



*LRZ-Newsletter February 2022: Enjoy reading and look for the signs of the springtime*

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## NEWS

### “We have quiet a lot planned for 2022”

New technologies, more services: Most recently, the Leibniz Supercomputing Centre (LRZ) has made its presence felt primarily in the area of quantum computing. But it is also working on many innovative IT services. "As with all technologies, the LRZ is always about providing reliable IT services for science and research," says Prof. Dr. Dieter Kranzlmüller, Director of the LRZ. The data centre in Garching has a busy year ahead of it, and users of its services can look forward to many improvements and innovations. "We are working at full speed to optimize and modernize many LRZ services," says Prof. Dr. Helmut Reiser, Deputy Director of the LRZ. „For more stable, faster internet connections, we are in the process of replacing more than 1,000 of our 6,000 WLAN access points. We will modernize our router backbone to increase resilience. In addition, the topic of information security is becoming increasingly important." Kranzlmüller and Reiser talk about what new services and security measures LRZ users can expect this year in an interview on the LRZ website. They also talk about their personal wishes for the year 2022, when the data centre in Garching celebrates its 60th birthday. [To the complete interview.](#)



*Prof Dieter Kranzlmüller (left) and Prof Helmut Reiser of LRZ.*

### “Driving forward the digitisation of TUM”

Alexander Braun, an IT expert with a doctorate in civil engineering, is the new executive vice president for digitisation and IT systems at the Technical University of Munich (TUM). The University Council elected him to the Presidential Board for a three-year term at the end of 2021. Braun thus assumes the role of Chief Information Officer (CIO): "On the one hand, it's about ensuring the operation of our IT infrastructure and scaling and developing it for future requirements," says [the new CIO](#), describing his duties. "In addition, I'm in regular exchange with our schools and faculties in order to take their needs for teaching and research

into account in our IT strategy in a meaningful way." Braun is a true "Münchner Kindl", studied civil engineering at TUM, earned his doctorate on digitisation in civil engineering and headed a research group at the Chair of Modeling and Simulation. As CIO, he succeeds Dr. Hans Pongratz, who was appointed professor at TU Dortmund University and moved to the Foundation for University Admission as managing director in fall 2021. As an executive, Braun has helped develop the digitisation of TUM's administration in numerous projects and knows the university's internal processes. As CIO, he will work closely with the Leibniz Supercomputing Centre (LRZ). "My biggest challenge as CIO at the moment is to drive forward the digitisation of TUM and its associated administration," he says. "At this point, the LRZ is of course also a reliable partner for network operations and the many other services in the area of the web, high-performance computing and more." You can meet TUM's new CIO in [our interview](#).



### Women's Power for Science

They rebuild crystals in the lab, develop new technologies in clean rooms, tinker with processors, design software: More and more women are choosing to study mathematics, computer science, natural sciences and technology, the so-called STEM subjects. As many as [28% of university graduates](#) in engineering are female, and as many as 40% in computer science. Many of them stay in research: Because, as a video of the scientists at the [Origins Cluster of Excellence](#) shows, it's fun, brings you in touch with interesting people all over the world, because persistence, but also ideas are in demand, as well as team spirit and curiosity.

## #WomenInScience



But as in business, too many women's careers break off when family planning begins and they have children: While women achieve parity at the bachelor's and master's levels, with 45% to 55% of degrees worldwide, according to the UNESCO Institute for Statistics, they remain underrepresented in the top echelons of universities and research institutes. Female founders receive significantly less venture capital, and female researchers speak less frequently at conferences. This must change - as the Women in Science Day on February 11 urges, as does the European Union in its research programs: "As long as women and other underrepresented

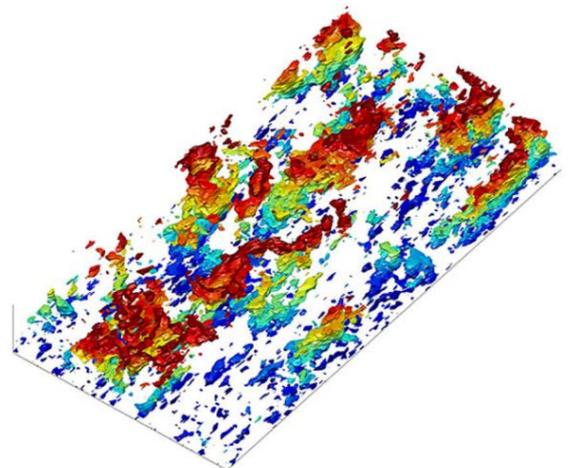
groups do not have their place at the table, Europe will not succeed in making full use of its human capital capacities," the [Horizon2020 program states](#). "If women remain underrepresented, this can lead to suboptimal outcomes." As a result, applications now include a focus on diverse team composition and receive more points when women lead projects. LRZ supports these demands, is committed to the Diversity Charter as an employer. And has participated medially in Women in Science Day. Between now and International Women's Day on March 8, it is also ensuring visibility on its social media channels for young female researchers and scientists who are changing supercomputing or using it to produce groundbreaking findings that can improve the world. You can discover 7 exciting personalities and interesting fields of work:

