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NEWS

The Future of Supercomputing – On the ISC Conference and Exhibition

"Shaping Tomorrow" or "designing the future" is the motto of the [ISC High Performance Conference](#): from **24 June to 2 July 2021**, technologies, strategies and methods will be discussed that can take supercomputing and the High Performance Computing (HPC)



community to the next level and into exascale times. This year, Europe's largest HPC event features representatives and partners from the Leibniz Supercomputing Centre (LRZ) as never before: As [Program Chair, Prof Dr Martin Schulz](#), Director at the LRZ and Chair of Computer Architectures and Parallel Systems at the Technische Universität München (TUM), has compiled the topics and sought lectures and speakers for them. "Our goal was to find speakers worldwide who have not yet been heard on the new technologies for supercomputing and who have yet to publish their research results," Schulz tells us in an [interview that you can find on the LRZ website](#). "It is an honour to be chosen as Program Chair. I like doing it because it's about networking with the community and the ISC is a nice event."

Schulz was supported by the organisational team of the ISC as well as by the program team, or rather: by Professors Gerhard Wellein and Georg Hager, both from the National HPC Data Centre (NHR) at Friedrich-Alexander University Erlangen-Nuremberg. Schulz's colleague Hans-Joachim Bungartz, also LRZ director and TUM professor of computer science, is responsible for the

"Applications and Algorithms" series of the invited part of the program. The ISC program includes many more contributions by LRZ users from Bavaria and staff. A selection - ordered by date:

28 June: [Prof. Dr. Xiaoxiang Zhu](#) has been modelling the future of cities, mobility and coexistence for years with the help of earth observation data. The TUM lecturer and head of Earth Observation Data Science at the German Aerospace Center (DLR) will open this year's ISC with a [lecture on the growing importance of artificial intelligence](#) methods in supercomputing.

- On the same day from 5 p.m., LRZ specialist [David Brayford](#) and colleagues will present the opportunities and [challenges of OpenHPC](#), technical requirements, tools and workflows.

29 June: How supercomputers help to decipher the processes of earthquakes and tsunamis and improve disaster prevention will be explained by LMU Professor and Ada Lovelace Award winner [Dr. Alice-Agnes Gabriel](#) in her talk from 2 pm.

30 June: For all its power - the supercomputing of the future must be energy-efficient and needs to be monitored closely. LRZ expert [Dr. Michael Ott](#) will [discuss the necessary measurements](#), suitable programmes and their functionalities with colleagues from other data centres starting at 2 p.m.

- Starting at 5 p.m., things will get practical – [in a workshop](#) HPC specialist [Michele Martone](#) from the LRZ will show the problems of differential equations with lowest values in simulations and how to solve them.

1 July: The amount of research data is growing, HPC is gaining importance in more and more scientific fields. [Dr. Volker Weinberg](#), lecturer and coordinator of the LRZ training program, discusses with colleagues from other institutions [how students can obtain computing resources](#) and how they can prepare themselves for working with algorithms in a roundtable,

2 July: Big Data needs supercomputers because they are able to carry out artificial intelligence processes. LRZ scientist [Dr. Juan Jose Durillo](#) and colleagues will show how Deep and Machine Learning can be developed, optimised and scaled on parallel systems in [a four-hour workshop](#) from 2 to 6 p.m.

- Containers facilitate access to data, software and codes regardless of location. In [a workshop](#), experts, including LRZ HPC specialist [David Brayford](#), will show the tricks and challenges.

- How compilation techniques can increase the performance of HPC systems and control the results is the focus of a workshop taking place digitally around the ISC, where LRZ staff member [Michele Martone](#) will show practical examples.

Already in the run-up to the ISC, on **23 June** during the Intel Dev Summit, [Elisabeth Mayer](#) from LRZ's Centre for Virtual Reality and Visualization (V2C) will present their visualization of the blood flow in human veins. The LRZ program "Future Technology" and the new test environment BEAST will again be the topic at the booth of Intel, where [Dr. Josef Weidendorfer](#) will explain it and show. **(vs)**



