



LRZ-Newsletter April 2021: The LRZ wishes happy holiday and sunny Easter. Enjoy reading!

NEWS

LRZ starts into the quantum computing age

Solving puzzles for science

Ideas for quantum processors

Calculating life

Figures of the month

WORKSHOPS & EVENTS

Wanted – Data projects for supercomputing

Register projects for SC21

Training camp for Data Analytics and Artificial Intelligence

Programming for HPC

Crash course for working with the Linux cluster

Quantum in a personal view

Software Design with C++

Faster Computing with Open ACC and Deep Learning

Informatik 2021 – IT, energy efficiency, environment and more

Introduction in C++

The Architecture Machine

Crash Course for the LRZ Linux Cluster

C for beginners

Projects sought for ISC High Performance

JOB OFFERS

MORE TO READ

INFORMATIONS & IMPRINT

NEWS

LRZ starts into the quantum computing age

The ribbon is cut: The [Quantum Integration Centre \(QIC\)](#) was inaugurated in mid-March by Bavaria's Minister President Markus Söder and Minister for Science Bernd Sibler at the Leibniz Supercomputing Centre (LRZ) in Garching. "In the LRZ Quantum Integration Centre, we bundle our quantum computing activities and drive them forward together with our partners in the Munich



Quantum Valley," explains Dieter Kranzlmüller, Director of the LRZ. "As a leading international computing centre, we are already working on building quantum computing hardware on site and developing concepts to make it available to researchers integrated in HPC systems and via our cloud. In our course programme, we are offering initial seminars for education and training, and as a supercomputing centre, we are naturally concerned with the question of how quantum computing can be combined with supercomputing. This will make quantum computing usable more quickly."

At the LRZ, scientists already have access to [powerful quantum simulators](#), such as the Atos Quantum Learning Machine (QLM), which was designed specifically for the development of new quantum algorithms. In addition, Intel's quantum simulator, installed and running on SuperMUC-NG, provides

researchers with up to 42 qubits. But this is just the beginning: this quantum offering will grow, as will the number of courses related to quantum computing.

However, quantum computing is still at the experimental stage. While the first quantum algorithms are already being created on simulators, there is a lack of reliable hardware, especially control units. In order to develop quantum processors (QPUs) and bring them to market maturity, manufacturers are now relying on co-design with users from industry and research and are also collaborating with data centres such as the LRZ. Together with the Finnish-German startup IQM, the Technical University of Munich (TUM), the Freie Universität Berlin, the Forschungszentrum Jülich and the chip manufacturer Infineon, the LRZ will develop a robust quantum computer in the next few years and put it into operation at the LRZ: "Digital-Analog Quantum Computing" (DAQC) is the name of the project funded by the German Federal Ministry of Education and Research (BMBF), which combines the technology of analog circuits with that of digital-universal computing units. Among other things, the system is to be integrated into the high-performance computer architectures at the LRZ, where it will accelerate applications and enable further services. You will find the stream of the opening with all discussions and greetings at [Youtube](#) (mostly in German). (vs)



Solving puzzles for science

Discover principles of order, thinking outside the box: [Sophia Grundner-Culemann](#) loves puzzles and brain teasers. Her favorite pastime brought her to the podium at the opening of the Quantum Integration Centre (QIC) at the Leibniz Supercomputing Centre (LRZ) and to a discussion with Bavarian Prime Minister Markus Söder and Bavarian Minister for Science Bernd Sibler on quantum computing. The PhD student at the Ludwig-Maximilians-Universität München (LMU) described to the two politicians and viewers during the live stream the risks posed by the new quantum computers for data security and encryption of existing IT systems. Sophia Grundner-Culemann deals intensively with cryptography: "This is based on number games and creates a connection between mathematics and computer science," explains the mathematician and computer scientist. Puzzles are part of the subject,



as is quantum computing as a potential code breaker. For her PhD at the Institute for Computer Science at the LMU, Sophia has been analyzing a cryptographic authentication concept for almost three years. "I have to look for assumptions or attack scenarios and solutions. Anyone who can use mathematics has many methods at hand to crack or build cryptographic systems. "

How [Sophia Grundner-Culemann](#) discovered cryptography for herself, what she wants to achieve in computer science, we describe on the LRZ website. There you will find other persons to watch, such as [Daniëlle Schuman](#) and [Bengisu Elis](#), who are researching future technologies with or at

the LRZ, developing new techniques and functionalities, optimizing supercomputing and IT. A look at the current course catalog of the LMU shows that Sophia is not only familiar with cryptography: Together with colleagues from the chair, she is responsible for the lecture [“Introduction to Quantum Computing”](#), which she helped develop. Registration closes on April 6th. (vs)

