*LRZ-Newsletter January 2022: A happy, successful new year 2022, stay curios*

# NEWS

## Help with Supercomputing

Addressing as many SuperMUC-NG compute nodes as possible simultaneously with algorithms is an art. But it is also necessary in order to use computing time efficiently, senseful and save energy. When dealing with data sets, memory issues also often cause problems. In about half of the computing projects for the supercomputer at the Leibniz Supercomputing Center (LRZ), questions arise about software, codes and storage. "That's why we've been intensively supporting computational projects since the end of 2019, and we provide researchers with a mentor," Gerald Matthias says, a PhD astrophysicist and head of **Computational X Support at LRZ**. "For users, the focus is on simulations and data, not necessarily on computing. They are, after all, primarily scientists who develop applications for their projects." The **mentors** help optimize codes, explain technology or keep projects running by reminding participants of requested computing times. Data specialist Dr. Yuanyuan Wang from the Technical University of Munich (TUM) was helped with access to the LRZ's data storage system (DSS) when analyzing satellite data. The research group of physicist Prof. Francesco Knechtli from the University of Wuppertal was helped by mentors with simulations and calculations of hadrons. Read more about the LRZ's Mentor:innen program and who uses it **on the LRZ website**

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## Car Racing with Artificial Intelligence

Driving around the racetrack at 218 or even 270 km/h. What is pure routine for Formula 1 drivers is a sensation for a racing car that drives autonomously: The car is kept on course only with the help of sensors and computers and, thanks to artificial intelligence, reacts independently to curves or obstacles even at high speeds. Also with the support of the Leibniz Computing Center (LRZ), the two TUM Chairs of **Automotive Engineering** and **Automatic Control** are developing and testing software and systems for autonomous driving vehicles. Motorsports is a vehicle to try out the technology on race tracks. For this purpose, modified race cars are equipped with the software. The **TUM Autonomous Motorsport team** has been extremely successful recently, not only achieving top speeds with its bolide, but winning awards in Indianapolis and in Las Vegas. "We are super happy with the results, our goal was 200 kilometers per hour, and we achieved that," says team manager Alexander Wischnewski. "During the races, we learned a lot about how parts of the software interact. Research projects often focus on a few specific or isolated issues; here we have the chance to look at the problems of a complete driving system." For a report on Team Autonomous Motorsport's work and how autonomous driving assistance is now hitting the roads, **click here.**


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## Design Process and Secure Applications

Sharing practical experience: The security team led by **Stefan Metzger,** Chief Information Security Officer of the Leibniz Supercomputing Center (LRZ) in Garching, is contributing two papers to the **29th conference of the Deutsche Forschungsgemeinschaft (DFN).** From February 2 to 4, the conference in Hamburg and online will focus on "Security in Networked Systems". During the DFN conference, LRZ specialists will demonstrate how organizations can set up an effective management system, for example for information and service security, and how they can establish two- or multi-factor authentication (MFA).

Data and IT service security starts with documenting processes to track results. Procedures can be systematized and assessed on the basis of the description of necessary processes and technology. Documentation of processes and results is mandatory for quality assurance. In this way, companies create a basis for pursuing goals and improving measures. "Anyone who starts with documentation should focus on the organizational and strategic aspects of the processes and initially establish a process-oriented mindset," explains Michael Schmidt, who is responsible for IT service management at the LRZ. Instead of complex, specialized management system tools, the LRZ experts recommend simple tools that are already available in the company, if possible: "Management system tools require specific information and figures to represent processes," Schmidt continues. "They thus direct

content, but in this way the danger grows that outdated processes are hidden behind elegant software functions." To prepare for its **certifications (ISO/IEC 20.000 and ISO/IEC 27.001),** the LRZ relied on Confluence wiki software. The text-based program made it possible to describe rules and procedures, and also to easily convert processes into workflows. Above all, however, the departments and teams became aware of strategies and the need for change while writing down the processes: "With a management system, it is more important than sophisticated technology that everyone involved understands it quickly and thinks along with it," says Schmidt, summing up LRZ's experience. "This then also serves information and service security, makes the organization and critical infrastructure visible."

