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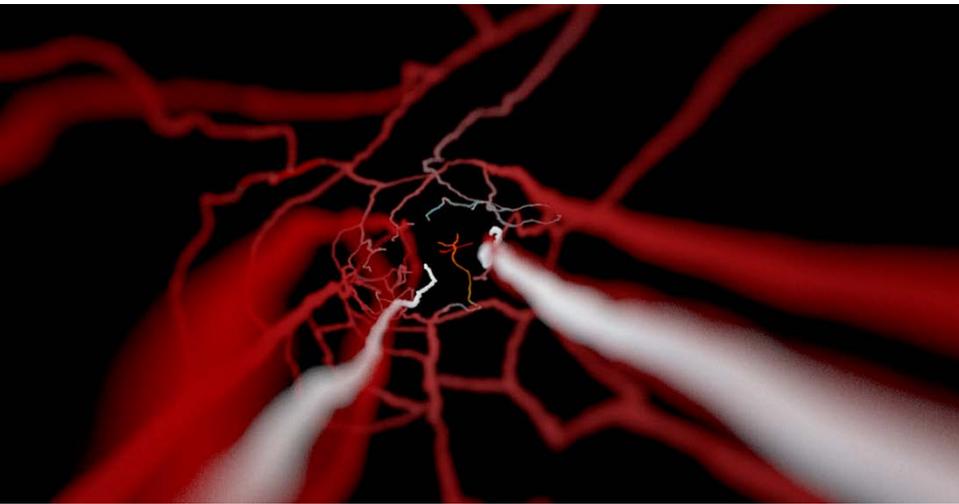
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**INFORMATIONS & IMPRINT**

## NEWS

### Excellent Research

Visualization and A fascinating project that is advancing diagnosis and treatment methods in medicine: Using measured values, data and images, supercomputers simulate and visualise a living human being, the Virtual Human. With the help of the Leibniz Supercomputing Centre (LRZ), the international research project [CompBioMed](#) has come a big step closer to this vision: Together with the LRZ Centre for Virtual Reality and Visualization (V2C), a research group led by the British physical chemist and computer



scientist Prof. Dr. Peter Coveney succeeded in modelling and [visualising the blood flow in the veins and arteries of a forearm](#). This resulted in tools to process complex data from flow simulations with graphical software. So the blood flow in other parts of the body can also be visualised: "One advantage of our workflow is that any images and media can be created from it and exported," says [multimedia specialist Elisabeth Mayer](#). "Anything is possible - a graphic, a short video clip, even a cinema film or a three-dimensional virtual reality application could be made from it."

The tool kit supports science in visualizing other flow phenomena in the human organism and is described in detail in the article ["Images](#)

[from the Organism"](#) on the LRZ website. With this pictures doctors can understand body functions or try out treatment methods. It is not without reason that this remarkable work is now in the run for the prize for the world's best scientific visualisation and will be presented during Supercomputing 2021 (SC21). It is just one of the contributions that LRZ staff and research partners will present during SC21. The international conference brings together the High Performance Computing or HPC community and takes place from 14 to 17 November in the USA and online. If you want to be there - here are the schedules (all local time CST):

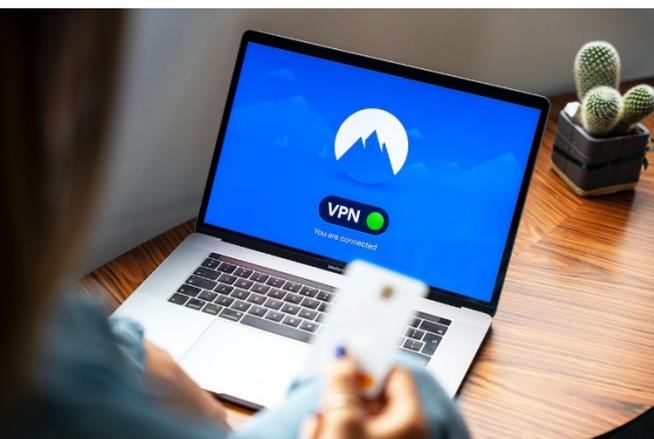
- **16 November, from 12: 15: "Operational Data Analytics"**: Bird of Feather discussion on energy efficiency in supercomputing. This is becoming relevant in view of the growing power of new systems. Hopes rest on the analysis of data from the systems and smart control. Dr. Michael Ott and Alessio Netti from the LRZ will discuss with colleagues how [data analysis of operating data](#) from HPC systems can be standardised and thus enable comparisons. [More information](#)
- **16 November, 14.30: "A Next-Generation Discontinuous Galerkin Fluid Dynamics Solver with Application to High-Resolution Lung Airflow Simulations"**: Presentation of the research report on the construction of a digital lung model by the Institute for Computational Mechanics at the Technical University of Munich (TUM). Professor Wolfgang Wall's team has already been working on the highly complex simulation for years and has added further parameters to it each time. With the support of the LRZ's Computational X team, not only a simulation code was developed, but also a highly scalable solver for calculating respiration functions. [More information](#)
- **17 November, from 12.15, "Open HPC Community"**: Open access to supercomputing resources, to research data and to tools - LRZ specialist David Brayford discusses with colleagues from other data centres in Europe and USA the technologies and processes how this works best. [More info](#)
- **17 November, from 12.15, "The Message Passing Interface: Version 4.0 and Beyond"**: LRZ Director, Prof. Martin Schulz, discusses the master release of the well-known programming scheme and how it can be further developed. [More Info](#)
- **17 November from 13.30. "SC Scientific Visualization & Data Analytics Showcase"**: The final of the competition and the presentation of the six best visualizations of the world. Elisabeth Mayer and the CompBioMed team will show the visualization of the blood flow in the forearm and explain how it was created with the algorithm HemeLB and the graphics software OSPRay. [More information](#)
- **17 November, from 16:30, "3D Acoustic-Elastic Coupling with Gravity: The Dynamics of the 2018 Palu, Sulawesi Earthquake and Tsunami"**: The European project [ChEESA](#) will present results of research on tsunamis and earthquakes and describe how they have also developed algorithms and software with the help of the LRZ and its supercomputer SuperMUC-NG. ChEESA also demonstrates first petascale production runs and scaling studies for a pilot demonstrator to compute the interaction of tsunamis and earthquakes. [More information](#)
- **17 November, from 17.15, "Integrating HPC with Quantum Computing"**: The BoF discussion led by Prof. Sven Karlsson (Danish Technical University), Prof. Martin Schulz and LRZ strategist Laura Schulz will focus on the integration of quantum and supercomputing. The question is when quantum processors are ready to work with HPC systems and which research areas will benefit from the combination. [More information](#)



