

LRZ-Newsletter March 2022: Enjoy reading and the first flowers

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"Bringing quantum computing into everyday research

The course for the future has been set: "In quantum computing, we are involved in eleven different projects to research the new



processors, to develop software stacks and programming environments, and to integrate quantum into supercomputing," Prof. Dr. Dieter Kranzlmüller, Director of the Leibniz Supercomputing Centre (LRZ), is pleased to report (on the photo left with Dr. Jan Goetz, IQM, at the start of the research project Q-Exa). "The practical handling of this future technology will be exciting." In the future, growing amounts of data are to be evaluated in real time if possible, High-Performance Computing (HPC) needs new concepts to increase computing power further and to accelerate computing for more energy efficiency: "Quantum computing could become a next developmental step for highperformance computing as accelerator," Dr. Martin Schulz, Professor of Computer Science at the Technical University of Munich (TUM) as well as a member of the LRZ Board of Directors, holds out the prospect. "The integration of quantum into supercomputers as well as the interaction of HPC, artificial intelligence and quantum could provide the necessary performance boost." Read on the LRZ website how the integration of quantum processors into the LRZ's supercomputers is being prepared and learn about the most important research projects in which the LRZ is involved. (vs)

"A clever thought usually has many mothers and fathers"

Mathematician, philosopher, inventor, cosmopolitan, today one would add networker: Gottfried Wilhelm Leibniz, who also gave his name to the Leibniz Supercomputing Centre (LRZ) in Garching, lived from 1646 to 1716 and left the world many theories and theorems. Leibniz worked towards the uniformity of scientific terminology; for example, the integral sign, the elongated S as a symbol for "everything" or a sum in mathematics originated from him. In his search for simplification and generalisation, he also developed the foundations for the dual number system, a universal language for mathematics (and informatics) with which all numbers could be represented by the digits 0 and 1 and which is the basis for digital binary codes. The prolific thinker and writer used every half-empty piece of paper to discuss phenomena in nature, mathematical solutions or new techniques. Prof. Dr. Michael Kempe is the master of these pieces of paper and writings, heads the Leibniz Archives in Hanover and is intensively involved with his life and work. In his book "Die beste aller möglichen Welten" (Fischer-Verlag) he condenses the rich work into seven days. Even for an intellectual polyathlete like Leibniz, the day had only 24 hours and the week only seven days", Kempe says, "I found it very attractive to show in an exemplary way what Leibniz tackled in one day and also how he kept getting lost, tangled up." In an interview with the LRZ, the historian explains why Leibniz thoughts are important for today and what we are able to learn from this " intellectual polyathlete". (vs)



Prof. Dr. Michael Kempe and his book about Leibniz

Time travel through universe

With the help of Thesan, the <u>largest and most detailed cosmological simulation</u> to date, an international research team shows how the radiation of the first galaxies changed the cosmos and led to the reionisation of interstellar hydrogen gas. "Other simulations have so far not been able to reproduce how galaxies influence the gas surrounding them in the young universe," explains Enrico Garaldi, a researcher at the <u>Max Planck Institute for Astrophysics</u> in Garching. "Thesan is the first simulation that quantitatively explains how the first galaxies change the gas around them." For the <u>Thesan project</u>, the MPA collaborated for three years with the Massachusetts Institute of Technology (MIT) and Harvard University. Reconstructing the early universe is challenging because it involves modelling extremely chaotic interactions, e.g. between gravity, gas and radiation. Thesan calculates these interactions with the highest level of detail and over the largest volume of any simulation to date. To do this, it combines a realistic model of galaxy formation with an algorithm that tracks the interaction between light and gas, as well as a model for cosmic dust. Thesan has a circumference of 300 million light years, simulates a billion years in the development of the universe and allows a glimpse of the time when the first stars began to shine there and their light heated the gas surrounding them - the starting point of all developments. For Thesan, 60,000 cores of the SuperMUC-NG together calculated around 30 million CPU hours, which would have taken 5,700 years on a desktop computer.



