



*Frohes Fest  
Happy Holidays*

*LRZ-Newsletter December 2021: Enjoy reading! We wish you happy holidays, an atmospheric end of year and a joyful start in 2022*

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## NEWS

### A Database for Service Optimisation

The Munich Scientific Network (MWN), wireless local area networks (WLAN), mail hosting, managed MACs and PCs: Behind every service provided by the Leibniz Supercomputing Centre (LRZ) for science and research are devices and network technology. They are inventoried in a central database, the [Configuration Management Data Base](#), or CMDB for short. "It contains hardware,



switches, monitors, routers, access points, but also items such as IP addresses of servers, i.e. everything that is necessary for the management of our IT services," says [Markus Gillmeister](#), computer scientist and responsible for user-related services at the LRZ. "This way we can keep track of everything, optimise our services and inform our customers in a more targeted and precise manner."

#### Transparency improves coordination

In the meantime, the [database lists](#) a total of 148,000 items, including almost 5,000 access points, 256 firewalls, 1,486 servers, the devices of almost 500 workplaces in the LRZ and at Munich universities, as well as 2,853 virtual machines. Four LRZ employees programmed the requirements for a uniform database that their colleagues had previously collected. The result was a long list - especially since each item in it is further specified, for example by the inventory number, with data on

invoice and warranty, on location and above all on the service to which it is assigned. The CMDB was developed for the certification of IT service management according to ISO/IEC standard 20,000, unites the contents of the most diverse documents, tools and lists that departments used to keep for themselves. However, it is more than just a list, it centralises information, shows the life cycle of devices, licences and dependencies between individual items, assigns these services and users and enables better internal coordination. "CMDB is a step towards the data-driven enterprise," Gillmeister explains. "Even though we still enter a lot of data manually, the database is already helping to automate services." If, for example, a firewall is set-up for a virtual machine, a tool in CMDB collects the necessary data on the network, server, necessary co-systems - and the protective measure can be activated with a few clicks. CMDB also stores whether it is still working.

#### Automated information and services

This enables control and management: if one of the 25 servers fails on which the groupware Exchange and the mail system run, the users of this service are notified. Before maintenance or when devices are replaced, users can now be addressed according to location thanks to the CMDB. The goal is for the LRZ systems to take over this task themselves one day: "We are feeling our way towards automated information," Gillmeister reports. "To do this, however, the CMDB data must be checked and optimised if necessary. We have entered it into CMDB from various systems and partly by hand, which unfortunately increases the error rate." Nevertheless - the advantages of CMDB speak for themselves: the IT departments of the Munich universities would like to access at least part of CMDB to keep track of equipment and services that institutes and chairs subscribe to from the LRZ. In the LRZ itself, the experts are already thinking about a status page: on it, traffic lights show how the IT services of the data centre are currently functioning. This service would also be fed mainly by the central inventory list CMDB. (vs)

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### Growth for the LRZ

The Leibniz Supercomputing Centre (LRZ) is growing with its tasks: in 2021, the [Future Computing programme](#) for exploring new supercomputing and high-performance computing systems took off. The [Quantum Integration Centre \(QIC\)](#) was opened. And -



with partner organisations - many new research projects from the high-tech agendas of Europe, Germany and Bavaria were attracted to Garching. "We are very happy about our success, it demonstrates that the LRZ enjoys a good reputation internationally, also among politicians and the public who fund us," says Dr. Jürgen Seidl, who heads Administration at the LRZ. "However, success comes with challenges such as the lack of space as well as a shortage of staff." New ideas are therefore in demand: the field of quantum computing alone will bring nearly [30 new colleagues](#) to the LRZ in the next few months. The library at Boltzmannstraße 1 in Garching is already being reduced in size, and corridors and halls are being converted to create more space for offices and workstations. [In the interview on the website](#) Dr Jürgen Seidl and Sabine Osorio, Head of Human Resources at the LRZ, report on how the growth at the LRZ can be organised and what innovations can be expected. "With every application we find more arguments

why experts would like to work at the LRZ," says Osorio. "Nevertheless, the LRZ must become more visible as an employer." For growth, the LRZ is also counting on digitisation and more flexible work schemes; working from home - introduced in the pandemic - is taking root and is now being supported with new tools.