- [Bengisu Elis](#) researches for supercomputing and improves node communication
- [Prof. Dr. Alice Agnes Gabriel](#) is dedicated to seismology, develops the formulas for calculating earthquakes and their impact, and was able to solve the mystery of why the 2018 tsunami in Palu, Indonesia, caused so much damage just by analyzing data.
- [Daniëlle Schumann](#) experiments with quantum annealers and develops new algorithms for them or adapts existing codes to the new computers
- Consultant [Dr. Tanja Hanauer](#) knows that people don't like to follow rules - and has therefore created a set of rules on how companies can visually remind employees of safety measures:
- [Sophia Grundner-Culeman](#) likes to puzzle and has therefore devoted herself to cryptography and IT security. She is developing ways to encrypt digital information and is also working on quantum computers, which she claims can crack ciphers more easily:
- [Elisabeth Mayer](#) illustrates research results with the means of visualisation and virtual reality. She builds presentation rooms on the Internet and simplifies workflows for the visualization of simulations in a team:
- [Ivana Jovanovic-Buha](#) uses mathematics and supercomputers to check the models on which Bavaria's flood warning systems are based, for example. With her work, she ensures more precise findings and thus better forecasts.

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### Calculating turbulences more easily

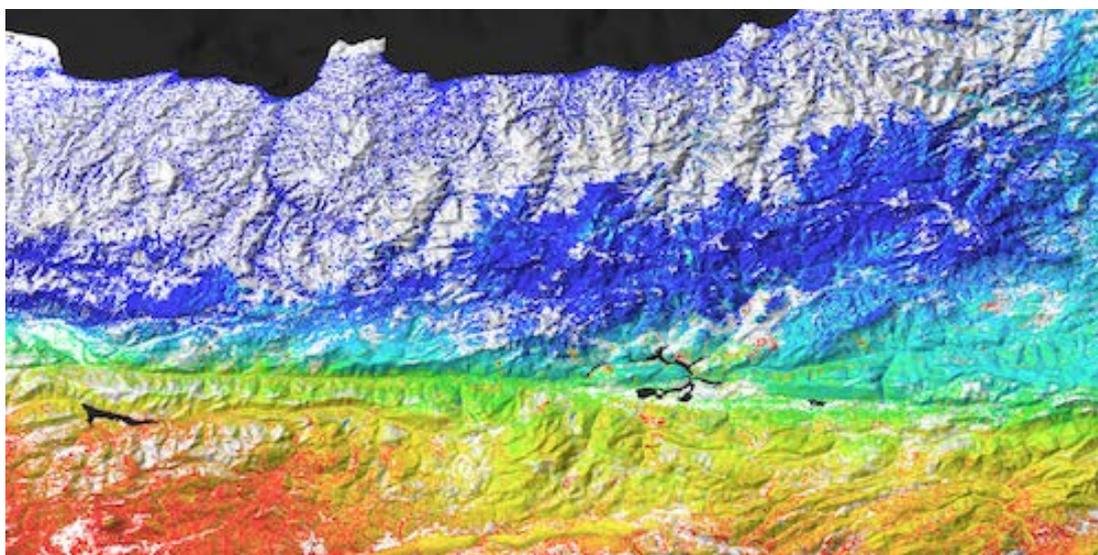
Simulating turbulence is a challenge even for supercomputers: The team led by [Dr. Martin Oberlack](#), professor of mechanical engineering and expert in fluid dynamics at Darmstadt University of Technology, set out to do something fundamental and made a breakthrough. They wanted to model the largest turbulence situation to date on the SuperMUC-NG at the Leibniz Supercomputing Center (LRZ) while simplifying the underlying calculations. Turbulence is statistical because we observe random behaviour," Oberlack explained in a report of [Gauss Centre for Supercomputing \(GCS\)](#) report on his research. "The Navier-Stokes equations describe it very well, and with them we can study the whole range of a turbulence down to the smallest scales, but that's also the problem - all scales play a role in turbulent motion, so we have to resolve them all in simulations." The many small vortices pose particular problems; calculating them overwhelms many a supercomputer. In vehicle construction, engineers therefore measure the turbulence of wings or car bodies in wind tunnels, but this is time-consuming and expensive. Oberlack and his team therefore tried to solve the turbulence calculations differently - they came across the [symmetry law of mathematics](#) and the logarithmic wall law, an aerodynamic law from the early 20th century by Theodore von Karman. These led to the conclusion: To represent a turbulence, it is not necessary to calculate each vortex



individually, but average values are sufficient. In order to prove this thesis, the 311,040 nodes of the SuperMUC-NG calculated together for about three years. Although this only proves the simplest case of turbulence on a flat surface, Oberlack's team is already working on new, more complicated scenarios - and aerodynamicists or engineers in vehicle construction can look forward to soon having a new, simpler set of formulas for calculating turbulence at their fingertips. (The picture of Sergio Hoyas shows UV-structures in the logarithmic layer, coloured by their distance to the wall.

