



## **LRZ-Newsletter March 2021**

### **NEWS**

- Quantum computing for science and industry**
- Computing power for artificial intelligence**
- Innovative processors in stresstest**
- Researching for supercomputing**
- "Computing time should be used for meaningful science"**
- Figures of the month**

### **WORKSHOPS & EVENTS**

- Combine Quantum computers with Supercomputers**
- Wanted – Data projects for supercomputing**
- Working with ANSYS Fluid Dynamics**
- Projects sought for ISC High Performance**
- Poster printing runs out**
- Register projects for SC21**
- Crash course for working with the Linux cluster**
- Software Design with C++**
- Faster Computing with Open ACC and Deep Learning**
- The Architecture Machine**

### **JOB OFFERS**

### **MORE TO READ**

### **INFORMATIONS & IMPRINT**

## NEWS

### Quantum computing for science and industry

The [Munich Quantum Valley \(MQV\)](#) kicks off: In various research projects, the Leibniz Supercomputing Centre (LRZ) and the [Walter-Meißner-Institut \(WMI\)](#), both institutes of the Bavarian Academy of Sciences and Humanities (BADW), are working on pioneering processors for quantum computing. The projects are funded by the German Federal Ministry of Education and Research (BMBF) with a total of 26.6 million euros. The aim is to increase knowledge about new ways of computing and, above all, to develop the first commercially viable hardware, software and services related to quantum computing.



This is where the hopes of science and industry are pinned: quantum computers will be able to process much more data much faster in the future and thus answer some research questions that are difficult to solve. The first prototypes are already being used in the fields of logistics, traffic planning, finance and material sciences to improve transport routes, traffic flows, cash flows and the composition of materials. But these computers are still error-prone; their processors work with no more than 50 quantum or qubits, their smallest units, and usually still have to be adapted for defined tasks. They are far away from standards, let alone market readiness.

#### New concepts, materials and techniques for quantum processors

But this is set to change in the coming years: "[From the basic research to the market](#)" is the name of the BMBF's funding program, which aims to develop new, innovative types of processors and business models. Under the leadership of the Finnish-German startup IQM, the Leibniz Supercomputing Centre (LRZ), Jülich Forschungszentrum, the Freie Universität Berlin and chip manufacturer Infineon are driving [digital-analog quantum computing \(DAQC\)](#) forward. The project combines simple, controllable analog systems with universal quantum computers whose computing power doubles with each additional qubit. Thus, processors with 5, 20 and 54 qubits will be created initially, as well as the methods and electronics to proof these control units. Last but not least, the DAQC control unit will have to prove itself in at least one industrial application. In the long term, science and industry should be able to access the new quantum computers via the cloud, which is why they are also to be integrated into supercomputers, initially the one at the LRZ. This is another way to create new services and offerings. The DAQC project will also contribute its experience to the European research project [OpenSuperQ](#). The launch event of the Munich Quantum Valley took place on March 4, 2021: Politicians and scientists described plans and objectives. The [recording of the event](#) is available online.

#### Computing power for artificial intelligence

Artificial intelligence (AI) needs computing power. That is why the Leibniz Supercomputing Center (LRZ) and the Munich Center for Machine Learning (MCML) are now bringing together knowledge and technology and jointly creating more computing power for basic research on AI. For this purpose, [MUNICH.ai \(Mcml Universal Cluster for High-performance AI\)](#), a cluster based on 8 DGX-A100 nodes from NVIDIA with a total of 64 Graphics Processing Units (GPU), has just been put into operation at the LRZ in Garching. The system brings it to 40 AI petaflops. "The additional hardware installed represents state-of-the-art technology and guarantees a standard that only Germany's leading AI centers can offer," explains Professor Thomas Seidl, Chair of Database Systems and Data Mining at Ludwig-Maximilians-Universität (LMU), Director of MCML and LRZ.