Ideas for quantum processors

Quantum computing is leaving the laboratories of physics and moving into the data centers. This is changing the environment, applications - and the associated terminology: terms such as processors, gates, control electronics are used differently in quantum computing and high performance computing (hpc), often with only subtle differences. That shows that the international community not only has technical issues to sort out, but also has to find a common language. This was evident during the recent virtual meeting of the [Bavarian Quantum Computing eXchange network \(BQCX\)](#), where vendor companies talked with researchers from the Finnish academic [IT center CSC](#) and the [U.S. Lawrence Berkeley National Lab \(LBL\)](#) about the design of quantum processors and quantum control processors. The lively, sometimes controversial discussions were moderated by [Prof. Martin Schulz](#), Member of the Board of Directors at the Leibniz Supercomputing Centre (LRZ) and Head of the Chair of Computer Architecture and Parallel Systems at the Technical University of Munich (TUM), and [Prof. Sven Karlsson](#) from the Institute of

Applied Mathematics and Computer Science at the [Technical University of Denmark \(DTU\)](#).

New measuring units for performance control

With the definition of processor and computer, speaker [Dr. Anastasiia Butko](#) from the LBNL (a computer scientist) immediately introduced her topic: the design of quantum processors (QPU) with regard to their integration in supercomputers. High-performance systems get these first computing units up and running and into everyday use. Similar to the LRZ Quantum Integration Center (QIC), the LBNL is preparing [the installation of QBU in its supercomputers](#), and the Department of Energy (DOE) is investing 150 million dollars for this ambitious goal. "The physical nature of quantum devices creates non-trivial architectural challenges for the control hardware that cannot be solved with the existing approaches," says Butko.

“Specialized hardware is required.” In order to develop this, other standards are required to test the new technology. Instead of FLOPS, computing time and energy requirements or the inexplicable number of qubits, the scientist recommends describing the performance of the QPU with the help of the gates that the qubits enter, as well as describing their frequency and depth.

Unlike the transistors of existing computers, qubits can assume not only the values 1 or 0, but also the intermediate states. In addition, the smallest computational and memory units of quantum computing are constantly interleaving in new connections or gates. While this potentiates computing power, it makes it prone to interference. QPUs from startups such as IQM Quantum Computer and Alpine Quantum Technologies (AQT) or from manufacturers such as Google or IBM are not yet ready for mass production. As the number of qubits in the processor increases, so does the sensitivity, but also the demands on the control electronics and their integrability and scalability. Functioning prototypes currently offer not much more than 50 qubits, but this is not yet sufficient for reliable computers for broad applications.

Challenges on the way to series production

With the help of specially developed [Rocket Custom Co-processors \(RoCC\)](#), standardized ISA control and algorithms from the [QUASAR](#) framework, the LBNL wants to build a first circuit (with the help of FPGA) to control QPU and try it out in its own system. Quantum processors could “soon” become programmable and ready for the market, Butko concludes her lecture. However, it is uncertain when they will run largely without interference. "The first commercially relevant results for quantum computing will come from a QPU that works in a supercomputer," says Jan Goetz, co-founder of [IQM](#). "This enables hybrid algorithms in which a part of the program is executed by a QPU instead of a classic HPC cluster." For this goal, however, new programming languages have to be developed, the calibrations of QPUs have to be changed and the workflows between the binary systems and the universal QPU have to be harmonized.

Because the technical basis for the use of QPU in the supercomputers is still missing, [Mikael Johansson](#) from the CSC in Espoo (Finland) does not expect the first components until the end of the 2020s: "HPC and quantum computing are not particularly similar, this limits the functions", he says and points out: "Perhaps the advantage of Quantum doesn't come from its computing power, but from its energy efficiency?" In any case, demands Thomas Monz, co-founder of the Austrian startup [AQT](#), quantum processors should be easily accessible with the help of supercomputing centers and easy to handle even for non-physicists and non-computer scientists. In this way, they could establish themselves and increase computing power in business and science. It would certainly also be helpful to arrive at a clear technical language: It isn't still defined what the terms “analog” and “digital” actually stand for in quantum computing. (vs)