Orchestrating Thousands of Computer Nodes

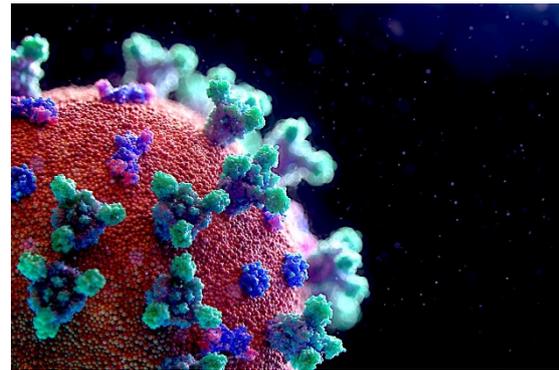


Working with accelerators, with GPUs or - soon - with quantum processors, more and more monitoring and optimisation on systems and codes: The HPC community is currently focusing on many strategies to take supercomputing to the next level or into exascale times. [Amir Raoofy](#) is also committed to this goal: The young computer scientist and engineer, born in Iran, is researching how parallel systems can process data and how the interaction of thousands of computing nodes can be improved. For his PhD thesis [Raoofy](#) sometimes works at the Leibniz Supercomputing Centre (LRZ) on SuperMUC-NG, the Linux cluster CoolMUC and, most recently, on the test environment BEAST: "We are in the data age, I am interested in which measured values or information can best be used to describe or analyse a computer system in order to better understand its work, to be able to intervene in the event of errors and to achieve more performance," he describes his interest in a [portrait on the LRZ website](#). The doctoral student, who was awarded the [Hans Meuer Award](#) during the ISC in 2020, also tells us what his work has to do with music and a choir. (vs)

On the Trail of the Corona Virus

Successful research: A team from the Technical University of Munich (TUM) and the Max Planck Institute of Biochemistry has tracked down [the attack tactics of the Corona virus](#) and revealed how it alters proteins in human cells on several levels in order to replicate. "This knowledge helps to better understand the virus and find starting points for new drugs," explains Dr. Andreas Pichlmair, Professor of Immunopathology at the Institute of Virology at TUM. The Linux cluster CoolMUC of the Leibniz Supercomputing Centre (LRZ) was also involved [in the research](#): in almost 6.5 million computing hours, mass spectrometry data from around 1200 experiments were analysed. "In each of these, we identify and measure the density of thousands of proteins from human cells, on average about 5000 per experiment," reports bioinformatician Dr. Alexey Stukalov.

Pichlmair's team documents their work in the [scientific journal "Nature"](#): The focus is on the interactions of human lung cells with the viruses SARS-CoV and SARS-CoV-2 (Corona). If cells defend themselves against the multiplication of intruders, complex protein signalling sequences are set in motion on both sides. In addition, proteins are supplemented and remodeled by molecules. The research team led by Prof. Dr. Andreas Pichlmair and Prof. Dr. Matthias Mann, who heads the Department of Proteomics and Signal Transduction at the MPI of Biochemistry, investigated these developments with the help of mass spectrometers and bioinformatic analysis methods. The result is a map that shows the different points of attack of the viruses, i.e. which of their building blocks bind to which proteins of the cells, remodel them by adding molecules and thus change their function.



A total of 1484 interactions between the building blocks of cells and viruses were traced. "To determine the proteins specifically affected by SARS, we applied a statistical model for each one and implemented it in the STAN modelling platform," Stukalov reports. "This approach provides a comprehensive analysis of the data, but is quite computationally intensive. Without the LRZ team, we would not have been able to complete our study in the tight timeframe." From April to October 2021, CoolMUC completed a total of 166 jobs. The result is something to be proud of: An openly accessible database now provides information on where Covid-19 attacks cells - knowledge that pharmacologists can now use to develop drugs against the symptoms of Corona and improve vaccines. Pichlmair and Mann's research was one of the [projects in 2020](#) that were granted accelerated access to the LRZ's computing capacities last year to fight Corona. (vs)

