LRZ-Newsletter October 2020

NEWS

New Head of Central Services of the LRZ: Dr. Jürgen Seidl

A warm welcome: Since October 1, Dr. Jürgen Seidl is head of the department “Zentrale Dienste” of the Leibniz Supercomputing Center (LRZ). Dr. Seidl, who holds a doctorate in history, is moving from the Bavarian State Library (BSB) to the LRZ. In his doctoral thesis, Seidl researched the corporate history of BMW and joined the BSB via the Bavarian Academy of Sciences (BAdW). Here he initially worked on library projects before moving to the administration of the scientific library. In his last position, Seidl was head of finance in the central administration department. In his private life, the new LRZ colleague likes board games, ice hockey and soccer - just to get to know him better, a few questions:

What attracts you to the LRZ? **Dr. Jürgen Seidl:** First and foremost, the excellent reputation of the LRZ and the very good experiences of my former department, the Bavarian State Library, with the LRZ were decisive for my application. After the job interview I could immediately imagine working here.

What are you particularly looking forward to? **Seidl:** To my new colleagues and exciting challenges. The foretaste that I was able to get in the weeks before I started has already been very positive. We were able to clarify many things in advance in a very unbureaucratic way, from workplace equipment to the LRZ mouth-nose cover with the "Stay Safe" imprint.

What drives you? **Seidl:** The desire to solve the tasks at hand as well as possible and prioritizing them in the right order, but sometimes just a good cup of coffee with delicious chocolate.

With whom in the computer, internet, IT scene would you like to discuss - and why? **Seidl:** With Dietmar Hopp - besides questions about ethical responsibility in IT, I would like to learn more about his great social commitment. Since I am also a big sports fan, soccer and ice hockey would take up a large part of this conversation.

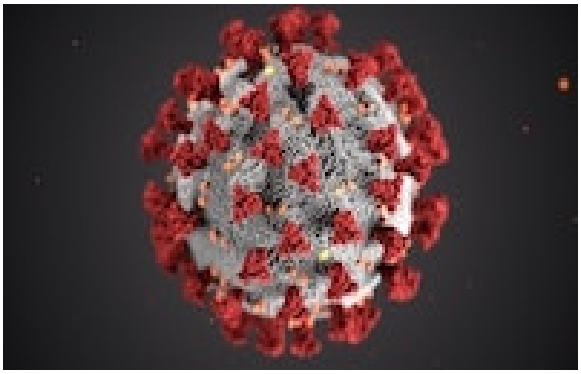
What function would you want to be invented for computers/smartphones right now? **Seidl:** Definitely beaming. That would save me the daily train ride from the Oberland – the region in the south of Munich - to Garching and elsewhere.

And which ones could you gladly do without? **Seidl:** Non-essential cookies or the fact that I have little or no control over my own data while surfing the Internet.

What relaxes you? **Seidl:** Time at home on the terrace with the family, preferably with an exciting board game. **(vs)**

Technology Donation for Corona Research

With technology against the Covid 19 virus: US chip developer AMD is supporting the search for vaccines against corona with high-end computer systems and access to Penguin-on-Demand (POD) clusters in the cloud, which are operated with the new second-generation EPYC and Radeon processors. In addition to 19 research facilities around the world, the technology donations will also be installed at the Leibniz Supercomputing Center (LRZ) and the High Performance Computing Center Stuttgart (HLRS). “Supporting world-class research with cutting-edge IT technology is the key focus at Leibniz Supercomputing Centre. This generous AMD donation puts us in the position to offer our partners in the domain of personalized medicine innovative artificial intelligence solutions”, Prof. Dr. Dieter Kranzlmüller, Director of the Leibniz Supercomputing Centre of the Bavarian Academy of Sciences and Humanities says. “While this allows them to address the immediate research needs around COVID-19 in much better ways, including working on improved diagnostic quality and speed, we’re implementing our vision to further integrate HPC and AI to be used in personalized medicine. This will enable our partners to establish high-impact improvements to the treatment of patients suffering from other diseases in the long-term.”