# MCML

Munich Center for Machine Learning



#### Innovative processors in stresstest

Getting to know other computer architectures and processors: The [BEAST \(Bavarian Energy, Architecture and Software Testbed\)](#) test environment at the Leibniz Supercomputing Centre (LRZ) stirs up curiosity. Computer science students from Ludwig-Maximilians-Universität (LMU) and the Technical University of Munich (TUM) get insights into the AMD, Marvell and Fujitsu processors (CPU) during the BEAST training course a system which also features graphics processing units (GPU) from AMD or NVIDIA for faster data processing: "BEAST offers the latest software and access to a wide variety of systems, which is very exciting for me," says Sergej Breiter, a master's student at LMU and a graduate of the first BEAST training course. The latest supercomputers are currently being equipped with the aforementioned processors, which is another reason why students are interested in the BEAST course, which TUM and LMU organized together with the LRZ in the 2020/21 winter term and for which applications are already being accepted for the summer semester.

A total of 26 computer science students took part in the first training course. In twelve sessions from November to February, they solved practical tasks in groups on BEAST's new control units as well as on computing nodes of Intel's SuperMUC-NG. "The goal of

the BEAST internship is to try out modern high-performance computer technologies, different computer architectures and memory hierarchies, to confront them with programming languages and software, and to compare experiences," explain lecturers Dr. Karl Füllinger (LMU) and Dr. Josef Weidendorfer (TUM), who lends the working group "[Future Computing](#)" at LRZ. The course also includes presentations by manufacturers, who provide insights into technical strategies and explain construction or functional methods. Registration to the BEAST internship: LMU <http://www.nm.ifi.lmu.de/teaching/> and TUM: <https://www.in.tum.de/caps/lehre>. More about [the BEAST-Internship](#) you will find on LRZ-Website. (vs)



## Researching for supercomputing

It's not easy to describe their subject. "When computer units are connected with a cable, they communicate with each other when computing. My job is to improve that communication," says [Bengisu Elis](#). That way the Turkish native explains to her parents what's behind her PhD work at the Technical University of Munich (TUM). The PhD student uses practical examples to teach her younger brother about her subject, computer science. Elis is researching the supercomputing of the future; in the communication



of components and processors, she is looking for ways to make high-performance computing more efficient, more sustainable, more powerful. In addition to the Linux cluster and the SuperMUC-NG of the Leibniz Supercomputing Centre (LRZ), its new test environment BEAST is now also part of Bengisu Elis' work environment: "BEAST is technically interesting and an extremely important tool for my work; I can use it to investigate different architectures."

We introduce [the PhD student on the LRZ website](#): Following [Daniëlle Schumann](#), the second portrait in a loose series of young scientists who are researching future technologies with or at LRZ, developing new techniques and functionalities, improving supercomputing or enriching research and science with it. Elis is intensively involved with the Message Passing Interface (MPI), a standard for communication between processors or control units. With her team at TUM, she has already been able to adapt the MPI control tool PMPI to more modern technologies: QMPI is the name of this possible successor, for which the team has formulated requirements and use cases and implemented a prototype.

She is currently working on its improvements. (vs)

## "Computing time should be used for meaningful science"

Came to stay: For the third time, [Prof. Dr. Peter Bastian](#) from Heidelberg University has been elected chairman of the steering committee for SuperMUC-NG at the Leibniz Supercomputing Centre (LRZ). Bastian heads the "Parallel Computing" working group at the Interdisciplinary Center for Scientific Computing (IWR): "We primarily develop efficient and robust methods for solving certain systems of equations," is how he describes his team's task. Bastian's deputy is [Prof. Dr. Gerhard Wellein](#) from Friedrich Alexander Universität in Erlangen-Nuremberg, who is also the spokesman for the Competence Network for Technical Scientific High-Performance Computing in Bavaria (KONWIHR). The steering committee is elected every two years and consists of a total of 15 scientists representing the LRZ and its parent the Bavarian Academy of Sciences and Humanities (BADW), as well as the German Research Foundation (DFG). The LRZ Steering Committee extends computing time and evaluates the scientific merit of research work. Last year, that amounted to about 70 applications. "Each member of the steering committee is responsible for his or her own area, commissions expert opinions from external parties and uses them to prepare a funding proposal," Bastian explains the

tasks. In the [LRZ-interview](#), he also discusses new regulations for the use of idle time at the SuperMUC-NG and why the LRZ supercomputer will not be old news for a long time yet. (vs)



*Prof. Dr. Peter Bastian, University of Heidelberg; Prof. Dr. Gerhard Wellein, Friedrich-Alexander-University, Erlangen*