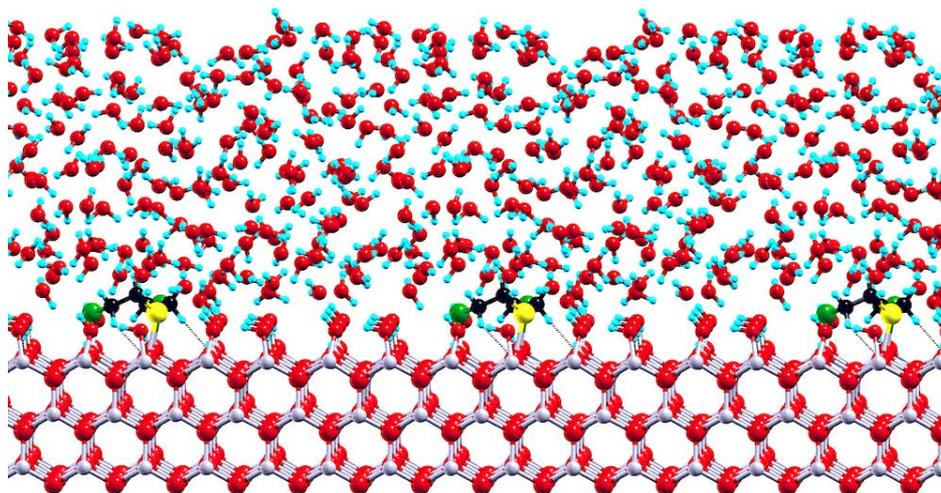
IT Technology and Services for Museums

It all started with films, but today more and more museums and exhibitions are using virtual, augmented and mixed reality to show art, science or natural phenomena (Screenshot left: virtual Caravaggio-exhibition). The 34 houses of the Bavarian State



Museums and Collections therefore need [more and more IT technology](#): "Museums no longer just show things on the wall, more and more new media are moving into the halls, presentations and didactics are changing," reports Lars Raffelt, who heads the IT Service Centre of the Museum Association. "You need IT and services for that. Someone also has to take care of laying fibre optics or cables or setting up databases. We realize that together with the LRZ." You can find out how the Leibniz Supercomputing Centre (LRZ) also supports the IT Service Centre, why museums are digitizing more and more exhibits and making them publicly accessible online, and why sometimes even a grandfather clock needs professional IT support in [an article on the LRZ website](#). (vs)

Calculate Faster with Car-Parrinello Molecular Dynamics

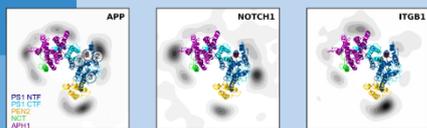


Car-Parrinello molecular dynamics (CPDM) is used by supercomputers in physics, chemistry or materials research to calculate and model the spatial movements of atoms and molecules. In the process, communication between the computing nodes in the parallel computer systems is increasingly proving to be a brake on the implementation of the algorithm on all computing nodes and their work. In cooperation with the Leibniz Supercomputing Centre (LRZ), a team from the Friedrich Alexander University (FAU) Erlangen has now succeeded in speeding up the CPDM program enormously and adapting it to the ever-growing number of computing nodes in modern parallel systems: CPDM can now be integrated and run faster on the SuperMUC-NG and other current supercomputers - making it easier to calculate formulas and develop new materials. A [short report](#) on the adapted algorithm can be found on the LRZ website, [the research report here](#).

P. Bastian • D. Kranzlmüller • H. Brüche • M. Brehm • G. Mathias
EDITORS

High Performance Computing

in Science and Engineering
Garching/Munich 2020



Figures of the Month

The new report volume “High Performance Computing” from the Leibniz Supercomputing Centre (LRZ) weighs **1196 grams**: It describes excellent science and research that could be realized and calculated from 2018 to 2020 with the help of SuperMUC-NG. On **280 pages** and in **619 photos, images or graphics**, the weighty work presents a total of **115 projects in 10 chapters** - among them are simulations of natural phenomena and from space, also of processes in the human body or of airflow around vehicles and other technology. This shows the wide range of HPC in the research fields today. Of course, the [work can also be read online](#). The PDF requires **25 megabytes of storage space** in low resolution and **103 megabytes in high resolution**, both works together **128 megabytes**: Enjoy browsing and reading. (vs)

WORKSHOPS & EVENTS

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 Result 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](#).

Quantum Computing in Practice

Register quickly: On **9 June 2021**, the [Bavarian Quantum Computing xChange](#) community of the Leibniz Supercomputing Centre (LRZ) will once again meet online to exchange ideas. This time, the Zoom meeting from 4 p.m. will focus on real applications for quantum computing. These are now becoming accessible to researchers and companies via cloud services, for example at the LRZ. So it's time to take a look at the practical challenges of the new computers: Machine learning methods are the focus of Dr Sonika Johri's lecture. The physicist works at the US manufacturer of quantum computers IONQ with processors whose compute units or qubits are created with the help of ion traps. She explains the specific functionalities of this technology. Dr Jeanette Lorenz, meanwhile, comes from the Fraunhofer Institut für Kognitive Systeme and traces the advantages of quantum computers over supercomputers. She will answer the question of what kind of algorithms already work on the first, still noisy quantum computers with a small number of qubits and how classical computers can cooperate with their new colleagues. [Informations and registration](#).