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## Quantum strengthens supercomputing

Bringing quantum computing into everyday research and developing it further: The Leibniz Supercomputing Centre (LRZ) of the Bavarian Academy of Sciences and Humanities (BADW) is purchasing a quantum computer from the Finnish-German start-up IQM. The Federal Ministry of Education and Research (BMBF) is funding this purchase with more than 40 million euros. Goals of the project ["Quantum Computer Extension through Exascale HPC" or "Q-Exa"](#) for short: To further develop the computer, thereby accelerating High Performance Computing (HPC) and building up know-how on the information technologies of the future: "With the Q-Exa project, we are opening a new promising chapter on our path to the quantum computer 'Made in Germany'," says Federal Minister Anja Karliczek, explaining the investment (in photo left with Jan Goetz/IQM). "The integration of a quantum computer into the infrastructures of the Leibniz Supercomputing Centre holds enormous potential for science and industry, Q-Exa contributes to making the quantum computer concretely usable for users from science and industry."



**Stabilising future technology**

For Q-Exa, a 20-qubit computer based on superconducting circuits will be coupled with the LRZ's HPC resources for the first time in Germany. Supercomputers are now reaching performance limits that can hardly be overcome with existing processors or with the help of artificial intelligence. On the way to exascale systems that can process the growing amount of research data, hopes also rest on quantum computers. They not only calculate on the basis of 0 and 1, their smallest computing units, the qubits, assume additional states and are thus supposed to process larger volumes of data in a shorter time. However, they are still difficult to stabilise, and basic programming environments and software for control and monitoring are still lacking. In the interaction of supercomputing and quantum computing, the new technology should therefore become suitable for everyday use and controllable, and on the other hand, HPC can thus reach higher performance levels: "Q-Exa is a key project for our activities in the LRZ Quantum Integration Centre and within the Munich Quantum Valley," says Prof. Dr. Dieter Kranzlmüller, Director of the LRZ. "The integration of quantum computing into supercomputers, especially at the exascale level, will accelerate research and opens up new opportunities for science and industry."

### Optimising and building know-how together

[Q-Exa's strategy](#) is co-design and cooperation: the 20-qubit quantum computer is supplied by the [Finnish-German startup IQM](#), with which the LRZ is already collaborating on in other research projects. "Together we are working to make European technology competitive and to develop the most promising hardware solutions for quantum computing here in Germany," says Dr Jan Goetz, CEO of IQM. Also involved in Q-Exa are Atos, a provider of HPC and quantum systems, and HQS Quantum Simulations, one of the leading providers of quantum algorithms for the chemical and pharmaceutical industries. With these partners, the LRZ will optimise both quantum and supercomputing. "Only by combining the world's most powerful computers with the potential of quantum computing will we be able to make the next big leap in supercomputing," Kranzlmüller continues. "Within the framework of Q-Exa, as a national supercomputing centre, we can not only have a significant impact on HPC, but also on the future technology of quantum computing - an exciting challenge." You can watch a [recording of the official press conference](#) with minister Anja Karliczek (from about second 20:00), and numerous media also reported on the first quantum computer: p.e. [Die Zeit](#), [Heise](#), [Businesswire](#), [The Quantum Insider](#), [All Electronics](#), [The Deep Tech Insider](#).

## Quantum Computing – a survey

Quantum computing, along with new memory and processor technology, is considered an important future technology for 16% of the supercomputing centres worldwide. 27%, like the Leibniz Supercomputing Centre (LRZ), are already building up their own resources and plan to develop new services from them. 73% of the supercomputing centres are planning to acquire the new technology. These are the most important results of a survey conducted by the media company IDC on behalf of Atos and IQM Quantum Computers, providers of quantum technology. The results were further elaborated and described from a practical view by LRZ strategist Laura Schulz, quantum specialists Ragnath Koduvayur of IQM Quantum Computers and Jan Wender of Atos, and Stephan Schenk of BASF, a potential user (picture below), in a streamed [online discussion](#).



The LRZ bundles its quantum activities in the Quantum Integration Centre (QIC) and is among the 9% of supercomputing centres that will integrate quantum processors into their high-performance computing or HPC resources. 48% of the centres surveyed want to remain competitive with quantum services, and 41% are driven by user demand. However, there are still hurdles due to laws, lack of experience and know-how, as well as staff shortages.

Quantum computers were also a topic at the Deutsches Museum, where Laura Schulz discussed the "[unimagined computing power of qubits](#)" with curator Luise Allendorf-Höfer, Professor Michael Hartmann from the Friedrich-Alexander-Universität Erlangen-Nürnberg, Wolfgang Kerler from the high-tech community 1E9 and quantum technician Martin Leib from IQM, who will soon be using them and what opportunities the new technology will bring to research and society: it's definitely worth seeing.