In the fight against the pandemic, AMD set up its own fund of technology and financial resources. In addition to the renowned Massachusetts Institute of Technology (MIT), as well as New York University (NYU) and Rice University in a first phase, other universities and institutes will gradually be provided with computing power until the end of 2020. Until the 4th quarter six GPU Compute Servers with one AMD EPYC-CPU each as well as eight AMD MI50 GPU with 32 Gigabyte RAM plus local NVMe storage will be installed at the LRZ. They support the **ongoing COVID-19 projects** in researching the virus' mode of action, simulating droplet infection and developing vaccines. AMD is donating a total of 12 petaflops of computing power to the research. Assembled into a supercomputer, it would rank among the top 500 fastest supercomputers. “AMD is proud to be working with leading global research institutions to bring the power of high performance computing technology to the fight against the coronavirus

pandemic," said Mark Papermaster, executive vice president and chief technology officer, AMD. "These donations of AMD EPYC and Radeon Instinct processors will help researchers not only deepen their understanding of COVID-19, but also help improve our ability to respond to future potential threats to global health." **(vs)**

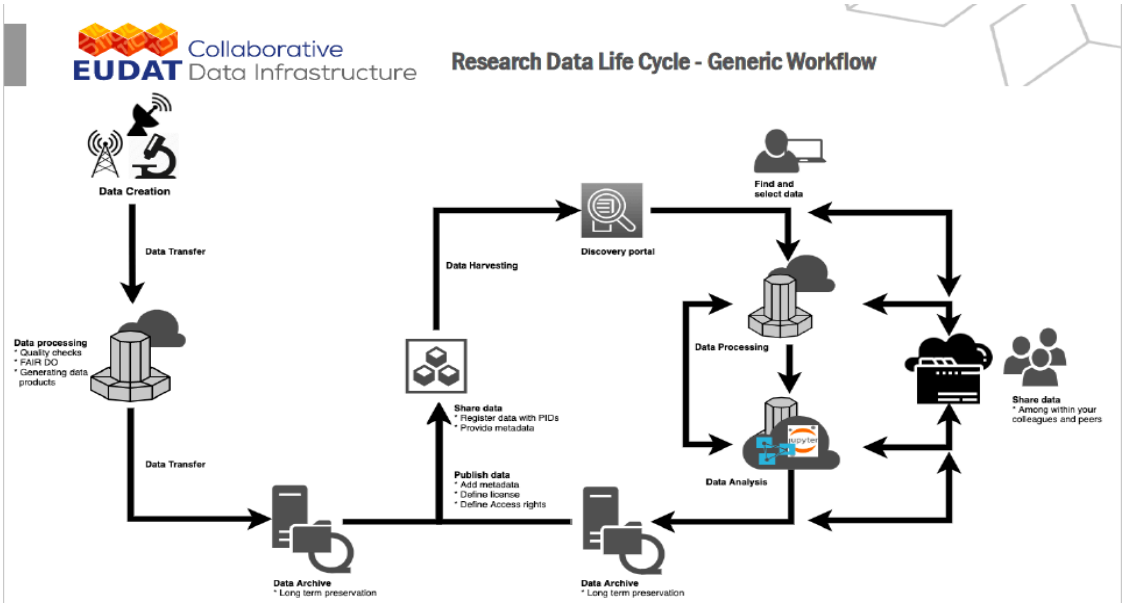
Nobel Prize for Astrophysicist Reinhard Genzel

Congratulations: **Reinhard Genzel,** Director at the Max Planck Institute for Extraterrestrial Physics in Garching, together with the physicists Andrea Ghez and Roger Penrose, has been awarded the prestigious 2020 Nobel Prize. "The Nobel Prize is a fitting honor for the team that has slaved for 30 years to make us better and better," comments the **Professor of Astrophysics**, who teaches at the Ludwig Maximilian University in Munich. Genzel and his team, like the co-award winners, have worked on the detection of black holes, they successful demonstrated it. These are now reality. Reinhard Genzel has an account at the Leibniz Supercomputing Center (LRZ). In the Universe Cluster of Excellence, the astrophysician and colleagues researched and modeled the development of the **G2 cloud** at the SuperMUC, and pictures of the simulation even made it 2014 onto the cover of the journal **"Nature".**

European Tools for Data Exchange

Europe is moving closer together - also in science and with the help of IT and cloud: The **European Open Science Cloud (EOSC)** planned by the EU Commission and the member states is taking shape. It will provide the technical infrastructure for the intermediate storage and archiving, for the retrieval, access and exchange of research data. The **EUDAT** Collaborative Data Infrastructure (CDI), a network of now 30 computer and data centers for research and teaching, is developing tools and services for this purpose. In the meantime, a good dozen open source-based programs and tools have been brought together under the umbrella of **EUDAT CDI,** which the astrophysicist and data processing specialist Johannes Reetz from the Max Planck Society's MPCDF data center presented in September at the Leibniz Supercomputing Center (LRZ): "The aim is to establish EUDAT CDI as a layer for data management and storage for the emerging European Open Science Cloud, while also integrating it into existing European HPC infrastructures.