## “We want to make the LRZ better known in the geophysics community”

Just under 10 percent of the research projects for which computing is done at the Leibniz Supercomputing Centre (LRZ) belong to geophysics and seismology. But many more are to come: That is why the LRZ is sponsoring the annual meeting of the [Deutsche Geophysikalische Gesellschaft \(DGG\)](#) from March 7 to 10, 2022, where geophysicists will exchange experiences and findings, discuss developments, and also new technologies. They can also get to know the computing centre based in Garching, its services as well as simulations and visualizations online. The focus is on the [mentoring program](#) for working groups that want to work with the High Performance Computers (HPC). "In the [CXS Lab](#), researchers find experts from different scientific domains," explains André Kurzmann, who holds a doctorate in geophysics. "Generally, questions about software, codes and large data sets come up in about half of all HPC projects. Each project gets its own mentor, and we take care of technical problems, such as when implementing applications or when memory requirements increase." The LRZ is still supporting geophysics primarily with modeling and simulation, but artificial intelligence methods are also likely to be in demand soon, Kurzmann says in an interview.



Satellite data illustrate tectonic plate shifts near Ordu/Turkey. Graphics: DLR/Sar4Tec

*Why does geophysics need supercomputing? What does it compute on the HPC resources of the LRZ?* **Dr. André Kurzmann:** Geophysics and seismology are classically among the pioneers in supercomputing, because for decades they have been processing a wide variety of data, for example on the history of the Earth, the composition of the Earth's crust, earthquakes and tsunamis, or from satellite data, and using them to calculate ever larger, more accurate models. In the meantime, the simulations are spatial, and the necessary calculations take days even on supercomputers. [Prof. Dr. Hans-Peter Bunge](#) from Ludwig-Maximilians-Universität and his team have simulated the development of the continents for many years, and today the model is three-dimensional and calculated in the highest resolution. With the help of SuperMUC-NG, [Prof. Dr. Alice Gabriel](#) from LMU and her research group were able to clarify why the tsunami that followed the earthquake in Palu, Indonesia, was so exceedingly strong.

And last but not least, the LRZ built [terabyte](#) together with the German Aerospace Center, via this high-performance platform for data analysis, remote sensing data are to be immediately analyzed on our supercomputers.

*Does geophysics already rely on artificial intelligence methods, which also require computing power?*

**Kurzmann:** The focus of geophysics projects at the LRZ is still on calculations and simulation, but machine and deep learning or pattern recognition are interesting in the field of tomography, for example, when geological layers are examined and visualized with radio waves. Artificial intelligence is also advancing the study of earthquake waves or remote sensing data.

*The CXS Lab at LRZ supports researchers in geophysics with a mentoring program. Why?* **Kurzmann:**

Computing time and supercomputing are valuable, we want to use them efficiently and therefore we support research teams. In the CXS Lab, they find experts from various scientific disciplines. In general, about half of all HPC projects involve questions about software, codes and large data sets. Each project is assigned a contact person. [Mentors](#) take care of technical problems, for example when implementing

applications or when memory requirements increase. And they often push the computing work by asking questions about the current status of a project. The program is very well received by researchers.



Where do geophysicists particularly often need help? **Kurzmann:** Geophysicists are do-it-yourself researchers who develop their own software and algorithms. They usually need help with specific problems, such as porting their code to the supercomputer or optimizing their algorithms when the workload of thousands of computational cores doesn't work.

You're a geophysicist yourself - which projects do you particularly enjoy as a mentor? **Kurzmann:** The projects where I can provide advice and practical support and maybe even take a project further. Sometimes projects get into one-way streets, so when I can help steer research questions in a new direction, it makes me happy. At the interface between medium-sized and large-scale projects, there is also often a need for advice on applications or technology. Here, too, I can contribute my experience and push projects forward.

The LRZ is presenting itself at the annual meeting of the German Geophysical Society: What are you presenting and why? **Kurzmann:** We want to make the LRZ better known in the seismology and geophysics community. To this end, we are presenting the SuperMUC-NG and the HPC resources, our services and successful work online on a special website. We also show how researchers can present their projects in the Mozilla Hubs. By the way, the [simulation of Professor Bunge](#) mentioned at the beginning can already be seen there.