**SC21**  
St. Louis, MO | science & beyond.

## Secure Access to LRZ's Services

130,000 users work in the Munich Scientific Network (MWN). All universities and numerous research institutes in the greater Munich area are connected to the Leibniz Supercomputing Centre (LRZ) and the Internet via this network. Students and staff can access all important services of their institutes from outside via the MWN - such as email, LRZ Sync +Share, data storage and more.



[Virtual Private Networks \(VPN\)](#) have been used here for years to ensure secure access and prevent misuse by third parties. For this purpose, a virtual, closed communication network is set up via the Internet between the user's computer and the data centre, which is protected against access by third parties, unwelcome eavesdroppers and other attacks from the Internet. The need for this is great: previously, 1500 to 2000 users per day simultaneously accessed the science network with the help of the LRZ's VPN, but during the pandemic there were immediately more than 6500 per day.

The VPN solution from a large network provider has been working without any problems for years. "The licences we had purchased expire in 2022," explains Markus Meschederu, who's responsible for data lines and routers in the network team. "The hardware used has also reached the end of its life cycle, which would result in high costs. Also, the solution used so far has increasingly moved away from a pure VPN." In the search for suitable

alternatives, the open source solution OpenVPN was initially evaluated, which is already in use in some areas of the LRZ. However, this revealed some limitations that are unfavourable for client operation: "With OpenVPN, users have to do a lot themselves, such as installing updates or updating the configuration," says Meschederu. For security and convenience reasons, however, those responsible wanted to automate as many tasks as possible on the client. Another VPN solution was found in the [EU project GÉANT](#).

### Easy-to-use open-source tool

In recent years, GÉANT has already established the international WLAN for research and teaching, eduroam, which forms the basis for WLAN access via the MWN. Another development of the project is [eduVPN](#), an OpenVPN client specially adapted for academic needs for almost all operating systems. Meschederu pointedly says: "eduVPN is a nice packaging for OpenVPN." eduVPN is now available for all common operating systems via the LRZ's self-service portals. The configuration is very simple: The users select their respective institute from a list at the beginning. They are then redirected to a website for authentication, and all other settings follow automatically. Unlike other VPN solutions, eduVPN stores the authentication for a certain period of time. If the connection is interrupted, e.g. due to the stand-by mode of the user's notebook or computer or due to fluctuations in the internet connection, the users do not have to log in again.

eduVPN is more convenient than the previous solution and offers the same security advantages. The decision to switch to eduVPN has therefore been made: "We are currently running eduVPN and the old system in parallel," explains Meschederu. There are few problems, the number of enquiries at the service desk is manageable. For new users, [eduVPN](#) should be the first choice: In the meantime, more than 5,500 users are already working with eduVPN, and at peak times around 600 are accessing the secure network at the same time. Meschederu is satisfied with the changeover: "We needed support from the developers on some issues, such as connecting our Radius servers for user authentication," he says. "That went very well, eduVPN was enhanced in that regard. Functionally, eduVPN also offers everything we need." Once the old licences have expired, the entire system will be switched to eduVPN - but why should users wait so long? (js)

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## "Weak Passwords are the Number One Cause of Damage and Annoyance"

Making it harder for data thieves: October was marked by [cybersecurity](#). On [Twitter](#) and [LinkedIn](#), the Leibniz Supercomputing Centre (LRZ) informed interested parties how they can protect notebooks, smartphones and, above all, their privacy in the home office from attacks. All recommendations came from the LRZ security team - Miran Mizani presents their work in [an interview on](#)