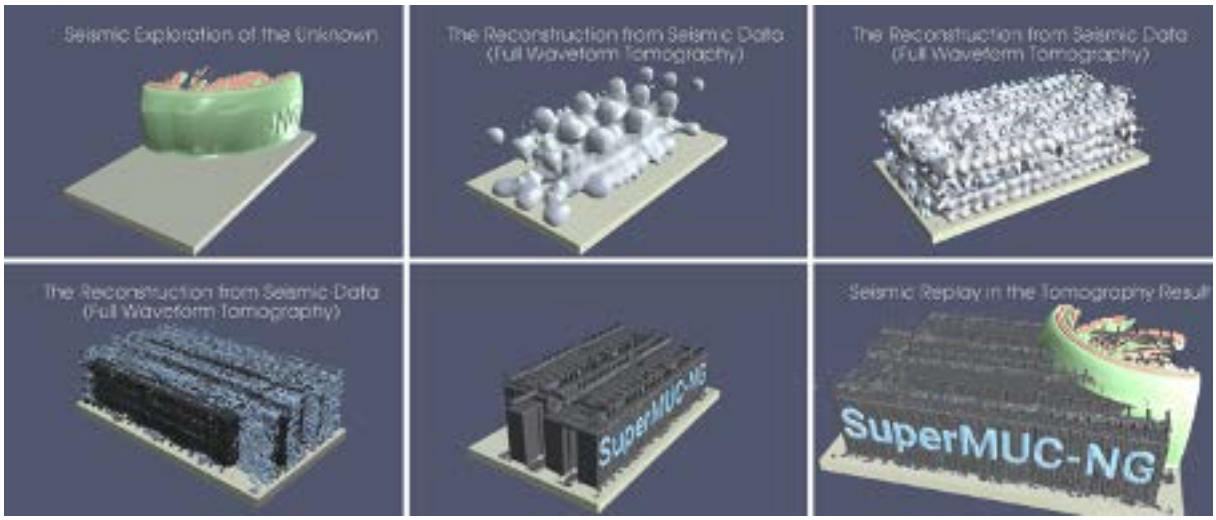
The services and projects primarily support (long-term) data storage and data management. As a partner of European research projects like **CompBioMed, GÉANT** or **LEXIS,** the LRZ already uses EUDAT services. Thus, own algorithms and applications are made accessible via the EUDAT software repository **GitLab.eudat.eu.** Meanwhile, the Research Data Management (RDM) team uses the EUDAT tools B2HANDLE, B2SAFE and B2STAGE to uniquely mark and identify measurement and simulation data, to protect them from damage caused by use, and to make them accessible. B2Find and B2NOTE also allow data sets to be equipped with meta-information on content, author, storage space and registered in databases so that they are easier to find online. B2ACCESS, however, serves as an identification tool through which users can register with EUDAT services via their own providers. B2DROP is an EUDAT service that can be compared to LRZ Sync+Share. "EUDAT offers secure tools, services and capacities for data storage and sharing of the European Data Space", Reetz promotes the initiative. Like the LRZ, EUDAT is also committed to FAIR(s) data exchange: Technology and systems, but above all the labeling of data records and distributed storage ensure that the information can be found, accessed, compatible and interoperable in the long term and can be reused by any researcher in its original state and without manipulation. It is quite possible that this will lead to closer cooperation between LRZ and EUDAT. **(vs)**



A test scenario for SuperMUC-NG

Algorithms won't become old, they are adaptable and can still be used even after major technology changes: André Kurzmann, who supervises the users of the supercomputers at the Leibniz Supercomputing Center (LRZ), worked on the algorithm of his doctoral thesis for advertising purposes and thus created **a model of the SuperMUC-NG**. "The aim was to show that the LRZ is well positioned in the geosciences and also supports seismic applications," says the geophysicist. "I also wanted to know whether the code would also scale across the entire SuperMUC-NG. It does."

