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Lifting a treasure trove of data



Extreme weather, droughts, melting glaciers, coastal erosion, even the development of cities over time: Currently, eight Copernicus Sentinel, the US Landsat and the radar satellites of the German Aerospace Center send approx. 19 terabytes of data per day about the current state of Planet Earth. To explore this gigantic treasure trove of historical and current earth observation data, DLR and Leibniz Supercomputing Centre build a [High Performance Data Analytics or HPDA platform](#) called terrabyte. The system connects [DLR's](#) satellite data archive in Oberpfaffenhofen with new, intelligently managed online storage of around 50 petabytes and the supercomputers of the scientific computing centre in Garching via a 10 gigabit/s line. In 2020, [DLR invested](#) 8 million euros on the procurement of the storage part, and the LRZ in turn supports and maintains the HPDA platform. With further funding from

DLR, terrabyte is now being expanded to include its own compute capacities that will enable data processing and analyses, with a special focus on using artificial intelligence methods. DLR's satellite data is to be used widely in the future; in addition to DLR, Munich and Bavarian universities will soon also have access to terrabyte.

Moving forward together

Energy-efficient supercomputing, new architectures and codes for high-performance computing, and above all the ever growing needs in science and research: the Leibniz Supercomputing Centre (LRZ) does not want to and cannot solve all the questions about its future on its own and is therefore being consulted by an [advisory board](#). Newly elected to this body were [Prof. Dr Gerhard Wellein](#) from the Friedrich Alexander University in Erlangen-Nuremberg and [Prof. Dr Stefan Dech](#), Director of the German Remote Sensing Data Centre (DFD) at the German Aerospace Centre (DLR), were, which has 28 members and includes representatives from the Bavarian Academy of Sciences, as well as Munich and Bavarian universities.



Wellein, a physicist, has been enriching the HPC community with his experience, knowledge and practical codes for more than 20 years. The multi-award-winning scientist teaches High Performance Computing (HPC) in Erlangen, has an excellent international network, is involved in the [Partnership for Advanced Computing in Europe \(PRACE\)](#) and in the [Bavarian competence network for scientific HPC, KONWIHR](#): "I have known the LRZ and many of its employees in high-performance computing for many years. I have come to appreciate their competence and high level of commitment," says Wellein. "I'm looking forward to getting to know new interesting research questions in the advisory board, which has a broad range of expertise."

Dech, a geographer, has also built up an international network. At [DFD](#), he researches remote sensing data for clues on climate change and environmental changes, and also deals with the methods and systems for analysing satellite data. "The LRZ can play a key role for climate and environmental research if it succeeds in lifting the enormous and rapidly growing treasure trove of satellite data for international research," says Dech. "Helping to drive that - I see that as a central part of my task as an advisory board member." Read on about the new advisory board members in [an interview on the LRZ website](#).



Better search and use of research data

Measurement data, interviews, images, social media data, statistics: In Research datas you will find not only one answer, so it should be made available to as many users as possible. This is the central goal of several projects of the National Research Data Infrastructure (NFDI), which brings together IT service providers such as the Leibniz Supercomputing Centre (LRZ) with research institutions, colleges and universities in Germany. Since 2018 and for the time being up to 10 years, the federal and state governments have been funding the development of open data platforms and portals for various scientific fields with 90 million euros annually, which will be equipped with new, smart analytical tools based on artificial intelligence and statistical methods.