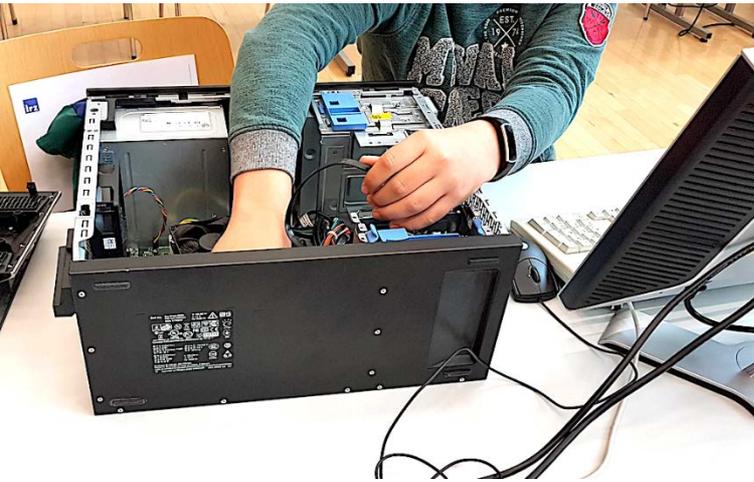


[the LRZ website](#). In his daily work, the computer scientist and his colleagues analyse security incidents, but also the tactics of attackers and optimise processes. "Whoever is responsible for services as an admin at the LRZ also takes great care of their security, which helps us a lot," he [says](#). "Weak passwords are certainly the number one cause and annoyance. Most of the time, attackers gain access to services and devices via compromised identifiers." In the interview, he also reports on the LRZ's latest security measures as well as research projects on this: So-called [cyberranges](#) are currently being set up in the LRZ cloud, which IT specialists like Miran can use to analyse cyberattacks and develop counterstrategies. Students who deal with data protection and cyber security are highly welcome in the team and find [meaningful tasks](#) at the LRZ to finance their studies.

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## School Trip to the LRZ

Trivia can be exciting: The fact that the adhesive mat in front of the computer room in the computing cube of the Leibniz Supercomputing Centre (LRZ) smacks when your foot is lifted on it immediately tempts you to jump and take lots of little steps. But then the SuperMUC-NG is even more interesting. "Do computers have feelings?" asks a pupil, and his friend immediately sees, "There's no keyboard here at all, how do you give the computer instructions?"



Rainer Oesmann, a member of staff at the LRZ, is today guiding six boys and girls from a sixth grade at Gymnasium Kirchheim through the computer cube, having to explain a lot of everyday things, sometimes even laughing a little. SuperMUC-NG, he says, has a name, but it shows less emotion and sometimes a few quirks. The commands to the mainframe come via data lines from the laptops and computers of the researchers at universities. And he already guides the group through the computer cabinets and explains to the children why it's as hot here as in a sauna: "There are 311,040 computing nodes working here and they produce quite a lot of heat." The boys and girls feel the different temperatures on the pipes of the water cooling system, look at the imposing gas cylinders of the extinguishing system and watch the whirring storage robots with thousands of tapes.

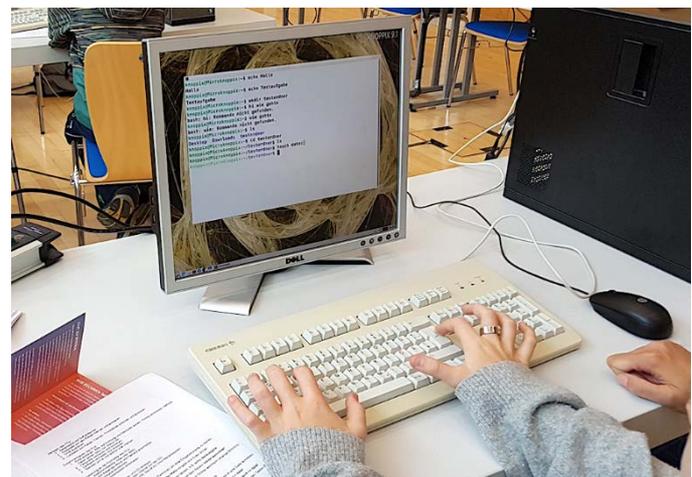
### Experience MINT Subjects in Practice

The LRZ goes schools: the scientific computing centre participates in the [TUMjunior programme](#), which is intended to arouse interest in mathematical and scientific topics and computer science, the STEM subjects, among schoolchildren. "TUMjunior is supported by the Bavarian Ministry of Education and is aimed at pupils in grades 5 to 10. Three excursions to different places of learning are planned for each class per school year," explains Dr Magdalena Kaden from the [School of Social Science and Technology](#) at the Technical University of Munich (TUM). Together with colleagues, the educator coordinates the programme under the direction of private lecturer Dr Jutta Möhringer, who initiated [TUMjunior](#), and evaluates its benefits. "When students see and experience technology and can even handle it themselves, their motivation to study it more intensively grows," she says. TUMjunior is intended to make it possible for students to experience and literally grasp the process of gaining scientific knowledge, which underlies all STEM subjects."