The second DFN talk is about IT security in practical and technical terms. Passwords alone do not make tools and services more secure. Many universities are therefore hoping for **two or multiple factor authentication (2FA/MFA),** which the LRZ introduced internally a year ago. Jule Ziegler, Miran Mizani, Daniel Schmitz, Stefan Metzger and Helmut Reiser describe not only how the catalog of criteria for the new system came about, but also how they chose and integrated the one that suited the LRZ out of 70 possible openly available or commercial solutions. Employees now no longer log in to LRZ systems using only a personally chosen password, but for critical web applications, services and systems they also use a random one-time password that generates a security token. Thanks to the management system and, above all, the documented processes, new organizational and technical procedures could be smoothly integrated into the IT service and information system. The LRZ is now bringing this experience to the Bayern2MFA project funded by the Free State of Bavaria: Together with the University of Augsburg, the computing center is advising Bavarian universities and research institutions on how to better secure their systems with the help of a 2FA and how to introduce it in practice.

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## "New Quality in HPC for Science and Research"

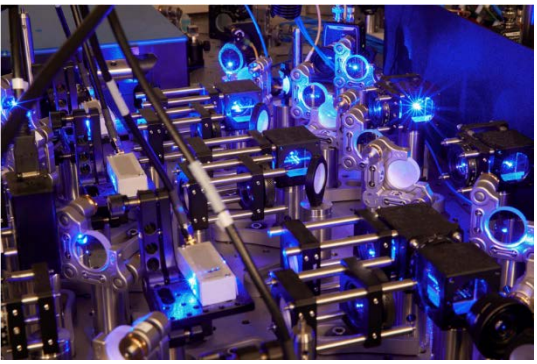
Powerful computing systems are no longer needed in science only for simulations and model calculations. Artificial intelligence methods are bringing new tasks to the High Performance Computing or HPC centers of universities and research institutes. The federal government is responding to this with the **National High-Performance Computing (NHR) program**. Nine university computing centers have been selected for the NHR and will now receive nearly 63 million euros per year for ten years to provide HPC resources as well as educational and consulting support. "Existing computing capacities and operating infrastructures played a role, as did expertise in HPC, educational offerings, competent user consulting, and proven research foci in the application disciplines," reports **Prof. Dr. Gerhard Wellein in an interview,** who heads the Computing and NHR Center at Friedrich Alexander University and is a member of the board of the NHR association. The **NHR** has already started its work, researchers can already apply for computing time at the NHR centers nationwide, and a common online platform for applications is in preparation. Read more about the NHR, the participating universities and the awarding process in the **LRZ interview.**

**The NHR Centres**

| NHR-Zentrum | Standort(e) | Zugang zu Rechenzeit |
|---|---|---|
| NHR4CES@RWTH | Aachen | **www.nhr4ces.de/index.php/applying-for-computing-time/** |
| NHR4CES@TUDa | Darmstadt | **www.nhr4ces.de/index.php/applying-for-computing-time/** |
| NHR@Göttingen | Göttingen | **www.hlrn.de/nutzungsportal** |
| NHR@Zuse | Berlin | **www.hlrn.de/nutzungsportal** |
| NHR@FAU | Erlangen | **hpc.fau.de/nhr-vormerkliste/** |
| NHR@KIT | Karlsruhe | **www.nhr.kit.edu/resources.php** |
| NHR@TUD | Dresden | **tu-dresden.de/zih/hochleistungsrechnen/zugang** |
| PC2 | Paderborn | **pc2.uni-paderborn.de/go/hpc-proposal** |
| Konsortium Süd-West | Frankfurt, Saarbrücken, Mainz, Kaiserslautern, | **https://www.rz.uni-frankfurt.de/hrz?legacy_request=1** |

## Constructing and Using Quantum Computers

Robust qubits and algorithms that work in hybrid systems: The Bavarian Quantum Computing eXchange community (BQCX) kicked off 2022 with talks by Ben Bloom, Chief Technical Officer (CTO) of the Berkeley, US-based startup **Atom Computing,** and Martin Ruefenacht of the quantum computing team at Leibniz Supercomputing Center (LRZ), both of whom touched on issues related to building quantum computers and operating them in supercomputers.