The LRZ is already directly involved in two NFDI consortia and won five more in 2021. The expertise of the Research Data Management, File and Storage Systems and Big Data and Artificial Intelligence teams is particularly in demand. The aim is to make research datasets easier to find and use internationally, and to do so for as long as possible. The LRZ has committed itself to the FAIR rules, according to which data should be findable,

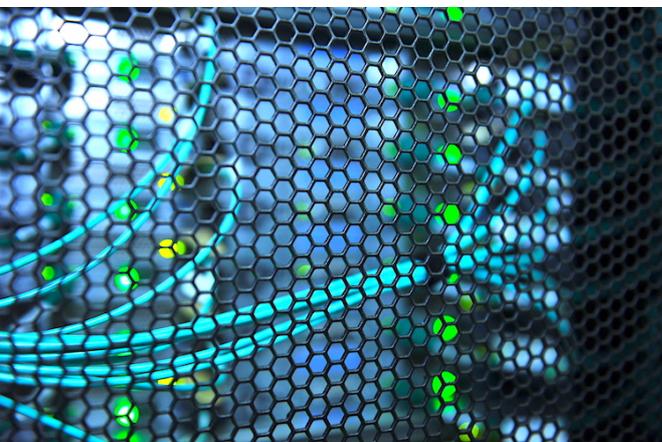
openly accessible, interoperable and reusable. "This simplifies the verifiability and sharing of research results", [Dr. Stephan Hachinger says in an interview on LRZ website](#). He leads the Research Data Management team. "A prerequisite for FAIR data management is the provision of research results with additional information." These standardised metadata are indexed by search engines and describe the content of data sets. In addition a checksum ensures that a data set has not been manipulated or changed during use.

NFDI projects with LRZ participation

- [BERD@NFDI](#): This project makes accessible data on the economic and labour situation as well as social developments and provides artificial intelligence and machine learning methods for evaluation. BERD@NFDI is led by the University of Mannheim.
- [FAIRmat](#) takes care of information and research results from the data-intensive material sciences, physics and chemical physics and is led by the Humboldt University of Berlin.
- [NFDI4Earth](#) focuses on the earth sciences. The LRZ is contributing its experience in setting up terrabyte and helping to simplify the use of simulation data. The Technical University of Dresden is leading this project.
- [PUNCH4NFDI](#), on the other hand, is creating a platform on which particle and astroparticle physicists can store their mass data and develop integrated data and metadata tools and file formats for this purpose. This project is organised by the German Electron Synchrotron (DESY) in Hamburg and Zeuthen.
- Finally, [Text+](#) addresses text- and language-based data from the humanities, i.e. information such as books, interviews, lectures, and aims to make them accessible for science. The LRZ supports the project with technical know-how.
- Since 2019, the LRZ has also been involved in the [German Human Genome-Phenome Archive \(GHGA\)](#), which will provide the technical infrastructure for data storage and analysis of information on human genetics and medicine under the leadership of the German Cancer Research Center in Heidelberg. The LRZ is also involved in the [NFDI Platform for Engineers \(NFDI4Ing\)](#); the leadership for this project lies with the RWTH Aachen. NFDI4Ing is particularly concerned with metadata in high-performance computing or supercomputers such as the SuperMUC-NG - a topic that is of great importance for all NFDI projects.

Discussing and improving the new Major Version MPI-4

In High Performance Computing (HPC), anyone who wants to address as many compute nodes of a supercomputer as possible and exploit the full performance, needs the Message Passing Interface (MPI). The programming scheme was developed for



message exchange in parallel computer architectures, has existed since the 1990s and has seen three major releases so far. The fourth one appeared in June 2021. MPI-4 offers about 150 new functionalities- and they will be discussed intensively by specialists from all over the world from 7 September 2021: For the first time, the Leibniz Supercomputing Centre (LRZ) will host [EuroMPI](#), the most important annual meeting that brings together all user groups. "In addition to the new possibilities, it will certainly be about the scalability of MPI-4 on the supercomputers of the Exascale generation, but also about better integration with accelerators such as quantum and graphics processors," says Prof. Dr. Martin Schulz, Director of the LRZ and Chair of Computer Architecture and Parallel Systems at the Technical University of Munich (TUM). "Probably partly in presence, partly virtually, pronounced MPI experts will come together at EuroMPI21."