In addition to the LRZ, TUMjunior classes also visit the TUM-Lab [experimental laboratory in the Deutsches Museum](#), the [ix-quadrat mathematics exhibition](#), the planetarium of the [European Southern Observatory \(ESO\)](#) or the [Botanical Garden](#), depending on the grade. The curriculum for Nature & Technology in Year 6 includes computers and computer science for the first time. Therefore, from October to December, a total of 17 sixth-grade classes from three grammar schools in Garching, Kirchheim and Unterföhring take a look around the LRZ in the mornings. There, under the guidance of LRZ trainees, they disassemble personal computers, look at hard disks and memory disks, circuit boards and processors, and reassemble them to then start a slimmed-down Linux programme and use it to create, save and change a file.

### Gaining Insight in Foreign Places

"Much better than at school," one boy comments and quickly turns back to the cables on the hard drive. "Today all technical devices are welded together, it's an absolute benefit for everyone that we can look inside a PC here and get to know the individual parts from the grey boxes," says Philipp Augat, who teaches German, history and computer science and works in the administration team of the Kirchheim grammar school. "A foreign place is much more interesting for the children, many technical questions can be better illustrated here."



At the LRZ, those responsible for training Petra Gärtner and Alessandro Podo prepared the visit of the school groups with the trainees and in cooperation with the teachers of TUMjunior, created a small manual for handling the technical components as well as the first Linux commands. Here, the children learn how supercomputers are built and what researchers use SuperMUC-NG for: for simulations of the Earth, for example, visualisations of turbulence in space and of blood flow in the body, or for calculations of flows. "We want to move away from guided tours, we want the students to be active at the learning sites themselves, to be able to experience science and technology in practice," says Kaden. "The respective excursions are systematically integrated into the lessons and are prepared and followed up using the TUMjunior materials."

### Making Research Tangible

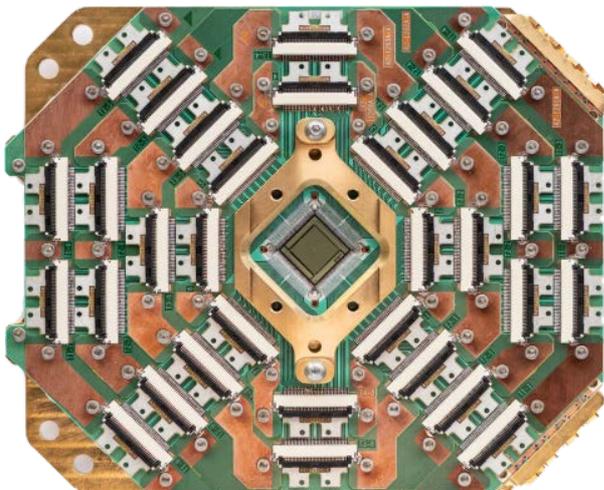
TUMjunior is still in the experimental stage, the three grammar schools are pilot schools. Teachers and students are still being interviewed for a study and their knowledge is being documented. If this confirms the pedagogical assumptions that science and

computer science become more comprehensible and interesting through practical experience and participation, the programme will be opened to other schools and throughout Bavaria. Pupils will then be able to visit even more places of learning; teachers, on the other hand, will find materials to go with the excursions, so that the subject matter and excursions can be meaningfully interlinked. "TUMjunior aims to further professionalise teachers so that they can embed methods such as excursions in their lessons," explains Kaden. "Children find their way around better, by the way, if they can visit a place of learning several times." It is quite possible that today's sixth graders will come back in two or three years: After all, there are many more interesting things to discover at the LRZ besides supercomputers - visualisation technology, for example, artificial intelligence and, above all, many exciting research projects. (vs)

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## Bringing Quantum Computing into everyday Research Life

Munich is no longer just a cosmopolitan city with a heart, but also the city for quantum computing: "In recent years, Munich has developed into an internationally visible centre for quantum research," notes Prof. Dr. Thomas O. Höllmann, President of the [Bavarian Academy of Sciences and Humanities \(BADW\)](#). "We are proud to be able to play a part in this." Two institutes of the Academy are intensively dedicated to the research and development of quantum computers: the Walther Meißner Institut für Tieftemperaturforschung (WMI) and the Leibniz Computing Centre (LRZ). They co-founded the [Munich Quantum Valley \(MQV\)](#). Now the Free State of Bavaria funds the initiative with 83 million euros to start with. The funding is dedicated for hard- and software for the computers of the future. "As a scientific computing centre, we bring together different technologies for [quantum computing](#) in one place in order to explore them intensively and use them to develop useful services for data-intensive science and research," says Prof. Dieter Kranzlmüller, director of the LRZ, describing plans for the funding.



Jobs for scientists and quantum experts have already been advertised at the LRZ, and the first technology, such as a quantum learning machine from Atos and an Intel quantum simulator with 42 qubits, is already in operation. In spring, the academic computing centre also bundled its quantum activities in the [Quantum Integration Centre \(QIC\)](#) and, together with partners such as the Technical University of Munich (TUM) and the Ludwig-Maximilians Universität (LMU), took part in national and international tenders.

