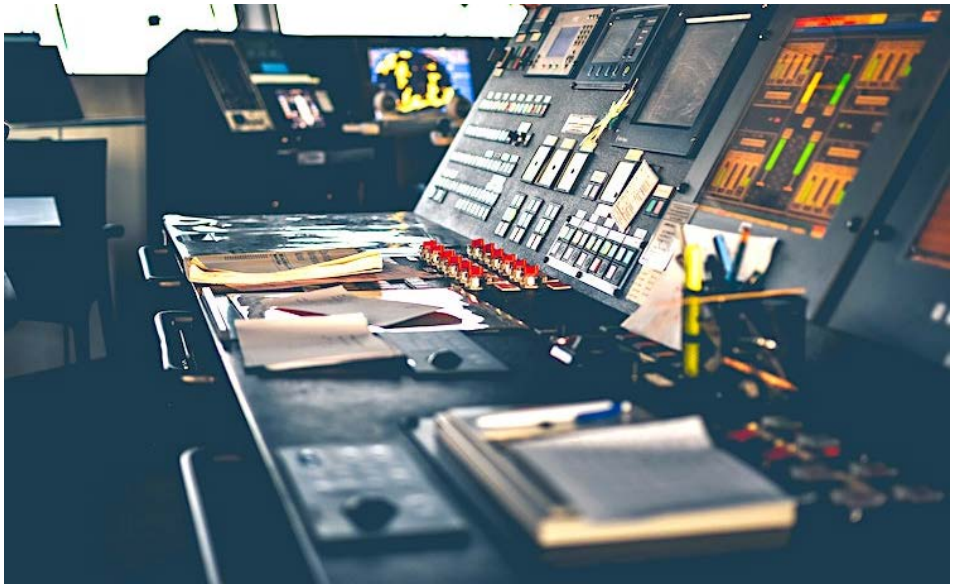
Our Topics:

News

Award-Winning Supercomputing Research



The more than 6480 compute nodes of the SuperMUC-NG contain around 15 million sensors that collect a wide range of data from the system. "In preparation for exascale times, high-performance computing systems are becoming increasingly complex," explains Alessio Netti, computer scientist at the Leibniz Supercomputing Centre (LRZ) in Garching. "For these systems to run stable, become more controllable and, above all, consume significantly less energy, we need more knowledge and thus more data". At the end of June, two projects which deal with operating data of high-performance computers, received awards: The jury of the ACM HDPC 2020 conference honoured the LRZ tool Wintermute in Stockholm as one of the most innovative analysis methods for High Performance Computing (HPC). At the ISC 2020 in Frankfurt, a research team led by Amir Raoofy from the Technical University of Munich (TUM) won the Hans Meuer Award for their work on 'Time Series Mining at Petascale Performance'.

Collecting and Evaluating the Right Data

Sensors already provide all kinds of information from supercomputers, for example on temperature, power, load and stress on components. The open source software Data Center Data Base (DCDB), which collects data from millions of sensors and thus enables the control of SuperMUC-NG and CoolMUC-3, has already been developed at the LRZ. In order to be able to monitor and operate hese systems efficiently, an analysis tool is needed, but above all a systematic approach for evaluating these data. With Wintermute, Netti presented a generic model at the digital edition of the HDPC conference and thus a basis for Operational Data Analytics (ODA). It is intended to provide as comprehensive a picture of supercomputers as possible and to enable forecasts and adjustments to be made to the technology. To this end, Wintermute processes information generated in components (in-band data) or sent by them (out-of-band data), either in a streaming process, continuously (online processing) or only when explicitly required (on-demand processing).

Using three case studies done on CoolMUC-3, the LRZ computer scientist shows which monitoring data can be used to detect anomalies in individual computer nodes, for example, in order to exchange or optimise them. Energy consumption can also be tracked and adjusted using Wintermute and selected data. The open source tool also shows where technology is causing bottlenecks in simulation and modelling. "Wintermute uses machine learning methods to make Operational Data Analytics more meaningful and thus more powerful," says Netti. "The tool was designed to be integrated into any existing monitoring system." The name actually refers to this: Wintermute is the name of an artificial intelligence that combines with another in a science fiction trilogy by William Gibson and becomes a - better - digital life form. The findings from Wintermute can help to improve computer systems of the future.