Developing MPI further

There are enough topics: the new version extends MPI to 64-bit data types for the first time and changes familiar ways of working. For example, the number of elements to be communicated can now be increased to well over two billion. Repeatedly executed work steps are better programmable via the so-called persistent collectives, and the tasks of an HPC code can also be portioned. Last but not least, error correction has been improved. "MPI-4 simplifies some of the functions of supercomputing," summarises LRZ staff member Dr Martin Ruefenacht, who worked on the major release and is co-organising the EuroMPI as Local Chair. "You can use and integrate work packages more easily."

The programme of the one-day conference contents lectures of speakers from the High Performance Computing Centre Stuttgart (HLRS) and the Rheinisch-Westfälische Technische Hochschule Aachen (RWTH), the University of Tennessee (UTC), where many recommended standards are implemented, The University of Tokyo, the Université Reims, the Lawrence Livermore National Lab (LLNL) and the Los Alamos National Lab (LANL) will be also represented. There will also be news from the research departments of Fujitsu and Intel. After the conference day on 7 September, the [MPI Forum](#) will meet, also in Garching: This committee of core developers and researchers deals with ideas and suggestions for improvements to MPI-4 and ensures that the programming language can continue to develop. Read on in the [interview with Dr. Mars-André Hermans](#) of RWTH, this year's programme chair of EuroMPI.



„The simple user problems are the annoying ones“

It has been celebrated regularly since 2000 and is meant to bring recognition: 2021 Systemadministration Day took place on July, 30. We, the users from Leibniz Supercomputing Centre (LRZ), said "thank you" to the specialists at [LinkedIn](#) and Twitter. Because they work hard every day to ensure that notebooks and workstations function, **networks** and the internet run reliably, software is available and regularly updated, cloudservices and high-performance computers are accessible. And because we don't always know how system administrators work, we asked Kevin Pötschke, who has completed his **training** at the LRZ.

Why did you decide to become a system administrator? **Kevin Pötschke:** I have been interested in computers for a long time and wanted to deepen my knowledge in this area. My brother also did the same training, so he probably infected me with it.

What are your tasks? **Pötschke:** Primarily, I create software packages for customers, that is, I receive an order to package an application such as Office or Chrome. To do this, I put the

software together and then install it via a silent batch script, i.e. a .cmd file that starts the installation without users noticing or having to react. Because the LRZ manages and distributes the updates, I deactivate the automatic updates and store a licence key or server if necessary. My other tasks include dealing with tickets from customers who have problems, for example with the anti-virus programme Sophos or with the connection of a network folder.

What do you particularly like to do? **Pötschke:** "What I like best is software packaging. It's always the same procedure, but the content differs from software to software

What user problems are annoying? **Pötschke:** Honestly? The very simple ones. Many of these simple problems and questions could be solved by a short search online or in the [LRZ documentation](#) itself

What is your professional dream or goal? **Pötschke:** I can't say at the moment, but for the time being I would like to stay at the LRZ and build up a professional foothold here.

Architect of virtual worlds



Admiring golden stucco, gliding over coloured marble inlays, looking at old paintings: There would be a lot to look at in the [chamber chapel of Electress Maria-Theresia](#) in the Schleißheim Palaces. But the room and its delicate works of art may no longer be entered. At the Leibniz Supercomputing Centre (LRZ), it has therefore been recreated in virtual worlds. [Elisabeth Mayer](#), a 3D specialist at the Centre for Virtual Reality and Visualisation (V2C), has helped to make the Gesamtkunstwerk accessible, at least in digital form: "Virtual or augmented reality applications help science through immersion to intensively explore and thus better understand phenomena from the environment or medicine or the arts," she says. "The challenge here is Big Data, the question is always how we can import and visualise enormous amounts of data in VR applications." We present the young scientist and her impressive work in [a portrait on the LRZ website](#). Elisabeth Mayer relies on game engines, has digitally recreated the SuperMUC-NG, constructs beer gardens and Christmas markets in the [Mozilla Hubs](#), creates the worlds for learning apps and is currently causing a furore in medicine and the supercomputing community with a

[visualization of blood flow](#) in the forearm.