Bloom, who holds a doctorate in physics and is a co-founder, demonstrated how Atom Computing is preparing a quantum platform with 100 qubits from **neutral atoms** consisting of an equal number of protons and electrons. To do this, the startup uses lasers of different wavelengths to process strontium-87 atoms and stabilize them as qubits in a vacuum. Additional lasers then excite these nuclear spin qubits to interact, which also leads to entanglements of the qubits. These entanglements are necessary for computing and should be maintained for as long as possible. Atom Computing estimates that the coherence time during which the qubits remain in this quantum state is up to 40 seconds. This is long compared to qubits made of superconductors or ion traps, which can only be activated for fractions of a second. In addition, the nuclear spin qubits can be flexibly controlled and selectively connected. In this way, Atom Computing aims to soon develop **larger platforms and processors.** "It's a promising technology," Xiaolong Deng, a quantum physicist with a PhD from LRZ, said after the lecture. "With atoms, **natural qubits** are created that are more robust and easier to control. We're working with the Max Planck Institute for Quantum Physics to try to create and stabilize qubits from other materials, so that's where these experiences and technologies are useful."

But how to deal with the new quantum processors? To make the future technology controllable and programmable, the first processors will soon be integrated into supercomputers, including at LRZ: "We suspect the integration of quantum computing could help improve supercomputing and vice versa. But this will not succeed with all problems," Ruefenacht clarified in his talk, referring to the differences between the two technologies. Classical and quantum computing are based on different physical principles, logics and solution approaches, and also (still) on different levels of computing power. Consequently, both require different algorithms. There are still only a few algorithms for quantum computing, but many for supercomputing. The only link between the two worlds - future hybrid algorithms will also be based on mathematical models. "A solution could lie in their composition," Ruefenacht continues. "Probably, when developing hybrid codes, we will have to think carefully about which parts of a problem are better solved with classical computing, and which, meanwhile, with quantum computing." The trick, then, will be to cleverly decompose computing tasks and define them as reciprocal steps for both systems.

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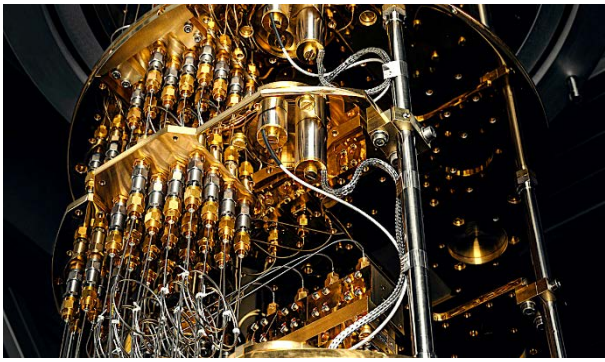
## Researching Quantum Computing

Bavaria's **high-tech agenda** is moving forward: In order to advance the research and development of quantum computing, the initiative **"Munich Quantum Valley" (MQV)** has now been formed as an association. The founding members are the Friedrich Alexander University, Erlangen-Nürnberg, the Ludwig Maximilian University and the Technical University in Munich, the German Aerospace Center, the Fraunhofer and Max Planck Societies as well as the Bavarian Academy of Sciences and Humanities with its institutes, the Walther Meissner Institute and the Leibniz Computing Center (LRZ). The goal of the MQV association is to accelerate the translation of scientific findings into practical products and market-ready technology. To this end, a center for quantum computing and technology is to be established over the next five years, as well as a technology park. The MQV is financed by subsidies from Bavaria and the federal government.