A Matrix for Sorting Data

Amir Raoofy, PhD candidate at the Chair for Computer Architecture and Parallel Systems at the Technical University of Munich (TUM) of Professor Martin Schulz, also works with data supplied by thousands of sensors from supercomputers or from the monitoring systems of power plants over weeks or even years. However, he is interested in how SuperMUC-NG and CoolMUC-3 handle the huge amounts of data. "Using matrix profile algorithms, time series can be searched for patterns and similarities," says Raoofy, outlining the problem. "But they are difficult to scale and are not suitable for HPC systems". However, the evaluation of large time series requires supercomputing: Anyone who wants to know under which conditions a gas turbine will run reliably and when the first components will be susceptible to repair should be able to check a lot of data. The computing power and capabilities of supercomputers make such analyses possible only in combination with scalable algorithms.

Raoofy and his collegues developed the now award-winning scalable approach (MP)N. This can be run efficiently on up to 256,000 computer cores - that is around 86 percent of the computing resources of the SuperMUC-NG. The fact that it delivers exact calculations was tested with performance data from the SuperMUC-NG. The

algorithm is currently being used to analyze data supplied by two gas turbines belonging to Stadtwerke of Munich. TurbO is the name of the project funded by the Bavarian Research Foundation. "In our experiments, we performed the fastest and largest multidimensional matrix profile ever calculated," reports Raoofy. "We achieved 1.3 petaflops per second." This means that supercomputers like the SuperMUC-NG can quickly and efficiently evaluate data from long time series - science and technology will know how to use this. **(vs)**

Back to Content

Supercomputing-Technology under Test

The Leibniz Supercomputing Centre (LRZ) will extend its testbed program using HPE'S Cray CS500 system with Fujitsu A64FX processors that are based on Arm architecture. Integrating the technologies in early autumn, the institute of the Bavarian Academy of Sciences and Humanities will be the first academic computing centre in the European Union to offer this innovative hardware for its users to explore. "As a world-class academic supercomputing centre, it is one of our core tasks to explore new and diverse architectures within our Future Computing Program. Together with our core partners, we look forward to exploring the capabilities of this technology and the benefit it brings to our users - especially in the area of HPC and AI", says Dieter Kranzlmueller, Director of the LRZ.

HPE's Cray CS500 system is based on the same Fujitsu A64FX processor used in the recently installed Japanese high-performance computer Fugaku currently #1 on the global Top500 list and is a central asset for the LRZ testbed program and its system known as BEAST (Bavarian Energy, Architecture and Software Testbed). The Arm-based architecture in the Fujitsu processors, integrated by Hewlett Packard Enterprise (HPE) will offer unique pathways for traditional modelling and simulation tasks while being equally suitable for data analytics, machine learning and artificial intelligence workloads. It will be available to core academic partners and select projects as well as next-generation HPC practitioners. HPE's Cray CS500 system features the Cray Programming Environment, a fully integrated software suite that maximizes programmer productivity and application performance. "HPC plays an increasingly critical role to meet key societal and economic challenges in areas like medicine, climate change, and risk management. We are committed to advancing HPC technologies by developing diverse architectures to support any workload need," Bill Mannel said, the Vice President and General Manager HPC, Hewlett Packard Enteprise. "We look forward to working with the Leibniz Supercomputing Centre to explore how alternative architectures can enable new HPC applications to bolster research and innovation, while improving performance and efficiency."