Figures of the Month

91 scientists are involved in a total of **13 environmental** and climate projects for which SuperMUC-NG and CoolMUC have so far completed around **130 million computing hours** and will continue to work. Some of these projects also deal with extreme weather conditions, heavy rain and flooding. You can find more than just figures about the research projects and the tasks of the LRZ on the [LRZ-website](#).

WORKSHOPS & EVENTS

MPI and the Next Performance Level for HPC

The Message Passing Interface (MPI) is the focus of the EuroMPI conference, which will take place on **September 7, 2021** at the Leibniz Supercomputing Center (LRZ) in Garching near Munich. Users and researchers will discuss newly proposed concepts of the programming scheme and extensions to the MPI standard, libraries and languages based on MPI, as well as necessary interfaces to other standards in parallel programming. Of course, it also deals with applications and their adaptations to new, more powerful computer architectures and networks. MPI goes Exascale. This year, Prof. Dr. Martin Schulz, Director of the LRZ, is responsible for the EuroMPI program. [Information & registration](#)

Iterative Solvers for Linear Systems

An online seminar for numerical scientists (computational science) and researchers working with linear equations for data analysis and modeling. The focus will be on iterative solvers for linear systems of equations from **September 8-10, 2021**. In addition to classical schemes and basics of multigrid techniques, Krylov subspace methods and highly efficient preconditioning methods will be presented and illustrated with practical applications. Practical exercises allow testing basic iterative solvers and deepen the understanding. [Information & registration](#)

Crash Course for the LRZ Linux Cluster

On **September 8, 2021**, beginners in high-performance computing (HPC) can learn about working on parallel computing systems. The focus of the one-day crash course is on computational fluid dynamics (CFD), i.e. the simulation and representation of flows and motions of and in gases or liquids, using the ANSYS programs as well as StarCCM+. The Linux cluster systems of the LRZ, their user environment and various access options are explained. Attention: This course was originally dated for September 15 and had to be postponed. [Information & registration.](#)



Telling stories with immersive techniques

Virtual, augmented or mixed reality are ideal for explaining research and science or for telling stories: Creators can apply with their projects for the European Creator's Lab until **September 12, 2021**. Here, game developers, designers, programmers, authors, journalists, students and researchers can find inspiration. Students and researchers can be inspired and learn with or from each other. Elisabeth Mayer from the Leibniz Supercomputing Center will be there as a mentor for virtual reality applications. The European Creator's Lab is organized by the XR Hub in Bavaria and will take place online from **November 15 to 19, 2021**. [Information & registration](#)

Thinking ahead with OpenMP

There are still plans for a face-to-face event: The international OpenMP workshop will take place in Bristol from **15 to 17 September**. During the three days, experts from all over the world will discuss how the OpenMP programming scheme can be further developed, point out future trends and jointly search for solutions to problems and questions concerning Open MP. The LRZ is actively involved in the standardisation of the programming language, without which little or nothing runs on the SuperMUC-NG. [Information & registration](#)

Building the Digital Twin

High performance computing (HPC) for medicine has many aspects: Supercomputers evaluate screening and other data with smart analysis methods, they visualize bodily functions or they model humans: CompBioMed is working on the "Virtual Human". The European center of excellence and research consortium invites to the conference from **September 15 to 17, 2021** and presents existing biomedical applications and software as well as methods for visualization, virtualization and simulation of body functions and the bone structure. The LRZ is represented with lectures on visualization and adaptation of existing programs and applications for exascale systems, Prof. Dr. Dieter Kranzlmüller and Dr. David Wifling from LRZ are responsible as Programme Chairs for the topic Methods. [Information & registration](#)

Informatics 2021 - Ideas for the Future of IT

Energy-efficient supercomputing, environmental research and artificial intelligence methods for parallel computer systems are the main topics of Informatik 2021 from **September 27 to October 1, 2021**. LRZ staff member Dr Maximilian Höb describes in a workshop how [energy efficiency in data centres](#) can be increased through artificial intelligence, monitoring and clever technology. The annual conference of the Gesellschaft für Informatik addresses students with the presentation plenum **"SKILL"**. Final papers are still being accepted until June 26, 2021. [Information & registration](#)