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## Figures of the Month

At the beginning of the year, the Leibniz Supercomputing Centre (LRZ) installed the 15,000th PC within the Munich Scientific Network (MWN); in the meantime, the number of PCs has already grown further to 15,065. But Apple devices are also in use at Munich's universities and colleges: So far, 1695 Macs have been set up at 24 faculties and departments. Because of the pandemic, many of these devices are not currently in regular use, but their number will continue to rise, the LRZ order book shows.



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## WORKSHOPS & EVENTS

### Annual Meeting of the German Geophysical Society

Exploring earthquakes or the nature of the Earth's crust, analyzing remote sensing data from satellites: from **March 7 to 10, 2022**, the 82nd Annual Meeting of the German Geophysical Society will focus on developments on the Blue Planet. The ÖRZ is a sponsor of this event, which will also be dedicated to data analysis and the latest technologies for modeling and computing measurements.

[Registration](#) is still possible

### 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](#)

### Quantum Computing in Data Centres

How do data centers actually use the future technology of quantum computing? On behalf of technology provider Atos and the startup IQM Quantum Computing, the market research company IDC asked scientific and commercial institutions. Raghunath Koduvayur, IQM's head of communications, will present the most interesting results at the Bavarian Quantum Computing eXchange network (BQCX) meeting on March 9, 2022. And Dr. Jan Goetz, co-founder of IQM, looks afterwards at how quantum processors could extend and complement the next generation of supercomputers. The BQCX virtual meeting starts at 4 p.m., more information at [www.bqcx.de](http://www.bqcx.de), registration at [bqcx@lrz.de](mailto:bqcx@lrz.de).

## Introduction to the HPC systems at LRZ

Using fluid mechanics as an example, you will get to know the Linux cluster of the LRZ: In the crash course on **March 9, 2022**, learn how to log in, set up a user environment, load files and folders into the system, and plan applications using SLURM. The practical exercises will focus on the programs ANSYS CFX as well as StarCCM+, with which especially computations of fluid mechanics are possible. [Information & registration](#)

## 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. The [EuroCC GCS](#) course and bootcamp on **14 and 15 March 2022** will teach the basics of programming, but also how to control your own codes and systematics. The LRZ organises this course together with the HLRS, Nvidia and OpenACC. [Information & registration](#)

## Quantum Computing – Technology and fields for application

[World of Quantum](#) is the name of a new trade fair in Munich, which will take place from **April 26 to 29, 2022** at the Messe München. In addition to companies and manufacturers, the Munich Quantum Valley (MQV) and the Quantum Integration Centre (QIC) of the Leibniz Supercomputing Centre (LRZ) will also present themselves at this exhibition. In the MQV, Munich universities, research institutes such as the LRZ, and companies are conducting research on the technology of the future and are also setting up training programs. At the World of Quantum, the consortium will present itself to a broader public for the first time. The new trade show is part of the already well-known Laser-Photonics.

## Computer centers - a place for girls

Drawing girls' attention to exciting careers involving information technologies or in computer science, getting them excited about technology, and offering practical insights into the day-to-day work of computer specialists: [Girl's Day](#) will take place again on **April 28, 2022**. As in previous years, the Leibniz Supercomputing Center (LRZ) will be taking part again in 2022. Girl's Day will take place virtually. At the LRZ, participating young women will be taken into virtual worlds and can build their own rooms in the Mozilla Hubs. [Registrations](#) start at the end of March

## Introduction to the HPC systems at LRZ

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

## Learn C++ and programme with it

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

## Programming for parallel systems

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

## ANSYS Fluent for Computational Fluid Dynamics

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

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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 [online](#). Here you can also read where to direct your interest. The equipment and furniture are free of charge for institutes,

chairs and other research institutions.

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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!

[Software developer DevOps](#) for IT service-management tools  
[Manager](#) for CRM system  
[Programmer](#) for IoT reserach projects  
[IT specialist / system engineer](#) for storage services  
[Technicl employee](#) for maintenance of communication networks

[HPC software engineer](#) for quantum software stack  
[IT spezialist oder system consultant](#) for more factors authentication  
[Scientific employee](#) for technical vulnerability-management  
[Scientific employee](#) for the security incident management  
[Scientific employee](#) for managed security services  
[IT-system administrator](#) for the development of operating- ans security concepts for Windows client systems  
[IT spezialist](#) for data security

[Projekt manager media design](#) for the relaunch of websites (BADW)  
[Clerk for Licences](#)

[Student Assistant](#) for software development of ITSM  
[Student Assistant](#) for the licence team  
[Student Assistants](#) 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](#).

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