### Software stacks in demand, but also exchange of ideas

This is now proving successful and bringing funding to Munich and to BADW. The focus of future research and development at the LRZ is on the everyday use of quantum computers in research and industry. Quantum processors and computers are still at the experimental stage. To reach market maturity, the technology of the future needs reliable operating systems, programming environments, software and more tools, as well as concepts for data security: "In order to be able to work with them, quantum computers need, in addition to the processors, above all control and steering tools," explains LRZ Director Prof. Martin Schulz. "We see developing these as a major contribution of the QIC at LRZ." Involved in projects such as Q-Dessi, [DAQC](#) or [BayQS](#) are not only the Munich universities but also the Fraunhofer Institutes AISEC and IKS, as well as processor manufacturers such as the German-Finnish start-up IQM. The optimisation of existing quantum processors will also be the goal of research consortia with LRZ participation: Quantum processors will be integrated into the supercomputing resources at the LRZ to increase their stability, provide reliable computing performance and control.

The data centre has equipped itself well for these tasks: Back in 2019, it founded [Bavarian Quantum Computing eXchange \(BQCX\)](#), a network for quantum enthusiasts from science, research, business and politics. This grew into a vibrant community that today reaches far beyond Munich and its Quantum Valley, where ideas and concepts for the tasks ahead are intensively discussed and exchanged. "At the LRZ, we provide researchers with computer resources and IT services," Kranzlmüller says in this regard. "As a result, know-how on research projects and new ideas accumulate here. At the LRZ, we therefore also see ourselves in the role of a networker, bringing researchers and interested parties together and offering them platforms for exchange and collaboration."

And on it goes with the projects: Q-Exa will promote cooperation with IQM. With funding from the Federal Ministry of Education and Research, the LRZ is purchasing a quantum computer from the young company for research purposes. The kick-off for the Q-Exa project will be a press conference with the Federal Minister of Education and Research, Anja Karliczek, next Monday, November 15. The Federal Ministry will broadcast it live on [the internet](#) and on [Twitter](#).



## Calculation Tasks for Quantum Computers

Plan regular deliveries to many different locations or explore the basics of quantum computing: The [Bavarian Quantum Computing eXchange \(BQCX\)](#) discussed fundamental issues and practical solutions in October. Organised in cooperation by Leibniz Supercomputing Centre (LRZ) and Munich Universität der Bundeswehr, Dr Sabine Tornow, who heads the quantum computing department at the CODE research institute, and Lilly Palackal, a doctoral student at the Technical University of Munich (TUM) and a student trainee at chip manufacturer Infineon, presented the results of their research projects.

To challenge quantum computers with highly complex computations, Tornow and her team are looking at many-body physics, a field, she says, "that is very well suited for testing quantum algorithms and finding working heuristics for today's quantum computers". To model the behaviour of open one- and two-electron systems, the scientist and her team work with different, widely used [quantum variational algorithms \(QVA\)](#), with an IBM quantum computer as well as classical computers: "QVA work iteratively and mainly solve optimisation problems," explains Dr. Mario Vera Hernandez from the LRZ Quantum Computing team. "In the first step, the quantum computer estimates a minimum value composed of diverse parameters. In the second step, a classical computer changes these parameters to improve the minimum value again." The results are then checked with error mitigation methods: a useful interplay for calculating other open systems in research, as Tornow sums up: "For short periods of time, the simulation on the quantum computer agrees very well with the exact results when error mitigation methods are applied." And the simulation could still be extended.

Mathematician Palackal's solution was much more pragmatic. She showed how manufacturers or trading companies can sustainably plan a regularly necessary supply of many locations or branches. Palackal solved the underlying allocation problem mathematically and with the help of the so-called [Unconstrained Quadratic Binary Optimisation formula \(QUBO\)](#) and with the help of a quantum annealer from D-Wave. "Quantum algorithms require a lot of creativity," Hernandez-Vera says appreciatively. "You have to resolve computational problems in terms and formulas that quantum hardware is suited to. This kind of matching of a mathematical representation and hardware requirements is one of the most important skills we need for new quantum algorithms."

The next BQCX meeting will take place on 8 December from 4pm. Students will present research projects before Bavaria's quantum community celebrates Christmas. Please sign up for the invitation list at [bqcx@lrz.de](mailto:bqcx@lrz.de).

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## Sudoku for Quantum Computers

Key clatter, concentrated mood, quiet discussions: 11 students from Ludwig-Maximilians-Universität (LMU) are programming an IBM quantum simulator in Lecture Hall 2 at the Leibniz Supercomputing Centre (LRZ) and trying to teach it to play Sudoku, the game with number squares. "For the first time, our [quantum hackathon](#) can take place here in the presence of people," [Sophia Grundner-Culemann](#), a doctoral student at the LMU Chair of Communication Systems and Systems Programming in Computer



Science, and Dr Tobias Guggemos say, a lecturer and quantum specialist at the Remote Sensing Technology Institute of the German Aerospace Center (DLR). Both presented the lecture ["Introduction to Quantum Computing"](#) in the summer semester with Prof. Dieter Kranzlmüller, head of the LRZ, and now some of the graduates are trying their hand at practical quantum problems for a week to deepen their knowledge. "We were looking for a sufficiently large room with good data connections for this, and we can also show the participants the supercomputer here," explains Guggemos. In addition to the LRZ, the German Space Operations Centre (GSOC) and the CODE research institute at the University of the German Armed Forces supported the workshop with know-how and technical resources.