Building an open search

Experience new search technologies, discuss strategies on how to break the dominance of Google, Bing, Yandex or Alibaba: The Open Search Foundation (OSF) invites you to the third Open Search Symposium #ossym from **October 11 to 13, 2021**, hosted this year by CERN in Geneva. During the digital conference, new tasks will certainly be distributed - the OSF is, after all, working on an open search index, harnessing data centers such as the LRZ or the CERN and many, many enthusiasts who are committed to openness and transparency on the Internet. If you want to get involved, network or learn more about innovative search technologies, this is the place to be. [Information and registration.](#)

Introduction to ANSYS CFX

10 lectures and about 5 practical exercises to get familiar with the ANSYS programs: This online course from **October 18 to 22, 2021** is intended for students and researchers with a good knowledge of fluid mechanics and the numerical methods to compute it. Initial experience in computational fluid dynamics (CFD) is welcome. Participants will get to know the ANSYS software package CFX and its functionalities and will learn the most important steps for its use on the LRZ Linux cluster and other high performance computers. Last but not least, possibilities for workflow automation with Python in combination with the CCL/CEL scripting language of ANSYS will be covered. [Information & registration](#)

Classifying texts with speech applications

We've been doing it in everyday life for a long time: using speech assistants, corresponding programs for processing speech (Natural Language Processing or NLP) are now spreading into research with AI assistants. The online course on **October 19, 2021** introduces NLP techniques for processing, analyzing, and generating text-based data. Researchers can use these techniques to create their own NLP applications and enable human-computer communication using chatbots, voice agents, and other speech applications. Deep-learning models are gaining importance because they generalize language, and transformer-based models, such as Bidirectional Encoder Representations from Transformers (BERT), are driving NLP further because their features provide high accuracy in text evaluation. In this course, you will learn how to use BERT and other language applications for text classification. [Information & registration](#)

Modeling with ANSYS Fluid

Calculating and modeling flows - this is where the ANSYS Fluid software package comes in. Over six days starting on **October 28 and ending on December 2, 2021**, this online course provides insights into the functionalities and possibilities that ANSYS Fluent offers researchers. Included are practical exercises with the program package, as well as an introduction of the Linux cluster of the Leibniz Computing Center. Last but not least, possibilities are shown to automate and individualize work steps of ANSYS Fluent with Python and the ANSYS script languages Fluent TUI and Fluent Expression. Participants should have previous knowledge of fluid mechanics as well as numerical methods for the calculation of flows. [Information & registration](#)

Trends in Supercomputing

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

Software Design with C++

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

The challenge of Quantum Computing

Quantum technologies are still young and in the experimental stage. But the community is already networking and discussing innovations, challenges and opportunities: from **29 November to 2 December 2021**, for example, at the European Quantum Technology Conference, which will take place virtually. Topics for lectures, workshops and tutorials as well as research posters can be submitted **until 19 July**. [Information & registration](#)

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, scientists or students 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. We will be happy to contact you.

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!

[IT-Systemadministrator](#) for Linux systems and for management of virtual servers and containers

[Site Reliability Engineer](#) for management and development of the LRZ Data Storage Archive

[IT-Administrator](#) for management and service with Window-clients

[System Engineer](#) for High Performance Storage

[System Engineer](#) for management and development of NAS environment and storage services like Bayernshare

[System Administrator](#) for management and service of Windows Clients

[Researcher](#) for Penetration Testing

[Research Engineer](#) for programming models

[Reserach Engineer](#) for characterization and programming tools

[Spezialist](#) for High Performance and Quantum Computing

[Account-Manager](#) for the support of clients in universities and research organisations

[Student Assistant](#) for the development of ITSM software

[Student Assistant](#) for the web backend und the BAYSICS portal

[Student Assistant](#) for the Servicedesk

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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- 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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