). "We will also take a closer look at which LRZ services cause many tickets in order to better organize the processes behind them in the future."

About 15,000 service requests or incident reports arrive at the LRZ’s service desk* each year and initiate work orders, first for the students who do the first level support, and then for LRZ experts if needed. Most requests are answered quickly and straightforwardly, but about 50 of them result in a complaint because the support did not satisfy the sender. These discussions are now being analyzed in order to improve processes or technology and to better support employees at the Servicedesk. "So far, most things are working well; even during the pandemic, the tone of the users did not become more impatient or aggressive," Vogel says. "But anyone who complains can quickly become a multiplier and damage the image of LRZ as a reliable IT service provider."

CRM is also a task motivated by the LRZ’s certification: In the summer of 2019, the LRZ had let itself certified for the first time according to ISO standards for IT service management (20000) as well as IT security (27001). The certificates are audited regularly and require constant optimization. "We don't want to offer 08/15 service," says Vogel. "That's why we strive to be understanding and to communicate with customers in search of solutions. That helps everyone involved, and it tells us where we can do more."

* By the way, students who enjoy working with IT technology and want to earn money on the side can regularly find job offers for student assistants at the LRZ.

Optimize together

The certifications of the Leibniz Supercomputing Centre (LRZ) are setting a precedent: In April 2020, the IT Service Centre (ITS) of the University of Bayreuth also received the certificate for information security according to international ISO/IEC standard 27001, and the next one according to ISO/IEC standard 20,000 for IT service management is in preparation. LRZ colleagues helped with their experience, analyzed processes at the university data centre and identified opportunities for optimization. This is how a consulting partnership came into being: To renew their certificates, the two data centers are now evaluating each other's IT security and service quality: "The audits encourage employees to get to know each other, so we can intensify the exchange of experience and cooperation," says Prof. Dr. Torsten Eymann, holder of the Chair of Business Informatics and Vice President of the University of Bayreuth.

After around 18 months of preparation, the LRZ had itself certified in summer 2019 as Germany’s first scientific data center in the disciplines of IT service management and information security. The IT team at the University of Bayreuth learned about this through working groups and news reports and sought help. Certificates must be renewed regularly and the analyses of relevant processes and the documentation of security or service measures must be repeated for this purpose: "In addition to audits by certification bodies, the standards provide for further examinations by independent auditors to ensure that the organization is constantly improving," explains Prof. Dr. Helmut Reiser, deputy director of the LRZ. "Only a few commercial auditors have experience with scientific or university data centres. This special know-how is more what both partners profit from the most in this partnership." The first mutual audits showed success, strengthen the desired exchange and cooperation, and have the side effect of being more cost-effective. In April 2021, a Bayreuth team will therefore again put the LRZ under the microscope and vice versa. Both data centers qualify interested employees as auditors, and the LRZ uses this knowledge to expand its consulting and services.

About us

Read and listen to more about the Leibniz Supercomputing Centre (LRZ): Also in January, there were reports about the scientific computing centre and its work, and employees also gave talks about their projects.

• Prof. Dieter Kranzlmüller, Director of the LRZ, explained to representatives of the polish Sano Centre for Computational Medicine how high-performance computing and the Leibniz Supercomputing Centre can help society and science, especially medicine. The
46 minutes for the presentation are worth to see: because of the description of the most projects for which SuperMUC-NG and the Linux cluster in Garching are used; but also because of the figures about supercomputing from Garching.

- Everyone is talking about Big Data, Artificial Intelligence (AI) and Machine Learning (ML) these days. But the fact that these future technologies need computing power and therefore a resilient IT infrastructure is usually forgotten. Dr. Nicolay Hammer, who heads the Big Data and AI team at the Leibniz Supercomputing Centre (LRZ), discusses this with the founders of the Munich-based startup Erium, a software provider from Munich. Data Scientists and interested parties can hear many practical tips about cloud computing and technical equipment for AI applications in the podcast.

- On the occasion of the Holocaust Memorial Day, which should not only be commemorated on January 25, the German Tagesschau asks a good question in its podcast: What if there are no more eyewitnesses because they have all passed away? The digitization of conversations and encounters could help cultural memory. The Tagesschau explains this showcasing the LeDIZ research project, for which Holocaust survivor Abba Naor was interviewed, filmed and finally virtualized. His digital alter ego is currently touring schools and universities and impressing students and teachers alike.

- Last but not least, here are two new photos from the computer cube and from the Max Planck Institutes Computing Center (MBCDF) in Garching. There, the cabinets of the HPC libraries have been pasted with pictures of projects: On the left the simulation of the blood flow of CompBioMed, on the right a decorative picture with light distortions.

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**Figures of the month**

At its peak, SuperMUC-NG manages 26.9 petaflops; the supercomputer also offers 719 terabytes of main storage and 70 petabytes of disk storage. Since its launch in fall 2019, it has already completed about 3.5 billion compute hours. Due to its innovative hot-water cooling and the 3,000 liters of water that flow through each of SuperMUC-NG’s racks per hour, it consumes 5% less power. Up to 45 degrees hot, the water absorbs the heat from the processors to cool them down. This generates energy for heating the offices, but also for other cooling systems. Over the course of a year, the LRZ saves a lot of energy and costs that can be used for science. And here’s another figure: according to the research institute Hyperion Research, every dollar invested in high-performance computing generates around $463 in revenue and around $44 in profit. Good to know.