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## Figures of the month

At the Leibniz Supercomputing Centre (LRZ) [software](#) is not only used, but also developed. A small but fine team takes care of this - a handful of software engineers develop useful tools for LRZ users or for the organization, in addition to other tasks. In planning and managing their tasks, they rely on **14 methods** such as Scrum, DevOp, Test-Driven-Development and Clean Code, but also on **20 tools** such as Git and GitLab, Docker, Python, TypeScript, OpenStack or VMware. Thus, in **6 Scrum sprints** or sub-projects and **1811 versions**, the commits, the [password reset system](#) were created: With this, almost **30,000 LRZ users** now create their passwords themselves online. Previously, they had to contact the LRZ service desk. Hummel is much more complex: In **7 sprints** and **2767 commits**, a system was created that will soon be able to manage the software for operating the approximately **1100 websites** that the LRZ hosts and organizes. Security and data protection features or PHP versions are then updated automatically. The team is ambitious - another 8 software projects, for example paperless HR processes, an electronic order book as well as the configuration of switches for do-it-yourself are already on the to-do list.

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## WORKSHOPS & EVENTS

### Combine Quantum computers with Supercomputers

On March 10, 2021, the [Bavarian Quantum Computing exChange \(BQCX\)](#) network will take off - with an exciting topic, top-class scientists and an interesting partner: The initiators of BQCX, Laura Schulz and Luigi Iapichino, organized this meeting with Prof. Dr. Sven Karlsson from the Technical University of Denmark (DTU). The March meeting will focus on the production of quantum computers, but more importantly on the integration of future technology into existing systems and supercomputers. Those who want to work with it today or to control quantum computing and its results, need classical control systems that should be extensible and enable real-time responses. This is the thesis of Dr. Anastasiia Butko at Lawrence Berkeley National Lab (LBNL, USA), who researches the cooperation between high performance computing and quantum technology. She will discuss initial results of her work with Prof. Dr. Sven Karlsson, Prof. Dr. Martin Schulz of the Technical University of Munich, Dr. Jan Goetz of IQM Quantum Computers, Dr. Mikael Johansson, of the IT-Centre for Science, Finland, and Prof. Dr. Thomas Monz, co-founder of Alpine Quantum Technologies (AQT), at the digital BQCX meeting. Deep insights into quantum computing and hybrid High Performance Quantum Computing (HPQC) are bound to happen. [Registration requested.](#)

### Wanted – Data projects for supercomputing

Companies, startups and scientists who need the computing power of supercomputers as well as clever analysis and data management tools for a Big Data project can apply to [LEXIS now and until June 2021](#). The European project, in which the LRZ is also involved, is looking for partners from science and industry to test the newly developed, powerful data platform and its tools, which has already proven itself in some specific research work, with the help of questions and applications from practice. The focus of LEXIS is on location-independent access to Big Data as well as its storage. LEXIS also supports the development of Artificial Intelligence and Machine Learning applications. The LEXIS platform is particularly suitable for issues in areas such as aeronautics, automotive, disaster control, medicine, pharmaceuticals, weather and climate information. More info and registration on [the Lexis website](#).

### 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: [research projects](#) and posters can be submitted 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.

## 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 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 ...

## 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](#)



## The Architecture Machine

A short video already stirs up anticipation: "The Architecture Machine" has been extended **until June 2021**. The exhibition at the [Pinakothek der Moderne](#) 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. Meanwhile, museum visits can even be scheduled again, [register your visit](#) at the Moderne Pinakothek.

## 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!

[Quantum Computing Engineer](#)

[Quantum Computing software Engineer](#)

[Researcher](#) for HPC and quantum computing integration

[IT-Architect](#) and Linux-Specialist  
[Electrical engineer](#) for the building management  
[Technical Specialist](#) for the web team  
[Systemadministrator](#) for client management Windows  
[Social Media Manager](#) for research projects  
[Office Assistant](#) for the KI-Agentur  
[Administrator Human Resources](#)  
[Specialist](#) for funding management  
[Student Assistants](#) for the servicedesk  
[Student Assistant](#) for frontend development

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## MORE TO READ

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

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## INFORMATIONS & IMPRINT

- 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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