The LRZ is bundling its quantum activities in the **Quantum Integration Centre (QIC).** "The strategy of the QIC is based on three pillars: We will provide quantum services to researchers, advise and train users and, as an academic computing center, accompany, research and help shape the further development of this technology of the future," says Prof. Dr. Dieter Kranzlmüller, director of the LRZ. Last year, the academic computing center in Garching already received **funding from the German Federal Ministry of Education and Research** (BMBF) for the purchase of a first quantum system and was also able to acquire remarkable research projects together with universities and institutes. "We are now opening the door to the quantum era," Kranzlmüller continued. "The integration of quantum into HPC systems can enormously enrich science and research and strengthen the power of the next supercomputers." Most of the research projects of the LRZ and its partners in the MQV are aimed at designing a Munich Quantum software stack that will make complete quantum systems easier to use. It will also be used to develop programming and software environments for a wide variety of application areas. Another project: Quantum computing is intended to complement supercomputing and give more power to the next exascale systems. Current projects with LRZ participation:

• **Digital-analog quantum computing, DAQC:** The German Federal Ministry of Education and Research (BMBF) is funding the construction and integration of a superconducting quantum system that mixes different technical designs, digital and analog quantum computing. In this project, the LRZ is collaborating with the German-Finnish technology company IQM, the chip

manufacturer Infineon, and the Austrian company ParityQC, as well as with the Forschungszentrum Jülich and the Freie Universität Berlin. The goal is a digital-analog processor with a calibration and control mechanism that will be integrated into the HPC environment as an accelerator.

• **Quantum computer extension by exascale HPC, Q-Exa:** With funding from the BMBF, a first quantum processor with at least 20 qubits has already been procured from IQM for this project. This is to be integrated into the next planned supercomputing generation. The LRZ is cooperating on this project with the startups IQM and HQS Quantum Simulation from Karlsruhe, as well as with Atos and the company science + computing in Tübingen.

• **Quantum-enabling Services and Tools for Industrial Applications, QuaST:** Funded by the Free State of Bavaria, QuaST deals with application software for quantum technologies, works on platforms for their use and also offers qualification opportunities. The Fraunhofer Institutes for Cognitive Systems (IKS), Applied and Integrated Security (AISEC) and Integrated Circuits (IIS) as well as the two Munich universities LMU and TUM and the LRZ contribute their expertise to this project.

• **Bavarian Competence Center for Quantum Security and Data Science, BayQS:** Quantum computers are considered fast computers - will also bring benefits to industry, but also risks. Funded by the Free State of Bavaria, BayQS is therefore working on software for this future technology, wants to work on platforms for its use and also offers qualification opportunities. The Fraunhofer Institutes for Cognitive Systems (OKS), Applied and Integrated Security (AISEC) and Integrated Circuits (IS) as well as the two Munich universities LMU and TUM and the LRZ are contributing their expertise to this project.

• **Munich Quantum Valley, MQV:** Within the framework of this broad and long-term promotion of the quantum technology location Free State of Bavaria, the parent company of LRZ and Walther Meissner Institute, the Bavarian Academy of Sciences, the two Munich universities of excellence LMU and TUM, furthermore the Friedrich Alexander University Erlangen Nuremberg, the Fraunhofer and the Max Planck Societies as well as the German Aerospace Center have joined forces. A lively cluster of research, companies and educational institutions for quantum computing is emerging in the MQV. The LRZ is involved in two subprojects of the MQV, **Q-DESSI** and **QACI:** Here, a software stack from firmware to programming environment and access portals is to be created, as well as the connections of quantum systems to supercomputing resources. In addition, users will receive support in the development of further quantum programmes.