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**WORKSHOPS & EVENTS**

**The Architecture Machine**

A short video already stirs up anticipation: The exhibition "The Architecture Machine" already started last year at the Pinakothek der Moderne. It traces the role of the computer in architecture and urban development - and it’s a story as worth seeing as it is exciting. Computers have long been helping with drawing, designing, even clarifying and presenting, and now they calculate traffic and other developments. In the Pinakothek der Moderne, this is told in multimedia and, among other things, in virtual worlds. The Leibniz Supercomputing Center (LRZ) supports the exhibition with technology and has advised the makers in advance. Unfortunately, the museums are closed due to Corona, but the video and pictures online will awaken anticipation. And if it gets boring on the holidays: It’s also worth taking a walk through the museum district and to the Pinakothek museums, where wonderful, atmospheric light installations can be viewed until February 12. By the way, "The Architecture Machine" has been extended until June 2021.
Building quantum computers

On February 10, 2021, the Bavarian Quantum Computing exChange (BQCX) network will also start up again - with an exciting topic, top-class scientists and an interesting partner: Laura Schulz and Luigi Iapichino, who initiated BQCX, organized this meeting with Prof. Dr. Sven Karlsson from the Technical University of Denmark (DTU). The BQCX network is growing...

To be able to work with quantum computers already today, classical computer controls are needed, which should be extensible and allow real-time responses. Dr. Anastasiia Butko at Berkeley Lab (USA) is researching how conventional and new technology work together. She will discuss the first results of her work at the digital BQCX meeting with Prof. Dr. Sven Karlsson, Prof. Dr. Martin Schulz from the Technical University of Munich, Dr.Jan Goetz from IQM Quantum Computers, Dr Mikael Johansson, from the IT-Centre for Science, Finland, and with Prof. Dr. Thomas Monz, co-founder of Alpine Quantum Technologies (AQT). Deep insights into quantum computing are pre-programmed. Registration requested.

Crash Course Linux Cluster

On February 10, 2021, beginners in High Performance Computing (HPC) can learn about working on parallel computing systems. The focus is on computational fluid dynamics (CFD), i.e. the simulation and representation of motions in gases and fluids, with the ANSYS programs as well as StarCCM+. The Linux cluster systems of the LRZ, their user environment and various access options will be explained. Information and registration

Register projects for SC21

It’s still quite a while away - the next Supercomputing (SC21) will start on November 14, 2021 - but the first submission deadlines have already passed: The trade fair organizers are accepting offers for workshops until February 19, presentations of research papers until April 2, and concepts for tutorials and panel discussions until April 30, 2021. Students who want to participate in SC21 free of charge as volunteers should get a move on quickly ...

Programming with OpenMP

With the spread of multi-core processors, shared memory programming is gaining importance. OpenMP is proving to be an engine for this. The high-performance, flexible programming model enables parallelism in researchers' applications. The three-day workshop from February 17 to 19 presents the basics of OpenMP programming and the "OpenMP Common Core" and introduces parallelism programming. Participants will learn the theory and practice their skills. Information and registration.

Programming with Fortran

Fortran is also a programming language widely used in science. The three-day online course from February 22 to 24 is therefore aimed at researchers with little or no experience. You will learn about different Fortran standards (95, 2003) and practical tools such as debuggers and syntax checkers, as well as how to use compilers and libraries and Fortran. Theoretical knowledge is deepened in exercises. Costs: 30 to 600 Euro. Information and registration.

Working with ANSYS Fluid Dynamics

The course starts on March 8, 2021, and lasts until May 17. Participants will learn the finer points of ANSYS Fluid Dynamics on 10 days. The program can be used to represent and model the flow of gases and liquids. From 10 a.m. to 12 p.m. and from 2 p.m. to 4 p.m. practical exercises and the handling of the ANSYS software package are part of the program. Costs between 50 and 120 Euro. Information and registration.

Projects sought for ISC High Performance

The International Supercomputing (ISC) 2021 is already looking for the presentations and projects that will inspire interested parties in June: HPC projects can be submitted until March 3, research projects and posters as well as talks for the PhD Forum until March 10. The ISC itself will take place digitally from July 24 to 2, 2021.

Poster printing runs out

In March 2021, the Leibniz Supercomputing Centre will cease printing posters. For a long time, posters replaced presentations during conferences and discussions and enabled group discussions. Now they no longer really fit in with the times. Therefore, the LRZ is giving up this service step by step.

Crash course for working with the Linux cluster

On April 14, 2021, beginners in High Performance Computing (HPC) can learn about working on parallel computing systems. The crash course focuses on computational fluid dynamics (CFD), i.e. the simulation and representation of motions in gases and fluids, using the ANSYS programs as well as StarCCM+. The Linux cluster systems of the LRZ, their user environment and various access options will be explained. Information and registration.

Software Design with C++

This three-day online course, April 21-23, 2021, focuses on object-oriented (OO) software design using the C++ programming language. Emphasis is placed on essential software development principles, concepts, languages, and practices that
researchers: use to create professional, high-quality code. The course provides guidelines for developing mature, robust, and code based on C++, but does not address specialties such as Template Meta Programming (TMP) or idiosyncrasies and curiosities of the language. Information and registration

Faster Computing with Open ACC and Deep Learning

The workshop at April 27-29, 2021 combines Accelerated Computing with OpenACC with the basics of Deep Learning for single and for multi-GPU. Participants will learn how to accelerate applications, how to train and deploy neural networks, and how to effectively parallelize training. The course is organized by the Vienna Scientific Cluster (VSC), LRZ, IT4Innovations as well as VIDIA. Information and registration

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!

Expert for parallel programming environment and libraries
Administrator Human Resources
Specialist for funding management
Administrator for High-Performing Storage
Storage Systems Engineer

MORE TO READ

Here you will find links to latest information from the german-european supercomputing community and our cooperation partners Publikationen of the Gauss Centre for Supercomputing (GCS): GCS-News und Inside Infolettern of he Gauss-Alliance
Publikations of PRACE: PRACE Digest, Jahresbericht

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