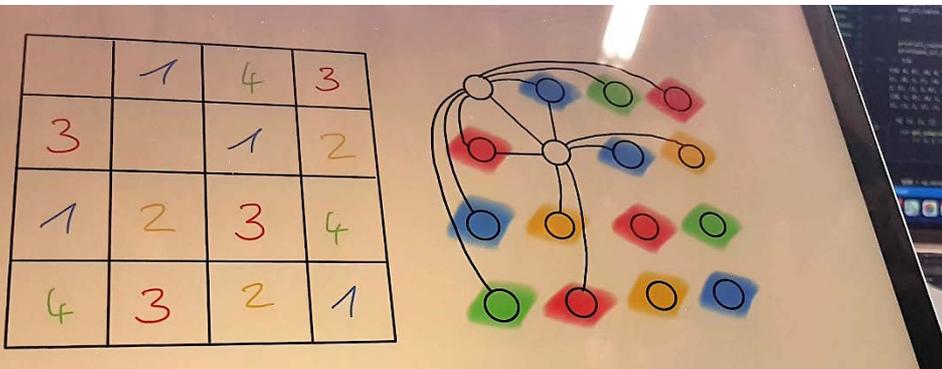
## Programming Combinatorial Tasks for Quantum Computers

The eleven participants initially started with small number squares of four and 8 boxes each, but the goal is to increase the size of the Sudoku squares in the course of the practical training, expand the algorithms and thus challenge an IBM simulator with 32 qubits, which is accessed via data line and cloud. "In Sudoku, numbers must not be duplicated in any row; mathematically speaking, this is a combinatorial task," Grundner-Culemann explains, "and it's made for quantum computers." Computers simply try out what people spend a good few hours puzzling over. They quickly find the required number combinations for a row and column. Quantum computers are faster at this because they cannot only calculate with 0 and 1, but also with more variants. But they also need guidance on what to calculate. "Classical computing presents all problems with 0 and 1, in quantum computing all values between 0 and 1 are possible," explains Viktoria Patapovich (photo above). She is studying mathematics and computer science, wants to try out the technology and meet people she can talk to about it. "So there are many more possibilities for finding solutions, but not via addition, but via the construction of quantum gates or entanglements." The research group turned Sudoku into a colour game and programmed the constraints - the quantum computer must not combine 'the same colours: with this

graph-colouring problem, Sudoku can also be solved. "Quantum computing is relatively new," says Maximilian Weiß (photo above), a 5th semester computer science and biology student. "You can't find solutions for many tasks on Google yet, so you have to sit down and try it out yourself, which is how you really learn to understand and use the resources."

### Working with QAOA and with Grover

Two well-known common algorithms from are used: The [Quantum Approximate Optimisation Algorithm \(QAOA\)](#) approaches the Sudoku question heuristically and allows smaller problems to be solved on quantum chips available today. [Grover's algorithm](#), on the other hand, guarantees a correct result with a certain probability, but is not yet practical to use on today's chips. Proving this is still a task in the hackathon. "The participants work out solutions for Sudokus with four, eight, 16 numbers, they discuss different ways of solving and learn to optimise circuits in the process," explains Guggemos. "The lecture and exercises usually deal with smaller problems, the hackathon gives time and space to tackle larger tasks." For the LRZ, there are also opportunities to draw attention to its own quantum resources, the Atos Quantum Learning Machine and an IBM simulator, which are now also available to researchers. In addition, the Bavarian Quantum Computing eXchange Community (BQCX) virtually connects



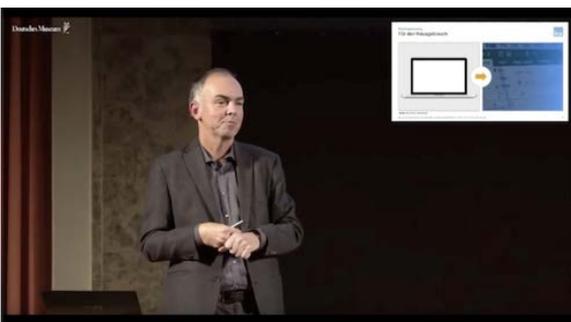
students with researchers and company representatives on the first Wednesday of each month. "Quantum computing combines physics, mathematics and computer science, requires a different way of thinking and a new logic, which interests me a lot," says Master's student Thomas Holger. "It's quite possible that I'll look for a quantum computing problem for my Master's thesis. There are already first possibilities to use it to encrypt the transmission of sensitive data more securely."

While Guggemos wanders around the room and supports the groups present as needed, Grundner-Culemann chats with the working group that is participating online in the quantum hackathon. The introductory lecture and the practical are already scheduled for the summer and winter semesters of 2022. "It would be cool if we could experiment with the LRZ's quantum resources then and get to know them better," says the PhD student.

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### The LRZ in Media

Supercomputing explained easily and clearly: Prof. Dr. Dieter Kranzlmüller, Director of the Leibniz Supercomputing Centre (LRZ), describes in a lecture at the Deutsches Museum the development, background and benefits of High Performance Computing (HPC) and illustrates this with impressive figures: Did you know that in 1969 14,245 flops or floating point operations per second were still needed to get three people to the moon and back safely? A cinch compared to the roughly two million flops that comparatively small smartwatches can deliver per second today, but often still not enough to cope with the increasing masses of data in research. Want more of these comparisons? Then take a look at [Youtube](#) (in German) and gather an hour of knowledge about supercomputing, SuperMUC-NG and fascinating research projects.