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### The Master of Models

The basis of simulation software and algorithms are mathematical models. These are regularly extended by more parameters and measured values, but still need to be maintained and checked. A task for computer scientists with a penchant for mathematics: **Ivana Jovanovic-Buha** is currently working on her doctorate at the **Chair of Scientific Computing,** part of the Department of Computer Science at the Technical University of Munich (TUM). She refines existing models by quantifying uncertainties and thus minimizing them step by step. The HPC cluster CoolMUC of the Leibniz Supercomputing Center supports her in this. Who benefits from this? All of us. Thanks to Ivana's work, the Bavarian State Office for the Environment and Consumer Protection now has software that can predict floods and heavy precipitation more accurately. This means better and earlier warnings are possible. The scientist told the LRZ enthusiastically and vividly about her tasks - **a lesson in modeling and the portrait of an exciting personality** you should get to know.

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## WORKSHOPS & EVENTS

### Searched – HPC Software for GPU

The **Competence Network for Scientific High Performance Computing in Bavaria (KONWIHR)** promotes software for High Performance Computing (HPC) from Bavarian colleges and universities and is increasingly looking for projects that require porting to Graphic Processing Units (GPU) until **March 1, 2022.** Smaller projects with a duration of up to three months and a funding volume of up to 10,000 euros as well as large projects with a duration of up to 12 months and a funding volume of up to 50,000 euros are particularly in demand. Background: the latest acquisitions at the computing center of the Friedrich-Alexander University in Erlangen, the Center for National High Performance Computing NHR@FAU, and at the Leibniz Computing Center (LRZ): While the **Alex cluster of the NHR@FAU** relies on 460 GPUs from NVIDIA, the **SuperMUC-NG**at the LRZ is currently being upgraded with **1000 Ponte Vecchio GPUs** from Intel. These resources are intended to be better utilized. They enable GPU programming models such as OpenMP, OpenACC, OneAPI, SYCL or CUDA. Applications can be submitted until March 1 at info@konwihr.de. The second annual deadline for submission is **September 1.**

### 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.**

## Securing the Networks

Log4Shell and many headlines from companies regularly show: the networked world is insecure. On **February 2. until 4, 2022,** the German Research Network (DFN) will dedicate its 29th conference to the topic of "Security in Networked Systems". The LRZ will be represented with two presentations: The colleagues describe how two-way and multi-way authentication can be introduced in practice. They will also show how processes and procedures can be documented, for example, for certification without special tools in a company's communication system. **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**

## ANSYS for Computational Fluent Dynamics

Consisting of 12 lectures and about 5 practical exercises, this seminar, which starts on **February 21** and runs until **March 28, 2022,** introduces the use of the ANSYS Fluid Dynamics software package CFX. 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**

## Programming with Fortran

You need Fortran and you are not so familiar with this programming language? Then this three-day course from **February 23 to 25, 2022** will be helpful. Here you will learn to program with the Fortran 95 standard and get to know the first functions of Fortran 2003. In addition, the instructors will show you useful tools for debugging errors and checking syntax. You will also learn how to use compilers and libraries. **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, Konwihr 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**

## 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**

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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**

## 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
**Administrator** for the CRM system
**IT Spezialist / Systemingenieur** for storage services
**Technical Specialist** for maintenance of communication networks

**IT-Spezialist or scientific researcher** für IT-Security und fürs Schwachstellen-Management
**IT-Spezialist** fort he Multiple Factor Authentification
**IT-Systemadministrator** for development of operation and security concepts Windows clients
**IT-Spezialist** for data backups
**Scientific researcher** penetration testing

**HPC-Software Engineer** für HPC Storage
**Sientific researcher** for management of HPC resources und scheduling projects (LRZ & TUM)
**Sientific researcher** for computing architektures and hardware design (LRZ & TUM)
**Sientific researcher** für input/output aspects und hybrides HP-/quantum computing

**Trainee** system electronics

**Student assistant** media design
**Student assistant** for ITSM software developments
**Student Assistant** web backend and the BAYSICS webportal
**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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