LRZ-Newsletter May 2021: Enjoy reading!

NEWS

Artificial Intelligence for the SuperMUC-NG

SuperMUC-NG has now been in operation at the Leibniz Supercomputing Centre (LRZ) for almost three years - time for an interim evaluation, but also for plans to upgrade the current system. In cooperation with Intel and Lenovo, the system will be upgraded to integrate high-performance modelling and simulation with artificial intelligence (AI) and deep learning methods. For this purpose, SuperMUC-NG Phase 2 will integrate next-gen Intel Xeon Scalable processors (codename Sapphire Rapids) as well as the new Intel GPU Ponte Vecchio based on Xe-HPC micro-architecture for HPC and AI. Intel's Ice Lake processors in turn make up the DAOS storage system, which accelerates access to large amounts of data.

To ensure that phase 2 of SuperMUC-NG continues to operate as energy-efficient as possible, the 240 Intel compute nodes are integrated into Lenovo's SD650-I v3 platform, which is directly cooled with warm water. "At the core of all LRZ activities is the user. It is our utmost priority to provide researchers with the resources and services they need to excel in their scientific domains," says Prof. Dr. Dieter Kranzlmüller, director of the LRZ. " Over the last years, we've observed our users accessing our systems not only for classical modeling and simulation, but increasingly for data analysis with artificial intelligence methods." These new techniques for processing data are shaping everyday research, requiring a lot of computing power, but most importantly, a different computer architecture and more flexible data storage. The new storage is expected to arrive in Garching in the fall of 2021, with the compute system expected to follow in the spring of 2022.

Preparations for the SuperMUC-NG mid-term review are in full swing. This will take place from **June 8 to 10** at the three-day "Status and Results" workshop. Scientists who have worked with the LRZ supercomputer will present their projects and simulations. Prof Volker Springel from the Max Planck Institute for Astrophysics is one of the participants. He challenged the SuperMUC-NG with the largest research project to date and models the formation of galaxies. Participants of the event will learn how the LRZ will improve supercomputing and the data analysis with the BEAST test environment, artificial intelligence methods and quantum processors. To read up on the research at SuperMUC-NG, the latest report volume has just been published. **(vs)**

SuperMUC-NG in virtual space

The SuperMUC-NG on an island, under a glittering disco ball, in the mountains, in a club or in a super cool modern living room: At Girls'Day 2021, the supercomputer of the Leibniz Supercomputung Centre (LRZ) traveled through virtual worlds of the Mozilla Hubs. There, 12 participants built their own rooms for it with the software Spoke and under the guidance of Elisabeth Mayer and Lea Weil, both employees at the Centre for Virtual Reality and Visualization (V2C). "The girls did not only learn how to use this virtual world and what you can do with it, but also a few basics about using browser-based software, 3D programs and virtual reality," Mayer explains.

Learning and experiencing how exciting technical professions can be - that is the goal of Girls' Day, in which the LRZ participates every year and which took place digitally for the first time in 2021. Female LRZ employees showed the high school students interesting software, online tools, and also their workplace. They described tasks, for example in the areas of research and development, of supercomputing as well as in the area of general user services and at the service desk. And of course, Petra Gärtner, who is responsible for vocational training at the LRZ, also presented the opportunities to complete such an vocational education at the supercomputing centre. "Better than school, simply something different and very diverse," said one participant, summing up the day's program from 9 a.m. to 3 p.m. And another: "I found the designing of the rooms very nice." Perhaps some of them will come back as trainees or students? **(vs)**

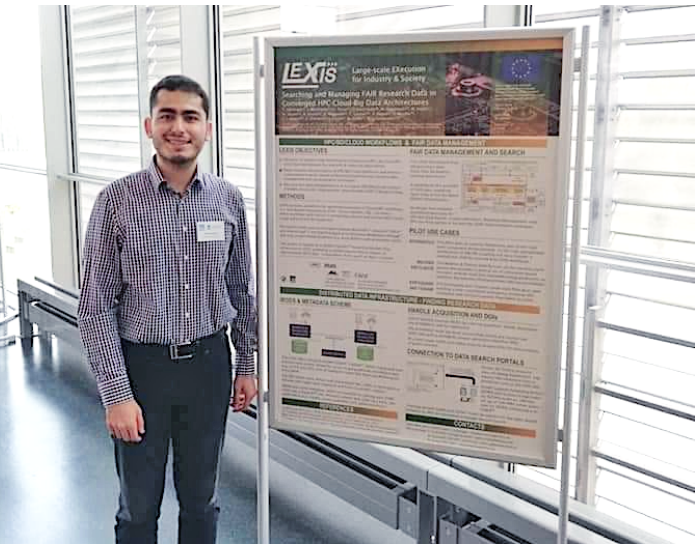
"Finding and inspiring the right specialists for the QIC"