"Wherever it says research and teaching in Munich, the Munich Science Network (MWN) and the LRZ are there," Prof.

Dr.-Helmut Reiser, deputy director of the Computing Centre, tells us in the [Cisco, Ingram Micro podcast](#) (in German). And much more about the work and the services that the LRZ no longer provides only in Munich and Bavaria, but also to researchers throughout Germany and Europe. Along the way, listeners learn why the LRZ cools its computers with warm water, how more than 311,000 processors are procured and how the next supercomputer will be built. Interesting: The successor to SuperMUC-NG will be built in teamwork and partnerships. Entertaining to listen to. Good questions, exciting and sometimes funny answers. Listen in.



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### Figures of the Month

Quite busy: Since it started its computing work in August 2019, SuperMUC-NG has been active for more than **4.9 billion** core hours, for **1,217,286** research jobs, especially astrophysics, material sciences, and increasingly also the natural sciences and medicine need the supercomputer's help in analysing big data. **1056** scientists and **397** projects were working on the SuperMUC-

NG. With its **311,040** computing nodes and its performance, it reached **8th place** among the Ttop 500 fastest computers in the world in 2019 - and it continues to keep pace: By mid-November 2021, SuperMUC-NG occupied **17th place** in the list - initial rumours suggest it could continue to hold on to top ranks when the supercomputer rankings are updated on November, 15. Much more important than the places remains its work for research and science ...

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## WORKSHOPS & EVENTS

### Trends in Supercomputing

The next [Supercomputing \(SC21\)](#) has already been scheduled. The US counterpart to ISC will start on **November 14, 2021**. For this conference and exhibition, the Leibniz Supercomputing Center is sending HPC and visualization projects into the race, research partners are presenting papers and have already been nominated for the prestigious Gordon Bell Prize. For the anticipation: The SC has opened a [Youtube channel](#), where you can already find some interesting insights into supercomputing.

### Experience Research and Art

Discussion panels, installations, exhibitions, workshops, participation and, above all, experience: the [first Hi!A Festival for Art and Research](#) has been running in Munich since October and will continue until **31 December 2021**. The Leibniz Supercomputing Centre (LRZ) is represented several times: On **15 November 2021** from 6pm, LRZ strategist Laura Schulz will discuss online with Luise Allendorf-Hütter (Deutsches Museum), Martin Leib (IQM), and prof. Michael Hartmann (FAU Erlangen) about the ["Unimagined computing power of qubits"](#) and the opportunities that quantum computing promises. The event will be broadcast live on [Youtube](#). Until **31 December**, the [LRZ's Centre for Visualisation and Virtual Reality](#) will also be showing online how supercomputers can be used to make research results visible and build them into virtual worlds. It's also a great place to learn, as the LRZ app ["Bridge of Knowledge"](#) impressively shows.

### Telling stories with immersive techniques

Virtual, augmented and mixed reality are ideal for explaining research and science or for telling stories: From **November 15 to 19, 2021**, the European Creator's Lab will deal with these topics, present works and give game developers, designers, programmers, authors, journalists, students and researchers the opportunity to network and develop projects together. The Creator's Lab is organized by the XR Hub in Bavaria and takes place online. [Information & Registration](#)

### HPC and Computational Fluid Dynamics at LRZ

On **November 17, 2021**, young scientists will be introduced to the use of the Linux cluster at the Leibniz Supercomputing Center (LRZ) and in particular to the possibilities of Computational Fluid Dynamics, i.e. the numerical representation of fluid dynamics. Introduced. Prior knowledge of HPC is not expected, but is certainly welcome. [Information & Registration](#)

### Software Design with C++

Object-oriented (OO) software design with the C++ programming language is the focus of this three-day workshop **from November 17 until 19, 2021**. Experts will discuss with participants the development principles, concepts, idioms and best practices for coding professional algorithms and applications. The course does not cover specialties of C++, but provides guidelines for developing mature, robust, and maintainable C++ code. [Information & Registration](#).

### The challenge of Quantum Computing

Quantum technologies are still young and in the experimental stage. But the community is already networking and discussing innovations, challenges and opportunities: from **29 November to 2 December 2021**, for example, at the European Quantum Technology Conference, which will take place virtually. [Information & Registration](#)

### Addressing the new GPU with CUDA C++

Compute-intensive CUDA C++ applications in high-performance computing (HPC), data science, bioinformatics, and deep learning can be accelerated by using multiple graphic processing units (GPU), which can increase throughput and reduce overall runtime. Combined with concurrent computation and memory transfer overlap, computations can be scaled across multiple GPUs without increasing memory transfer costs. In this course on **November 30, 2021**, participants will learn how to write CUDA C++ applications and improve application performance. [Information & Registration](#)

### Stimulate compute nodes properly

Even application developers familiar with OpenMP and MPI often don't know exactly how much performance their code could achieve in the best case. This online course from PRACE on **December 1, 2021**, therefore covers performance engineering approaches at the compute node level and provides an understanding of the interactions between software and hardware. If you want to properly utilize compute nodes you must start at the core, socket, and node level, where the code that does the actual compute work is executed. We will introduce the basic architectural features and bottlenecks of modern processors and compute nodes. [Information & Registration](#)