Calculating life

The Linux cluster at the Leibniz Supercomputing Centre (LRZ) has grown: The [Faculty of Biology](#) at the Ludwig-Maximilians-Universität (LMU) has its own computer network for the analysis of genetic material. "In recent years, biology has developed more and more into a quantitative science. We are now producing amounts of data on the scale of Google and Youtube," explains [Prof. Dr. Jochen Wolf](#), who heads the Department of Evolutionary Biology. "We therefore need our own computer resources plus



storage space with fast input and output performance." At the LRZ, the Linux cluster was expanded by 13 computing nodes with a total of 512 CPU cores and 15 terabytes of main memory and with a LRZ Data Science Storage (DSS) system made up of 166 16 terabyte hard disks and 24 SSD drives with 3.8 terabytes each combined. An Infiniband HDR network ensures the desired fast connections. "This brings together around two petabytes of usable storage volume and sufficient computing power plus I / O power to process large amounts of data," says computer scientist Stephan Peinkofer from the LRZ.

Computer technology for genome analysis

The LRZ advised the faculty on the acquisition, organized the remote access and operates the system, which was installed in a few weeks after delivery of the components and which will only be used by the biology faculty. "Life is defined by genetic material, we

want to use this system to analyze the genomes of bacteria, plants, animals and humans," says [Prof. Dr. Korbinian Schneeberger](#) from the Chair of Bioinformatics in Genetics and Genomics. The human genome alone contains around three billion base pairs and around 25,000 protein-coding genes. Relationships between living beings or their phylogenetic developments can be derived from these natural data sets. Genomes also stand for specific characteristics and capabilities of an organism and determine how these behave under environmental influences, such as heat or food intake. In Munich, for example, they are using genetic material to research how species of crows evolved in the bird world and how yeasts adapt to their environment. The interaction of genes and molecules in photosynthesis or the neurological performance of humans and animals is also of great interest to researchers.

From April, the dedicated cluster will gradually replace various servers and isolated IT solutions of the 44 working groups at the faculty and - according to Wolf and Schneeberger's hopes - encourage more exchange, synergies and joint projects among researchers. The biologists at LMU are investing around 800,000 euros in their own large computer, half of which was financed by the German Research Foundation (DFG), the other half by LMU. In the run-up, Wolf and Schneeberger were able to test a smaller version of their system at the LRZ. "The LRZ offers the necessary infrastructure and the experience to operate the hardware and supported us very well with this acquisition," says Wolf.



Preparation for supercomputing

The team is currently preparing for operations of the cluster, providing access and installing the first software. Wolf estimates that this could also set a precedent in other disciplines. "It is quite conceivable that the system will continue to grow after 5 years of funding, we expect usage inquiries from neighboring research areas at the LMU." The [need for quickly accessible computing power](#) is also increasing in bio and veterinary medicine, in the genom centre or in chemistry. Wolf and Schneeberger now answer questions from colleagues more often about computer technology and device applications. It is quite possible that the faculty's own computing systems will increase the demand for even more computing power and supercomputing for research in the long run. In any case, further growth can be expected for the LRZ Linux cluster. (vs)

Figures of the month



Supercomputing pays off - US market research company [Hyperion Research](#) has calculated the financial benefits of high-performance computing (HPC) in **763 projects**: According to this, **every dollar** invested generates more than **\$ 500 in sales** and **\$ 47 in profit** or savings potential. The balance sheet of the HPC looks even better in science: There **every dollar** invested generates **1,264 dollars in sales** and a profit or savings potential of almost **111 dollars**: Today, simulations are used to solve traffic problems, support disaster control and analyze environmental and climate developments . Last but not least, with the help of supercomputing, effective vaccines were found **a year and a half** after the outbreak of the corona pandemic. (vs)

WORKSHOPS & EVENTS

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](#).

Submissions 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 conference organizers are accepting offers for 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 ...

Training camp for Data Analytics and Artificial Intelligence

Four days full of techniques and methods for electronic data analysis: The virtual training camp for scientists who want to build smart systems for their research starts on **April 6 and ends on April 9, 2021**. It takes place digitally. In addition to instructors from the Leibniz Supercomputing Center (LRZ), professional data specialists from Intel and other institutions will teach. Participants will not only be introduced to the computer resources and the data cloud of the LRZ, they will also gain insights into existing training modules and algorithms from Intel libraries. [Info and registration](#).