## Supercomputing for SME and Science

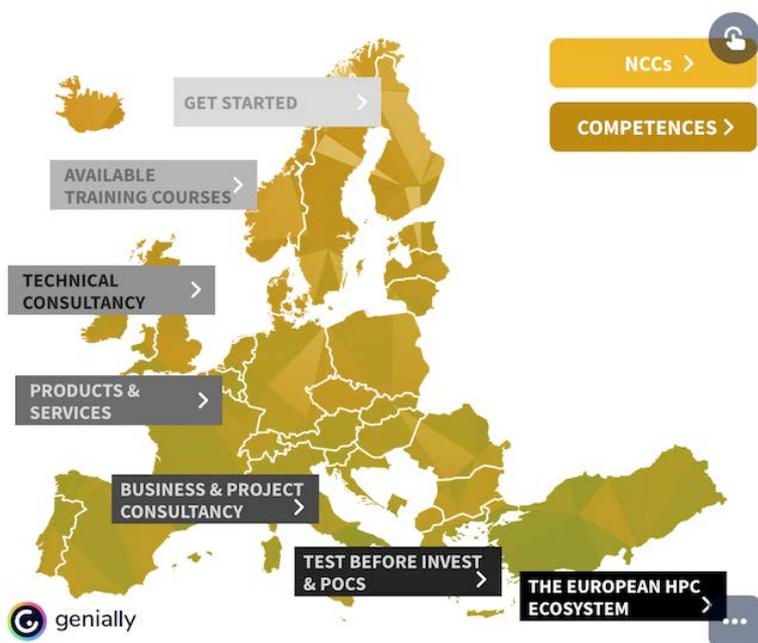
Getting to know and [controlling artificially intelligent systems](#) for data analytics or [programming new graphics processors \(GPU\)](#) and adapting them to individual needs: These are the topics of the two bootcamps that the [National Competence Centre \(NCC\)](#) for High Performance Computing (HPC) is launching in February and March next year at the Leibniz Supercomputing Centre (LRZ). The two two-day courses are not aimed at researchers and scientists only, but also at small and medium-sized enterprises (SME). "[EuroCC](#) aims to make supercomputing, HPC and artificial intelligence better known and easier to access in Europe and in Germany," LRZ specialists Kathrin Bild and Maja Piskac summarise the goal of the project, which started in September 2020.

"Moreover, EuroCC will act as a contact point to bring science and business together and to enable technical innovation." Success stories will convey how SME and research institutions can benefit from HPC and improve their offerings or results, as well as demonstrate the alternatives to the usual cloud services and advantages of supercomputing technologies.

This co-aligns with the goal of [European Union](#) to strengthen its own solutions for computer and internet use and data processing, as well as artificial intelligence and innovative IT technology. In doing so, EU wants to reduce the dependence of the economy and science in its member countries on IT offers from the USA and Asia, because these often do not meet the stricter requirements and demands in Europe - for example, when it comes to data protection or labour law. The project is building on the existing HPC centres in 33 European countries. EuroCC and - at the national, German level - [EuroCC GCS](#) are to network these more closely with each other by autumn 2022,

position themselves as national competence centres for smart data processing and complex calculations and make them better known in economy and research. GCS stands for [Gauss Centre for Supercomputing](#), the cooperation of LRZ, High Performance Computing Stuttgart (HLRS) and Forschungszentrum Jülich. As in the other member countries, half of the project is funded by the European Horizon 2020 programme and half by the state, in this case by the Federal Ministry of Education and Research. The HLRS is coordinating the work for EuroCC and EuroCC GCS; at the LRZ, computer scientist Piskac and mathematician Bild are working on specific tasks as task leaders.

At the halfway point of EuroCC, the first milestones have been reached: "On the EuroCC and EuroCC GCS portals, the national competence centres are listed with their focal points; here you can also find an info page on how to use HPC, as well as an overview of training and further education offers," Bild and Piskac report. The two bootcamps that take place at the LRZ and in cooperation with NVIDIA are also listed there. Further workshops with other partners are being planned. The interactive list of 33 competence centres is to be expanded in the upcoming months to include more data centres and HPC institutes that conduct research together with companies, tinker with software and process big data. In addition, experts in HPC, HPDA and AI in Germany can list their competences through a survey available online. Furthermore, it is planned to include the institutions of the Gauss Alliance and the National High Performance Computing (NHR) with their focus topics in the map. In addition, the openly accessible software, tools and smart systems are to be better specified for their use. Interested parties should soon be able to click through the site and find useful offers that can kick-off their journey in HPC.