## Schroedinger's Suite for Material Sciences and Pharmacology

Schroedinger offers a special software package for modelling molecules and biological substances. Its applications are the focus of the two-day workshop from **6 to 7 December 2021**, which the LRZ is organising in cooperation with the software manufacturer. Material scientists and pharmacists will learn how Supercomputing supports their research and work. [Information & registration](#)

## Research around Quantum Computing

Shortly before Christmas, the Bavarian Quantum Computing eXchange (BQCX) will meet again: On **December 8, 2021**, young scientists will present their research questions and projects in the network. These will also be of interest to older users. Afterwards, they can celebrate and network at the virtual Christmas party. Registration: [bqcx@LRZ.de](mailto:bqcx@LRZ.de)

## HPC and Computational Fluid Dynamics at LRZ

On **January 19, 2022** young scientists will be introduced to the use of the Linux cluster at the Leibniz Supercomputing Center (LRZ) and in particular to the possibilities of Computational Fluid Dynamics, i.e. the numerical representation of fluid dynamics. Introduced. Prior knowledge of HPC is not expected, but is certainly welcome. [Information & Registration](#)

## Artificial Intelligence for Research

Making research smarter: On **1 and 2 February 2022**, the focus will be on artificial intelligence in research. Participants will learn how to integrate AI methods such as pattern recognition, machine and deep learning into their research projects and how to efficiently evaluate large amounts of data. The agenda includes useful AI tools, data processing and the construction and concepts of neural networks and deep learning models [Information & registration.](#)

## Programming with OpenMP

Anyone who wants to operate supercomputers needs OpenMP. The programming scheme has proven itself in computing on parallel machines and shared memory since 1997 and is constantly being revised and adapted. In three days from **8 to 10 February 2022**, this PRACE online course will teach the basics and many tricks and concepts that simplify the everyday coding of researchers. [Information & registration](#)

## Coding for parallel systems

Besides OpenMP, OpenMPI also helps to get parallel computer systems with hundreds or even thousands of computer nodes going. From **8 to 10 March 2022**, specialists from LRZ, Konwihl and the Computing Centre of the University of Erlangen will reveal tricks for their own algorithms and introduce the basics of supercomputing. Participants will also learn which systems they can use for computing in Germany and how best to address them. [Information & registration](#)

## Programming and addressing GPU

Graphic Processing Units, or GPUs for short, expand the possibilities in computing and programming. They are suitable for artificial intelligence and smart applications and are activated with the programming languages, CUDA C, OpenACC, OpenMP or stdpar. On **14 and 15 March 2022**, participants will learn the basics of programming, but also how to control their own codes and systematics. [Information & registration](#)

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## 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 [here online](#). Employees of universities and authorities can register their interest under the mail addresses [<althardware@lrz.de>](mailto:althardware@lrz.de) or for furniture under [<GM@lrz.de>](mailto:GM@lrz.de). The equipment and furniture are free of charge.

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## 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!

### [Administrato for CRM-System](#)

[IT Specialist](#) for the maintenance of LRZ's communication networks

[IT Specialist System Integration](#) for the management of MAC clients und mobile devices

[Site Reliability Engineers](#) for the development of the Data Science Archive and storage solutions

[System Engineer](#) for the development of cloud storage solutions

[Software Developer DevOps](#) for IT service management tools

[IT System Specialist](#) for Webhosting

[IT Specialist](#) for security and penetration testing

[IT Specialist](#) for IT security, analysis and protection against cyberattacks

[Programming Specialist](#) for Supercomputing Applications and GPU  
[HPC Expert with focus on Biomedical](#)  
[HPC Expert with focus on Bio-Chemistry and Life Science](#)

[Trainee for System Electronic](#)  
[Trainee for IT Specialist System Integration](#)

[Student Assistant](#) for media design  
[Student Assistant](#) for development of ITSM software  
[Student Assistant](#) for web backend and the BAYSICS portal  
[Student Assistant](#) for service desk

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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

- 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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## INFORMATIONS & IMPRINT

- The LRZ Newsletter is published in German and English. You can find the latest and former editions on the [LRZ-Website](#).
- You have problems displaying the newsletter? Please send a description of your problem to <pr-team\_AT\_lrz.de>. Thank You!
- 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](#).

### Editor:

Leibniz-Supercomputing Centre (LRZ) of the Bavarian Academy of Science and Humanities  
Boltzmannstraße 1  
D-85748 Garching  
Phone: +49-89-35831-8000  
Telefax: +49-89-35831-9700  
E-Mail: pr-Team\_AT\_lrz.de; newsletter\_AT\_lrz.de  
Twitter: [LRZ\\_DE](#)  
LinkedIn: [Leibniz-Rechenzentrum](#)

### Editorial Office: PR-Team

E-Mail: pr-team\_AT\_lrz.de; newsletter\_AT\_lrz.de  
Photos: E. Mayer/LRZ; SC21; P. Lagson/Unsplash; Fly d'Art/Unsplash; S. Vieser/LRZ, D-Wave; MQV; Deutsches Museum; Cisco  
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