Numerous media reports, many "likes" and followers in the social media: The opening with high-ranking politicians and scientists brought a lot of attention to the Quantum Integration Centre (QIC) at the Leibniz Supercomputing Centre (LRZ). Luigi Iapichino, who holds a doctorate in astrophysics, heads the Quantum Computing team at LRZ. He is assisted among others by Stefan Huber, who holds a doctorate in quantum physics, and who will provide future users with access to the two simulators and support them in their daily work. Interest in working with the Quantum Learning Machine (QLM) from Atos or the 42-qubit simulator from Intel is growing in the Bavarian science community. At the beginning of May, the QIC organized an introductory course for the QLM with Atos - this is now a prerequisite for using the simulator: "With a limited user group, we can document initial experiences and instructions as well as get to know better users' requirements, after which we will systematically expand this," say Iapichino and Huber. In an interview on the LRZ website, the two explain the QIC's latest plans, how researchers can use the new quantum techniques themselves, and what research tasks in the field the LRZ is currently preparing.

Since 2020, the supercomputing centre has been involved in the QuantEx project, testing new quantum algorithms with the SuperMUC-NG and systems on site. With the Technical University of Munich, Infineon and the startup IQM, the QIC will also develop and test quantum processors, and with the Fraunhofer Institute for Applied and Integrated Security it is exploring technology and software issues: "We are now building structures for this," reports Iapichino. The QIC is currently still looking for employees and a space for a test lab. "If we achieve a similar reputation in quantum computing as the LRZ as Supercomputing Centre in five years, that would be a great success," Huber and Iapichino believe. "That's less about the systems, a big desire is to find the right specialists for the QIC and get them excited." Read more in the interview on the website. **(vs)**

Research data from the cloud

Access to research data from anywhere and at any time: What has long been state-of-the art for private photos, letters and files for internet users around the globe is now being worked on feverishly in high-performance computing (HPC). "For simulations and modeling, significantly larger amounts of data have to be moved, and in addition, no two supercomputers are built the same way," says Mohamad Hayek, outlining fundamental challenges. "In supercomputing, data transfer is therefore a much more complex matter." For about two years, the engineer and computer scientist has been working in the Research Data Management team to make Big Data accessible to scientists from Bavaria, Germany, Europe, stored on the servers in Garching and other supercomputing centers. "I can learn a lot for my subject in the process and deal with new techniques and tools," he says. "I like that."



Mohamad Hayek is one of a remarkable group of researchers the LRZ continuously features on its website. The engineer and computer technician is changing and improving supercomputing with his ideas. For the European project LEXIS - the acronym stands for Large Scale Execution for Industry and Society - he is responsible for the technology of the planned cloud platform. In about two years, this has been created with the help of the data management software Integrated Rule Oriented Data System (iRODS) and with B2SAFE, a program from EUDAT for storing large amounts of data. Tested several times and scientifically documented, the first users are already retrieving data and integrating it into an HPC system of their choice. It is quite possible that this will become an international standard and service for research. The portrait on the website describes how Mohamad works, what he studied in Beirut, what his future plans are, and also how the LEXIS platform was built. **(vs)**

Turbulence causes a sensation

It's breaking records and is electrifying science lovers: The most detailed simulation of interstellar turbulence to date. SuperMUC calculated more than a trillion resolution elements, in total, more than 65,000 compute cores worked for it. The simulation required more than 100 snapshots, stored intermediate results, and around 130 terabytes of main memory. The scientific journal "Nature Astronomy" reported on it in detail and devoted its April cover to the research paper in which the team led by Dr. Ralf Klessen of the Ruprecht Karls University in Heidelberg and Dr. Christoph Federrath of the National University Canberra located the sound barrier. Astrophysicist Luigi Iapichino accompanied the research project at the LRZ and explained in a virtual discussion

in Australia in April on how such a simulation can be accomplished in supercomputing systems. **(vs)**

Figures of the month

Without personal computers (PCs), notebooks and tablets, nothing works at the universities: At the beginning of April, the Leibniz Supercomputing Centre hosted **13144 Windows PCs** within the Münchner Wissenschaftsnetz (MWN) at the two Munich universities. In Corona times, however, only a portion of these, namely **8808 devices,** are currently being switched on again and again. That the digital efforts are constantly increasing at the chairs, is shown by the fact that **463 additional MWN-PCs** have already been planned and prepared for installation. In addition to PCs with Windows or Linux operating systems, scientists also like Apple computers: **732 MacBooks** and iMacs are maintained by the LRZ, and these are particularly popular with biologists **(87)** and lawyers **(69)** at Ludwig-Maximilians-Universität (LMU), as well as with educators at the Technical University of Munich (TUM **- 65**). This department also has the most tablets in use, **namely 333** out of a total **of 833 distributed** across the universities. **(vs)**

WORKSHOPS & EVENTS

Wanted – Data projects for supercomputing

Companies, startups and scientists who need the computing power of supercomputers as well as clever analysis and data management tools for a Big Data project can apply to **LEXIS** **now and until June 2021.** The European project, in which the LRZ is also involved, is looking for partners from science and industry to test the newly developed, powerful data platform and its tools, which has already proven itself in some specific research work, with the help of questions and applications from practice. The focus of LEXIS is on location-independent access to Big Data as well as its storage. LEXIS also supports the development of Artificial Intelligence and Machine Learning applications. The LEXIS platform is particularly suitable for issues in areas such as aeronautics, automotive, disaster control, medicine, pharmaceuticals, weather and climate information. More info and registration on **the Lexis website.**