## Analysis and Exchange of Big Data in Europa

Measurements, images, statistics, analyses: The data of a study usually answer more questions than the first ones asked, and elaborate, time-consuming experiments are too expensive to repeat. Therefore, the analysis of research data on various supercomputers and the exchange of data is becoming more important in Europe. Researchers should be able to do their



computing where the systems fit their requirements and are quickly available. "They often want to analyse and model their data on different supercomputers, as automatically as possible, easily and independently of location," says PhD physicist and head of the Research Data Management team at the Leibniz Supercomputing Centre (LRZ) Stephan Hachinger, outlining the problem. What is part of everyday life for users – the exchange of data – is a highly complex task in High Performance Computing (HPC). Tera- to petabytes are often processed here, which "despite fast networks, cannot be easily moved back and forth between strongly secured, heterogeneous systems", says Hachinger. User-friendly workflows for processing, analysing and exchanging data between locations are therefore required.

### Simplifying Complex HPC and Cloud Workflows

Big Data analysis, simulations and workflows on different supercomputers, as well as data exchange between European HPC centres have been at the focus of the EU project "[Large-Scale Execution for Industry and Society](#)", or [LEXIS for short](#) (Funding number: H2020 GA No. 825532). Coordinated by the [Czech national supercomputing center IT4Innovations](#), 17 institutes, companies and data centres, including the LRZ, have developed workflows and HPC and cloud technology. The result is the LEXIS platform, which builds on existing cloud systems, networks and supercomputers in Europe and organises the data flow. Users from research and industry can find tools at <https://portal.lexis.tech> that efficiently start and simplify analysis and simulation processes. Data is prepared and made available in the background for the next work step. The [portal also offers](#) practical tools for managing data based on [EUDAT services](#). Companies and researchers can process Big Data in the Czech Republic even though it is stored in Germany or Italy and vice versa, and collaborations can work together on data projects across Europe.

The [FAIR principles](#) play a major role in data management in the LEXIS system. According to these, research data should be findable, accessible, interoperable and reusable. Standardised metadata therefore indicate what individual data sets contain, how they were created and with which programmes they were created: "Within LEXIS, data is easily findable and it is immediately apparent how and for what purpose it can be further used," explains Hachinger. Although the LEXIS project will end in 2021, the portal and platform will continue to exist: Developed and optimised with partner organisations from the fields of meteorology, geophysics, polar and marine research and aircraft technology, the [first companies and research groups](#) are now testing the platform with Portal. One example is CompBioMed, an international project and centre of excellence for computational biomedicine, others are the specialised software manufacturer Pharmacelera from Spain or OpenEngineering from Belgium.

### New services for the LRZ?

The LRZ takes positive stock of the work on LEXIS. In addition to simplified processes and tools, several publications were produced. "We spent a long time looking for solutions for workflow control, for example in the processing of weather and climate data," Hachinger also adds. "EUDAT's combination of workflows and data management is exciting because it enables European computing from different locations." LEXIS will be used and further developed in the coming years. At the LRZ, they also hope for further collaborations with LEXIS partners, especially with the IT4I and the Irish supercomputing centre ICHEC. The platform and experience should flow into European HPC projects such as [EuroCC](#) or the work with the [Open Search Foundation \(OSF\)](#). And to long term, the LRZ itself could also benefit from the technology and thus expand its services. These possibilities are currently being explored. "This project has also brought us forward as a team," says Hachinger. "We were able to learn a lot about cloud and HPC technologies and project work, and saw how far we can get when the goal is clear and the team spirit is right." (vs)



Photo shows the LEXIS-Team of LRZ: Jirathana Dittrich, Dr. Stephan Hachinger, Dr. Rubén Garçia Hernandez, Elham Shojaei, Mohamad Hayek, missed is Johannes Munke



## Discover Bavaria Digitally

Paintings, sculptures, photos and more: 370,000 masterpieces from 110 museums and cultural institutions in Bavaria have been digitised for [Bavarikon](#) since 2012. In the meantime, they can be put together to form a wide variety of exhibitions. A current one, for example, shows [Jewish life in Regensburg](#), the most actual present [Bavarian lifestyle and handcraft](#). "Virtual exhibitions bring the richness of Bavarian history and culture into the home, workplace or school," said Bernd Sibler, Bavarian Minister of Science and Arts, at the opening. Bavarian traditions and festivals such as the Further Drachenstich, the

Oberammergau Passionsspiele and the Limmersdorf Lindenkerwa are presented in photos, videos, paintings, but also in audio formats through interviews or stories. The result is an astonishingly diverse, often interesting, sometimes quirky picture of Bavaria: well worth seeing and listening to.