Programming for HPC

Students and scientists who want to use the High Performance Systems or supercomputers of the Leibniz Supercomputing Center (LRZ) or the Gauss Centre for Supercomputing (GCS) for their work are the addressees of this 3-day workshop from **April 13 to 15, 2021**. They will learn the technology of SuperMUC-NG and supercomputers at the High Performance Computing Center in Stuttgart (HLRS) as well as from the Forschungszentrum Jülich, and also the first codes of the programming languages MPI and OpenMP. Experienced instructors from the Friedrich-Alexander-University Erlangen and the LRZ will also show the biggest pitfalls when addressing parallel systems. Thanks to the support of the KONWIHR network, the course is free of charge for students of Bavarian universities, participants from other groups pay 600 Euro. Participation only possible via the waiting list. [Information and registration](#)

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](#)

Quantum in a personal view

Push Quantum wants to introduce students to quantum computing, for example in hackathons during which participants solve real tasks from companies with the help of annealers and simulators, or in digital meetings with managers and specialists from companies that supply products for quantum computing. On **April 20, 2021**, Prof. Ignacio Cirac, lecturer at TUM and director of the Max Planck Institute for Quantum Optics, will introduce himself and talk about the opportunities with quantum. On **May 11, 2021**, Dr. Christophe Jurczak, Investor and co-founder of Le Lab Quantique, shareholder at Quantonation and board member at Nord Quantique, will describe how quantum computing can help the pharmaceutical industry find new drugs or decipher molecular structures. [Registration](#)

Software Design with C++

This three-day online course, **April 21 until 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 to 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 NVIDIA. Participation only possible via the waiting list. [Information and registration](#)

Informatik 2021 – IT, energy efficiency, environment and more

Until **April 30, 2021**, the Gesellschaft für Informatik is looking for papers and ideas for energy- and resource-efficient supercomputing for its annual conference Informatik 2021: It is about controlling and optimizing the work of high-performance systems as well as about the use of waste heat or more sustainable computer architectures, information about the format and submission can be found [here](#). Informatik 2021 also includes the lecture plenary "[SKILL](#)", here students of computer science present their ideas for the future and for existing applications. Proposals for workshops and talks will be accepted until **May 9, 2021**. Other topics for Computer Science 2021 also include [Artificial Intelligence](#) and [Environmental Research](#). Papers, talk topics and workshops are still being sought for these parts of the program as well. Submission deadlines are **May 31, 2021**, and **June 26, 2021**. The [program for Informatik 2021](#), which is held **September. 27-October. 1, 2021**.

Introduction in C++

With C++, machine-oriented and abstract applications can be programmed in equal measure. In the 4-day this course from **May 3 to 6, 2021**, introduces participants to the important functions and possibilities of C++: the most used terms, control structures, templates, as well as tricks for debugging and program management. Cost: 35 to 780 euros. [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.

Crash Course for the LRZ Linux Cluster

On **June 1, 2021**, beginners in high-performance computing (HPC) can learn about working on parallel computing systems. The focus of the one-day crash course is on computational fluid dynamics (CFD), i.e. the simulation and representation of flows and motions of and in gases or liquids, 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](#)

C for beginners

C is one of the most widely used programming languages, is used in the development of software as well as processors, and other languages such as C++, Java, PHP or Perl are also based on it. In three days from **June 21 to June 23, 2021**, participants will learn how to use C in their everyday lives. Of course, it's not just about the basic codes and programming, but also about debugging, version management, tips & tricks. Cost: 30 to 600 euros. [Information and registration](#)

Meeting Point ISC 2021

From **July 24 to 29, 2021**, [International Supercomputing \(ISC\) 2021](#) will open what is expected to be its virtual doors. Europe's largest meeting place for supercomputing will showcase ideas for computer architectures and innovative applications. Sustainability and energy consumption are already set topics, and there will certainly also be discussions about how artificial intelligence and machine and deep learning methods can accelerate supercomputing. Last but not least, there is sure to be talk about quantum computing and what is expected to be the next generation of accelerators, Quantum Processing Units QPU). The LRZ takes part at this conference.

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!

[System-Engineer](#) for the further development of the HPC storage infrastructure at LRZ

[System Engineer](#) for the development of storage services, e.g. BayernShare

[Astrophysist](#) for development of applications and consulting of HPC-users

[IT-Architect](#) and Linux-Specialist

[Electrical engineer](#) for the building management

[Office Assistant](#) for the secretariat of LRZ

[Administrator Human Resources](#) for the Bavarian AI-Agency

[Specialist](#) for funding management
[Student Assistant](#) for backend development
[Student Assistants](#) for the servicedesk

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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