The Thesan-Simulation: The graphic show 6 characteristics of the young universe. Graphic: MPA

Tracking earthquakes and tsunamis

Tectonic plate movements, breaking rocks and towering tsunami waves: A research team led by seismologist <u>Dr Alice-Agnes</u> <u>Gabriel</u>, professor in the Department of Geophysics at Ludwig Maximilians University (LMU) Munich, is using high-performance computing (HPC) to trace the origins of earthquakes and tsunamis - and develop the basis for a warning system for natural disasters. It recently published its results in the journal <u>Nature Geoscience</u>, and the <u>Gauss Centre for Supercomputing (GCS)</u> also reports on the work: "The growth of HPC hardware made this work possible in the first place," Gabriel is quoted. "We need to understand the workings of mega-subduction systems, this helps us to better assess the hazards in subduction zones. It's unclear



which geological faults can actually cause earthquakes of magnitude 8 and above and increase the risk of a tsunami developing." Earthquakes and tsunamis involve a wide variety of forces: the shifting of tectonic plates, physical laws that cause rocks to break and slide under maximum stress, and the propagation and growth of waves. Moreover, not every earthquake triggers a tsunami; the strength of the quakes plays more of a secondary role. Calculating such complex relations requires high computing power. In recent years, the team used the supercomputers of the Leibniz Supercomputing Centre (LRZ)-SuperMUC and SuperMUC-NG – and has created high-resolution simulations of various earthquake-tsunami catastrophes from measured values and data. Par example they have modeled the devastating seaquake on 26 December 2004 in the Indian Ocean, you see its spreading on the map left. And in the process the team

has continued to refine the algorithms. At the SuperMUC-NG, it has now been able to combine several models, and this detailed simulation points to three essential features that significantly determine the occurrence of tsunamis: the stress along the fault line at tectonic plates, the rigidity of the rock and the strength of the sediment layers. In the meantime, the team is working on using artificial intelligence and machine learning methods to extract even more knowledge from the earthquake data, they further improve its models and prepare them for the next generation of supercomputers, the <u>exascale-computers</u>. "We need physics-based HPC models for urgent response computing so that we can react quickly after dangerous events," Gabriel says. "If scientists know which geological structures can cause geohazards, we can rely on some of these models to provide information for hazard assessment and operational hazard mitigation."

When citizens do science IT is needed

Web technologies are part of the game when students conduct research and science involves citizens in research. Most citizen science projects in Germany have built web or mobile apps and websites, tools for research tasks and presence in social media. This is the result of a <u>case study published by the research team</u> at Leibniz Supercomputing Centre (LRZ). "We wanted to know how Citizen Science projects are structured and what they offer in terms of information technology," says Anudari Batsaikhan, LRZ staff member who oversees the contribution to the Bavarian citizen science program BAYSICS here. "Our results show that



the use of web technologies is already very well established in both natural and social science projects." For the study, the team looked at 112 projects listed by the Citizen Science platform <u>"Bürger</u> schaffen Wissen" (photo left). 76 of them focused on habitat research, 36 were dedicated to social issues including history and culture; 23 of the programs target citizens' participation from worldwide, 9 across Europe, the rest in Germany and its states. It doesn't work without an Internet presence - most citizen science projects (78 %) therefore present themselves in a web app, 43 % on a website. Mobile apps are used by 29 %. More than half of the programs (57 %t) rely on one platform, while 43 % combine several. Take for example BAYSICS: Bavaria's citizen research on the effects of climate change provides information via a website, a web app and a mobile app. Like most other citizen science projects, BAYSICS uses

Twitter, Facebook and additionally Instagram to disseminate news and enable participants to communicate with each other. At BAYSICS, interested parties can participate mainly via the web app for <u>making observations</u>. They also find several tools for analyzing data. In addition to such tools, Citizen Science projects primarily offer information materials for research and self-study. "In terms of e-learning, projects could technically provide more tools," Batsaikhan said. "There is also room for improvement in data sharing between Citizen Science projects or between individuals and organizations involved." Only 5 of the programs provide an interface so that data can flow into other information channels, such as those of research institutions or schools. "When developing IT and web-based tools, the goals that Citizen Science programs, in addition to readily available web technology, to provide participants with tools for research and communication. "The more topics a project has researched and the more flexibility it wants to offer participants, the more attention should be paid to interfaces for data exchange." Efficiency is also important in Citizen Science – data sharing can create synergetic effects enabling avoidance of repetition and cross-project data analysis. **(vs)**