The Leibniz Supercomputing Centre (LRZ) stores the Bavarian cultural treasure, which is being digitised under the leadership of the Bavarian State Library, on its servers and makes the digitised material accessible to research and society. Bavarikon comprises around 100 TB of data and occupies 100 servers. Some of the exhibits from [Bavarikon](#) are also set up in the [virtual worlds](#) of the LRZ's Mozilla Hubs. This exhibition is also worth a visit.



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## Figures of the Month

Supercomputing is an economic force: the new exascale systems, which are currently being planned worldwide and some of which are already being built, are driving business. The market research company [Hyperion Research](#) forecasts a growth in turnover of almost **8 %** for the next few years. By 2024, around **25 billion** US dollars will be invested in supercomputers, with the lion's share of just under **13 billion** dollars flowing into large computer systems such as the SuperMUC-NG, **4.5 billion** dollars into smaller systems and just **under 7 billion** into new exascale architectures. Because small and medium-sized enterprises and research organisations need more and more computing power for growing amounts of data and are relying on smart, artificially intelligent methods for evaluation, this particular market is currently becoming very differentiated. It can also be observed that companies and institutes are not only buying computers and processors, but are spending more money on storage and cloud technology, accelerators such as graphic processing units (GPU) as well as smart technology. **25 billion dollars** for supercomputing - that's a lot of money. But it is worth it in economic terms, especially in science: **every dollar** invested leads to new expenditure on technology, materials and, above all, personnel; Hyperion also calculates a profit or savings **potential of 111 dollars** per dollar. Supercomputing is used, for example, to develop vaccines and new medicines, to model the consequences of climate change or environmental catastrophes such as earthquakes and to plan protective measures against them.

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## Figures of the Year

The Leibniz Supercomputing Centre (LRZ) as an employer: In 2021, the LRZ welcomed **48** new colleagues and students as research assistants. **65** positions were advertised and **400** applications were received. **130** interviews were held. Not all positions could be filled by the end of November; some application procedures are still ongoing. The **263** staff members (as of Nov. 2021) have recurring questions about contracts, working hours and leave time. These added up to **10596** by the end of November. The LRZ continues to grow. You can currently find **19** job offers [on the website](#) – for IT specialists, HPC engineers, quantum experts and students: So we are looking forward to hearing from you!

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## WORKSHOPS & EVENTS

### Experience Research and Art



Discussion panels, installations, exhibitions, workshops, participation and, above all, experience: The [first Hi!A Festival for Art and Research](#) will run in Bavaria until **31 December 2021**. The Leibniz Supercomputing Centre (LRZ) will be represented several times: With a live stream of the discussion on the ["Unimagined computing power of qubits"](#) with LRZ strategist Laura Schulz, Luise Allendorf-Hütter (Deutsches Museum), Martin Leib (IQM), and Prof. Michael Hartmann (FAU Erlangen). 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. In addition, the [Bavarian Institute for Digital Transformation \(BIDT\)](#) presents virtually what artificial intelligence and digitalisation are doing in business and research.

## 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.](#)

## Securing the Networks

Log4Shell and many headlines from companies regularly show: the networked world is insecure. On 3 and 4 February 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](#)

## 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. 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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## 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!

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

[IT specialist and scientific staff](#) for IT security and for the vulnerability management

[IT specialist or system consultant](#) for the multifactor authentication

[IT system administrator](#) for the development of operations and security concepts for Windows client systems

[IT-Specialist](#) for data backups

[IT-Specialist/System engineer](#) for Storage services

[IT system administrator](#) for Linux environments  
[IT system administrator](#) for Windows clients  
[IT-system administrator](#) für Mac-clients and mobile devices  
[HPC software engineer](#) for quantum computing  
[HPC expert with focus on biomedicine](#)  
[HPC expert with Focus on biochemistry and life science](#)  
[Programmer](#) for scientific IoT projects

[Apprentice](#) for System electronics

[Clerk](#) for the management of licences

[Student assistant](#) for media design

[Student assistant](#) for ITSM software development

[Student assistant](#) for the web backend und the BAYSIC portal

[Student assistants](#) for the 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](#).
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- You can subscribe or unsubscribe the LRZ-Newsletter via our [website](#).
- Current information about the LRZ and about courses and events can also be found on [Twitter](#) and [LinkedIn](#).

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