Informatik 2021 – ideas for future

The Gesellschaft für Informatik is looking for ideas for the IT of the future and for optimizing existing applications for its annual conference in the fall. **"SKILL"** is the name of the presentation plenary for students of computer science, they can submit proposals for workshops and presentations until **May 9, 2021.** Papers and workshops about **energy effiency** – for this sessions the LRZ is responsible – will be taken until **May, 17,** this deadline has been extended. Other topics of the Informatik 2021 include e.g. **Artificial Intelligence** and **Environmental Research**. Papers, talk topics and workshops are also still being sought for these parts of the program. Submission deadlines are **May 31, 2021,** and **June 26, 2021.** The **Informatik 2021** will take place September **27-October 1, 2021.**

Quantum in a personal view

Push Quantum wants to introduce students to quantum computing, for example in hackathons during which participants solve real tasks from companies with the help of annealers and simulators, or in digital meetings with managers and specialists from companies that supply products for quantum computing. On **May 11, 2021,** Dr. Christophe Jurczak, Investor and co-founder of Le Lab Quantique, shareholder at Quantonation and board member at Nord Quantique, will describe how quantum computing can help the pharmaceutical industry find new drugs or decipher molecular structures. **Registration**

The Architecture Machine

A short video already stirs up anticipation: "The Architecture Machine" has been extended **until June 2021**.The exhibition at the **Pinakothek der Moderne** traces the role of the computer in architecture and urban development - and it's a story as worth seeing as it is exciting. Computers have long been helping with drawing, designing, even clarifying and presenting, and now they calculate traffic and other developments. In the Pinakothek der Moderne, this is told in multimedia and, among other things, in virtual worlds. The Leibniz Supercomputing Centre (LRZ) supports the exhibition with technology and has advised the makers in advance. Meanwhile, museum visits can even be scheduled again, **register your visit** at the Moderne Pinakothek.

Crash Course for the LRZ Linux Cluster

On **June 1, 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 will be explained. **Information and registration**

SuperMUC-NG in science

For about two years the SuperMUC-NG at the Leibniz Computing Center(LRZ) has been working for science. Now a first résumé is drawn. Researchers will report on their projects and experiences with the system, which consists of over 311,000 computing nodes, at the **SuperMUC-NG Status and Results Workshop** **from June 8 until 10. 2021**. Participants in the virtual event will also learn how the LRZ will shape its next future, improve and accelerate supercomputing, and what role artificial intelligence, high-

performance data analytics and quantum computing will play. They can also learn about the new BEAST testbed and its computing resources. **Information and registration**

Performance control for supercomputers

The **Virtual Institute - High Productivity Supercomputing** (VI-HPS) at RWTH Aachen University has developed a software package for the performance diagnosis of supercomputers and applications, which can be used to test and optimize your own algorithms before use. In a digital 5-day webinar from **June 14 to 18, 2021,** the LRZ and VI-HPS will present this program suite, its elements and various fields of application. Interested parties should have first experiences with parallel computer systems and highperformance computing, they can check and improve their own applications in the course with the lecturers. **Information and registration.**

C for beginners

C is one of the most widely used programming languages, is used in the development of software as well as processors, and other languages such as C++, Java, PHP or Perl are also based on it. In three days from **June 21 to June 23, 2021,** participants will learn how to use C in their everyday lives. Of course, it's not just about the basic codes and programming, but also about debugging, version management, tips & tricks. Cost: 30 to 600 euros. **Information and registration**

News about supercomputing

From **July 24 to 29, 202**1 **International Supercomputing (ISC) 2021** will open its virtual doors. Europe's largest meeting place for supercomputing will showcase ideas for computer architectures and innovative applications. Sustainability and energy consumption are set topics, and there will certainly also be discussions about how artificial intelligence and machine and deep learning methods can accelerate supercomputing. Last but not least, there is sure to be talk about quantum computing and what is expected to be the next generation of accelerators, Quantum Processing Units QPU). The Leibniz Supercomputing Center will be represented with its own workshops, talks and presentations during ISC 2021.

Trends in supercomputing

The next **Supercomputing (SC21)** has already been scheduled. The US counterpart to ISC will start on November 14, 2021. The **registration deadlines** for papers, presentations and workshops have just expired, and the initiators are already working on the program. Leibniz Supercomputing Center will also participate in this international conference and trade fair with numerous projects and presentations.

JOB OFFERS

You will find an international and diverse team in Garching, that is constantly growing. We have various job offers out at the moment please visit the **career page** of the Leibniz Supercomputing Centre for more information. We are LRZ - and curious about you!

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
Newsletters of the Gauß-Alliance
Publikations 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**.
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