Researching, programming and teaching for IT security

The <u>CODE research institute</u> welcomes a new dual leadership team: the <u>governing body of the Universität der Bundeswehr</u> München (UniBw M) has appointed Prof. Dr. Wolfgang Hommel, who worked as team lead and researcher for the Leibniz-Rechenzentrum (LRZ), as Executive Director and Prof. Dr. Michaela Geierhos as Technical Director. Hommel takes over from Prof. Dr. Gabi Dreo Rodosek, who is focusing more on her own research again, including on network security through artificial intelligence (AI). Geierhos in turn follows Hommel: "For the future, it is important to further sharpen CODE's profile," says the new leadership duo. The research institute is dedicated to topics from cyber and IT security as well as smart data and wants to open up quantum computing for the German armed forces and authorities. Its leadership duo is well equipped for this: Hommel has held the professorship for IT security of software and data at UniBw M since 2016, and his colleague Geierhos has been appointed professor of data science in 2020. The establishment of further research groups in the areas of privacy and applied cryptography is planned for 2022. In <u>the LRZ interview</u>, the CODE leadership team explains its plans and goals.



The new leadership team of CODE, Prof. Michaela Geierhos and Prof. Wolfgang Hommel

Bundesverdienstkreuz for member of LRZ Advisory Board

High honour for a member of the advisory board of the Leibniz Supercomputing Centre (LRZ): Prof. Dr. Martin Wirsing was awarded the Bundesverdienstkreut am Band by Bundespräsident Frank-Walter Steinmeier. Markus Blume, Bavarian <u>Minister for</u> <u>Science and the Arts</u>, presented it to him at the beginning of March (see photo left): "You have rendered great services nationally and internationally in science, research and teaching," Blume said. "Today, programming is about to become the fourth cultural



technique with a key significance for all areas of the economy and life." Wirsing has been an <u>elected LRZ advisory board</u> <u>member</u> since 2019, was vice-president of Ludwig-Maximilians-Universität München (LMU) and held its chair of programming and software engineering. There, Wirsing taught and researched the working processes of computers and the methods of programming. "It's surprisingly great to get a medal," he says with a laugh. "Never expected to get a medal myself." The mathematician and computer scientist is the author and editor of 20 books on software, IT systems and programming languages, he published around 200 scientific studies and headed various European research projects. Wirsing studied mathematics at the LMU and in Paris, worked at the Technical University of Munich (TUM) for a long time for the computer science pioneer and LRZ co-founder Prof. Dr.

Friedrich Bauer, was appointed to the chair of computer science at the University of Passau in 1983 and moved to Munich to the LMU in 1992. "As a professor of computer science, Martin has enriched teaching and research, and as vice-president of LMU he has continuously worked to improve study conditions," comments colleague Dieter Kranzlmüller, also a professor at LMU's Department of Computer Science and Director of the LRZ. "Great commitment and a well-deserved award!" Wirsing is almost glad that the pin is only worn rarely and on special, ceremonial occasions: "After all, I belong to the generation of 68," he says. "We were actually suspicious of medals. But the Federal Cross of Merit is really an honour that touches me, and it is a democratic award, anyone can nominate anyone for it." **(vs)**

Figures of the Month

Sharing is Caring: Since **2020**, the LRZ has been associated with <u>URLhaus</u> by <u>abuse.ch</u>, a non-profit initiative for IT and cybersecurity that emerged from a research project at the University of Bern. This collects characteristics that indicate the compromise of websites and IT systems. These so-called Indicators of Compromise (IOC) are mostly malware, they are listed by URLhaus and qualified according to activity, type, source, domain or URL. Since registration, the LRZ has reported **more than 1,000,000**, or more precisely: **1,004,496** malware URLs. Thus, the LRZ has become the top reporter of the useful service. **99** % of the malware are Mozi files - a malware family for Linux systems that builds on the source codes of older malwares and is preferably used for Distributed Denial of Service attacks (DDoS). "You have helped remove **1,002,304** malware pages. Thank you very much," writes the URLhaus system to the LRZ security team. We are happy to join in.