For his **doctoral thesis in 2012,** Kurzmann modeled the upper earth's crust using sound waves and other artificial waves. Such 2D and 3D tomography provides data that can be used to visualize geological structures and help track down raw materials such as oil or coal underground or plan tunneling work. The algorithm that Kurzmann developed became one of the first test cases of the SuperMUC-NG in 2019. Using artificial seismic data acquired in three million computing core hours, he built a model of the new supercomputer at the LRZ. "It is only a small model, but the seismic tomography contains around 170,000 3D simulations," explains Kurzmann. The resulting short video should be presented during the annual meeting of the **German Geophysical Society** with the special LRZ services for geophysicists, seismologists and geologists. Corona thwarted this plan, and now the simulation can be found on YouTube, while the algorithm is available as open source software on GitLab **(vs)**



Figures of the month

If several programmers are working on a software at the same time, they should be able to store and manage the different versions. The version management software Git and the cooperation environment GitLab based on it, which the LRZ offers to its users, helps them to do this. At Gitlab.lrz.de, around 15,000 users actively use the tool and are currently working on 40,000 programming projects with it. Including all files in the version management (repository), the large file storage (LFS) for large files and containers, the data volume is about 10 terabytes. Recently, the LRZ switched from the "Community Edition" to the educational license "GitLab Enterprise Edition". This allows LRZ users to use the functions of the commercial GitLab version for teaching and research purposes. The way to **LRZ-GitLab**. **(vs)**

WORKSHOPS & EVENTS

Supercomputers seeking work

The Partnership for Advanced Computing in Europe (PRACE) is now allocating computing time at European supercomputers. Application deadline is **27 October 2020.** Interested parties can find **online all information** on the various systems, including the SuperMUC-NG, as well as the requirements for access to High Performance Computing (HPC) in Europe.

Introduction to the supercomputer of LRZ

An introduction to high-performance computing and a crash course in computational fluid dynamics, the representation of flows on the computer, will be given in this half-day online workshop **on October 14.** It is intended for beginners and shows the work on the Linux cluster of the LRZ. **Informations and registration**

Introduction in ANSYS Fluid Dynamics

This is what future engineers and scientists need: ANSYS Fluid Dynamics is a bundle of programs for the calculation and visualization of different flows. The introductory course to the most frequently used program on the supercomputers of the LRZ will take place online every Monday from **October 19, 2020 and December 14, 2020** from 10 a.m. to noon and from 2 p.m. to 4 p.m. **Informations and registration**

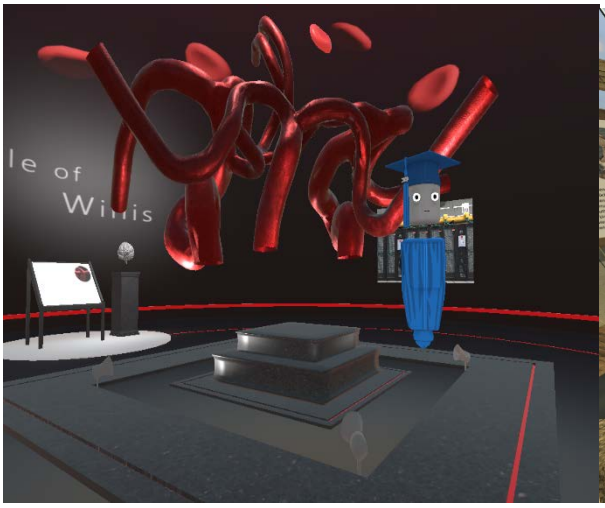
GRoW shows it's research

The summer has shown that life needs water, but many regions in Germany are running out of water. Between 2017 and 2020, the Global Resource Water (GRoW) project brought together almost 50 universities and research institutions with more than 30 companies, public authorities and associations to analyze water supply and climate change and to channel water consumption more efficiently in the future. The result is 12 practical collaborative programs and more than 40 case studies on regional and international solutions for water consumption. The GRoW project, which is financed by the Federal Ministry of Education and Research and in which the Leibniz Supercomputing Center (LRZ) was also involved, is inviting participants to its final conference from **20 to 21** October, 2020 at the Umweltforum Berlin and on the Internet. Research partners will present results and solutions to conserve water reserves and better control water consumption.

Munich Medientage: LRZ visualizations at the virtual event

Off to virtual reality: Like many conferences and trade fairs, Medientage München is taking place digitally this year. From **October 24 to 30, 2020,** media professionals, broadcasters and publishers will present their media productions and new ideas. The Leibniz Supercomputing Center (LRZ) will be there for the second time. The Center for Virtual Reality and Visualization (V2C) presents current projects in the virtual rooms of the Media Days. "The visitors of the Medientage look at our visualizations and simulations with different eyes and enrich our work with valuable suggestions. We are already very curious to see how the exchange will work out in a virtual environment this year," says V2C employee Lea Weil.