Tools & Tricks for HPC

The [Virtual Institute - High Productivity Supercomputing](#) (VI-HPS) at RWTH Aachen University has developed a software package around performance diagnostics of supercomputers and applications, which can be used to test and optimize algorithms before deployment. This suite of programs will be the focus of the 5-day Tuning Workshop from **June 14 to 18, 2021**. 12 experts from international data centers will explain how to use the tools, show their tricks, talk about their experiences and help participants improve codes. Interested parties should have some experience with parallel computing systems and high performance computing. [Information and registration.](#)

Computer Science for A Better Future

Researchers and scientists from the fields of mathematics and computer science will meet in Krakow from **June 16 to 18**: There, during the [International Conference on Computational Science](#), they will discuss trends in computational disciplines and methods, as well as software and research applications for physics, chemistry, biological and environmental sciences, medicine and engineering, and increasingly also the arts. The motto of the event is Informatics for a Better Future. Of course, solutions for security and data protection are also on the agenda. Prof. Dr. Dieter Kranzlmüller, head of the Leibniz Computing Center, has put together the main program together with computer scientist Prof. Dr. Maciej Paszynski from AGH University in Krakow. [Information and registration.](#)

Making Waves for Research & Teaching

Networking, IT technology and services, tools - GÉANT is the umbrella of all national networks that take care of the digitalisation of research and teaching in Europe. From 21 to 25 June, GÉANT invites you to its TNC conference, which will take place online for the first time this year and can be attended free of charge. "Making waves" is the motto, because digitisation and IT are changing and reshaping the coasts in a similar way to waves. For one week, lectures, discussions and workshops will focus on platforms for researchers, networking between researchers and projects, tools for data analysis, the management of research data, the security of data and its users. Of course, the experiences from the last Corona year with online courses and digitalisation offers for universities and research institutions will also be discussed - one question is how IT and the internet support student mobility. Studying and researching simultaneously in Munich and Lyon or Perugia is now becoming a reality. [Information and registration](#)

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 until end of 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](#).

New Technologies for Supercomputing

Artificial intelligence methods, data analysis, new tools and techniques for supercomputing - the Association for Computing Machinery ACM, the Swiss Computing Center CSCS and SIGHPC Education invite you to the #PASC21 conference. From **July 5 to 9, 2021**, the focus will be on methods, tools and many tricks for supercomputing. The LRZ will be represented at the five-day program with a lecture on artificial intelligence on parallel systems. [Information and registration.](#)

Deep Learning and GPU Programming

The OpenACC and CUDA programming languages can be used to accelerate HPC applications, but also to train neural networks and use them for pattern recognition or data analysis. In this four-day workshop from July 12-15, 2021, participants will also learn how to parallelize the training of deep and machine learning systems on multi-GPU. The online workshop combines lectures with hands-on exercises. [Information and registration.](#)

Crash Course for the LRZ Linux Cluster

On **July 21, 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. [Information and registration.](#) The course will be repeated on [September 15, 2021](#).

News about Supercomputing

From **July 24 to 29, 2021** [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.

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 and 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**. 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 and registration](#)

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.

Software Design with C++

Object-oriented (OO) software design with the C++ programming language is the focus of this three-day workshop from **September 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 and registration](#).

USED THINGS FOR FURTHER SERVICE

The LRZ is GIVING OUT used furniture. Interested parties from universities and research organisations please contact as soon as possible under the mail address <althardware@lrz.de>. The furniture is of course free of charge. We will get in touch soon.

- **Filing cabinet**, derived timber products, gray front, 5 shelves. Dimensions: 100 x 227 x 44 centimeters.
- **Steel cabinet**, gray, dimensions: 89 x 103 x 42 centimeters
- **Two steel cabinets**, gray, consisting of coat racks and shelves. Dimensions: 120 x 194 x 43 centimeters
- **Steel cabinet**, consisting of 4 lockers, gray, dimensions: 120 x 180 x 55 centimeters
- **5 lockers**, consisting of 3 units each, including bench, blue. Dimensions: 89 x 170 x 55 centimeters

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!

[System-Administrator](#) for the management of Windows-clients

[Web- und Data Base Administrator](#) for the LRZ-data base server

[IT-Architekt and Linux-Specialist](#) for the IT-supply of the Bayerischen Staatsbibliothek

[System-Engineer](#) for High Performance Storage

[System Engineer](#) for the development of storage services, e.g. BayernShare

[Account Manager](#) for clients of LRZ

[Staff referent](#)

[Staff officer](#) for present- and application management

[Associate](#) for Finance and Funding

[Student Assistant](#) for digitalization tasks

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

[Student Assistants](#) 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

[Publikations](#) of the Gauss Centre for Supercomputing (GCS): GCS-News und Inside

[Infoletters](#) 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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- 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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