WORKSHOPS & EVENTS

Smart Technics for science

Artificial intelligence (AI) techniques help in the analysis of research data. Therefore, NVIDIA, EuroCC GCS and OpenACC.org have developed an online bootcamp for researchers to learn how to use AI tools, techniques and algorithms. The two-day course will take place on **7 and 8 April 2022** and will teach step-by-step core concepts of deep neural networks, how to build deep learning models, and how to control accuracy. Information and registration

Data analysis with methods of Artificial Intelligence

Getting to know the techniques of evaluating and analysing Big Data with Artificial Intelligence (AI) methods: That is the plan from **19 to 22 April 2022** at the LRZ's Data Analysis Week. Among other things, participants will learn about high-performance computers and AI resources at the LRZ, as well as container techniques and, above all, the most diverse methods for evaluating and analysing large amounts of data using artificial intelligence and machine learning. In addition to lecturers from the LRZ, specialists from Intel will show tricks for using the latest AI-capable processors. <u>Information and registration</u>



Quantum Computing – Technology and fields for application

World of Quantum is the name of a new trade fair in Munich, which will take place from April 26 to 29, 2022 at the Messe München. The Leibniz Supercomputing Centre presents together with the Munich Quantum Valley (MQV), the Munich Centre for Quantum Science and Technologies (MCQST) and the institute for lifelong learning of TUM. Visitors are able to know opportunities for qualification and the project QL3,

also the activities to embed quantum processors in supercomputers and all the research activities in Munich. The new conference and fair is a part of the Munich's trade show Laser-Photonics.

#WomenInScience



Compute centers - a place for girls

Drawing girls' attention to careers in STEM subjects, getting them excited about technology, computers, informatics and offering practical insights into the day-to-day work of computer specialists: <u>Girls' Day</u> will take place again on **April 28, 2022.** As in previous years, the Leibniz Supercomputing Center (LRZ) will be taking part again in 2022. Girl's Day will take place virtually. At the LRZ, participating young women will be taken into virtual worlds and can build their own rooms in the Mozilla Hubs. <u>Registrations</u> start now.

Programming GPU for deep learning

Graphic Processing Units (GPU) are also made for artificial intelligence (AI) and machine deep learning applications. From **10 to 13 May 2022**, researchers can learn how to prepare and programme these new processors for their own tasks in an online course organised by the Partnership for Advanced Computing in Europe (PRACE). Experienced instructors from European supercomputing centres will introduce the programming models on OpenACC and CUDA, show how to use GPUs and how neural networks can be trained with them. Information and registration

Introduction to the HPC systems at LRZ

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

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Learn C++ and programme with it

The C++ programming model is made 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. How to use C++ skillfully you will learn 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, usage of memory 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

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 <u>online</u>. 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.

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 <u>career page</u> of the Leibniz Supercomputing Centre or send an <u>unsolicited application</u>. We are LRZ - and curious about you!

Manager for the CRM-System

IT specialist für die Betreuung von MAC- und mobilen Geräten Project manager media design for relaunches of web sites (BADW) IT specialist for expansion of hosting environments

Expert HPC and parallel Computing for life sciences and chemistry HPC Software engineer for the quantum software stack IT specialist or system consultants for the multi factors authentification Programmer for IoT research projects Software developer for the research data management IT specialist for data storage and backups

<u>PR manager</u> for science and online communication <u>Administrator</u> for licenses

<u>Student assistant</u> for pr and content <u>Student assistant</u> for ITSM software development <u>Student assistant</u> for the licence team <u>Student assistants</u> for the service desk

MORE TO READ

Here you will find links to latest information from the german-european supercomputing community and our cooperation partners

- The <u>newsletter</u> 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

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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