During the Media Days, exhibitors will present themselves in Mozilla Hubs, virtual spaces similar to those in video and online games, through which visitors navigate via smartphone, tablet, notebook or with virtual reality glasses. Practical: You don't need to create an account for this; all you have to do is click on a link and users are right in the middle of the digital exhibition. The V2C team is developing special rooms for the Medientage München to present three projects to visitors. For this purpose, the complex, data-intensive 3D simulations of CompBioMed as well as the 3D models of art-historical objects are reduced and processed so that they can also be accessed via browser and with less powerful devices. "Most models and textures in our visualizations are too complex for Mozilla Hubs. Therefore we have to reduce the polygon and pixel density significantly without losing too much information", explains Kristian Weinand, also from V2C. During the Medientage, the services of the LRZ and the V2C will be presented in three to four virtual rooms based on the work for projects like CompBioMed, MOOSAIK and some art historical objects**. (vs)**



Tips & Tricks for more Security

Cybercrime is constantly growing and finding more and more ways to defraud Internet users: a task for CONCORDIA, the name stands for "Cybersecurity Competence for Research and Innovation" and since 2019 has been networking universities, scientific data centers such as the LRZ as well as more than 50 companies from Europe, which are working on technical solutions for more security and data protection in the Internet and IT. On October **28 and 29, 2020,** CONCORDIA will offer insights into its work and present practical security solutions and offers for users, companies and organisations during virtual open days. Visitors can expect exciting lectures, valuable contacts and useful advice. Participation is free of charge if interested parties register with the LRZ code COD2020P018. Registration here.

Support for HPC-Users

In April it had to be cancelled due to Corona, at **October 26, 2020** it is taking place online: At the Extreme Scaling Workshop scientists can adapt and optimize codes to the needs of the SuperMUC-NG with the help of LRZ specialists and experts from Lenovo and Intel. "The workshop helps participants to make optimal use of the computing time they have been given, and helps

us to better utilize the SuperMUC-NG and learn about the applications that will be part of everyday life in a few years' time," explains Dr. Gerald Mathias from the HPC support team. An application with a large scale HPC project is required for the workshop.

SC virtual - to get a taste of the HPC community

Another digital fair: Supercomputing 2020 will also take place virtually or digitally this year, from **November 9 to 19.** This will provide an opportunity to gain an insight into the HPC community, new technologies and topics. To participate in tutorials and workshops or lectures, admission is required. But the exhibition from **November 17 to 19** can be visited free of charge - by appointment

Ideas for less Energy Consumption

Politicians discover the power of hackathons. From **November 13 to 15, 2020** the Bavarian State Ministry for Digital Affairs is organizing such a code festival and the Leibniz Supercomputing Center (LRZ) is part of it: #FutureTech4Climate is looking for codes, programs, apps and other technical solutions to slow down climate change. The LRZ is committed to ideas for energy saving in supercomputing and presents consumption data from SuperMUC-NG and colleagues for discussion. Participants should know programming languages and have first experiences in evaluating Big Data. You will find more information online at the State Ministry soon and too on our homepage.

C++ for software-engineering

Object-oriented software design with the programming language C++ is the focus of this online course **from November 18 to 20.** Participants will learn the most important programming concepts and procedures. The goal is to produce robust, reliable code that can be maintained and further developed. Informations and registration

Handling the supercomputers of LRZ

Those who could not participate in October will get another chance to get to know the Linux cluster of the LRZ **on 9 December.** The half-day online course explains the handling of the cluster and the most important applications to calculate and display flows in the cluster. Informations und registration

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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!

Researcher with focus on data bases for our Web-Team (m,f,d)
Tech-Specialist with focus on data bases for our Web-Team (m,f,d)
Data Architect for a High Performance Data Analytics-Platform (m,f,d)
Client-Manager for MAC- and Mobile Devices (m,f,d)
Client-Manager for Windows (m,f,d)
Storage Administrator (m,f,d)
Working student for front end development (m,f,d)
Working student for Web, Java Script & Type Script (m,f, d)
Working student for the Service-Desk (m,f,d)

MORE TO READ

Here you will find links to latest information from the german-european supercomputing community and our cooperation partners
PublikationS of the Gauss Centre for Supercomputing (GCS): GCS-News und Inside
Infoletters oft he Gauß-Alliance
Publikations of PRACE: PRACE Digest, Jahresbericht

INFORMATIONS & IMPRINT

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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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Fotos/Graphics/illustratione: CDC, EUDAT, Max-Planck-Institut, V2C-LRZ, A. Kurzmann/LRZ, S.Vieser/LRZ