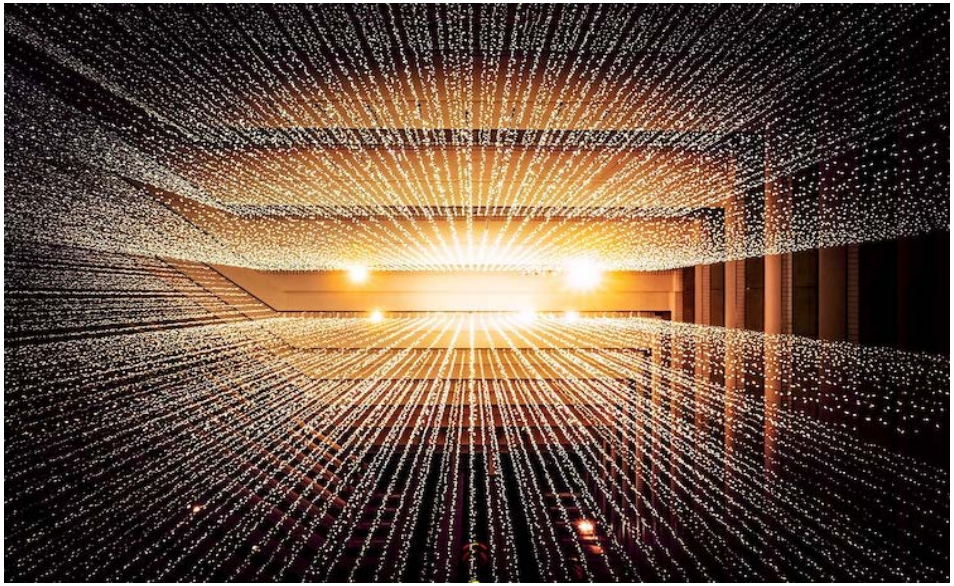
Exploring Diverse Architectures for Future Computing

Each of the Fujitsu A64FX Arm-based processors will be equipped with 32GB of second-generation high bandwidth memory (HBM2). The servers are connected by an EDR-Infiniband network. The system comes with an Open-Source (GCC/LLVM) software stack as well as a Cray Programming Environment supporting the vectorised processor units.

HPE's Cray CS500 offers LRZ users and HPC specialists evaluation and research opportunities for the processors' performance on real-world applications and in comparative studies to both regular CPUs and GPUs. As a pioneering centre for energy-efficient HPC systems and data centre infrastructure, LRZ is also highly interested in evaluating the performance per watt the system can deliver. "The Scalable Vector Extension (SVE) architecture, the high memory bandwidth with HBM2, and the Cray Compiler Environment and software stack are a few of the things we are excited to explore and better understand in support of our users and their scientific work," says Josef Weidendorfer, team lead Future Computing at LRZ. **(lp)**

Back to Content

The Hope for Quantum Computers



The economic stimulus package with which the German government intends to reactivate the economy includes around two billion euros for the construction and development of two quantum computers. Scientists rely on the better computing capabilities they promise for data-intensive research: quantum technology electrifies researchers, politics and industry. The Leibniz Computing Centre (LRZ) has already been working on this topic for some time - and this is now paying off in terms of research projects and international contacts. One year after its start, the Bavarian Quantum Computing eXchange (BQCX) is increasingly successful in inviting scientists and managers from all over the world with exciting topics to the meetings on every second Wednesday of a month: In June, for example, Dr. Travis Humble from the Oak Ridge National Laboratory (ORNL) and Dr. Max Henderson, senior researcher at manufacturer Rigetti, discussed how quantum computers support science and machine learning. At the end of June, Dieter Kranzlmueller, head of the LRZ, demonstrated at the event "Reclaim the Future" why it would be worthwhile for Europe to develop its own quantum technology.

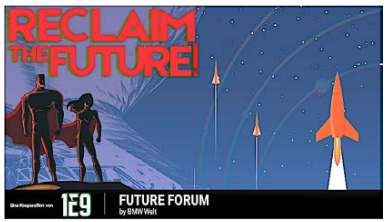
Different Technology, Comparable Results

Quantum computers are still in an experimental state. They work with qubits that assume their superposition states in addition to the values 0 and 1. Humble, head of the Institute of Quantum Computing at ORNL, explained how qubits can be stabilized by chemical, physical and/or mechanical methods, using the first quantum processors from D-Wave, IBM, IonQ. They are called "Noisy Intermediate Scale Quantum" or NISQ devices because these systems have small scales and are not error-corrected, i.e. they are unreliable. The ORNL tested their performance of NISQ systems from different vendors using algorithms from chemistry and materials science. Although they were constructed differently, the first quantum systems produce comparable results, says Humble: "NISQ devices can be used to test the concepts of quantum computers and their suitability for scientific computing. Hybrid Variational Quantum Eigensolvers or VQE require a good knowledge of how best performance is achieved. Quantum computing for materials science is, however, limited by the topology of the processors.

Source of Inspiration for Research

Henderson presented in his talk an overview of the relationship between quantum computing and machine learning. Quantum computers will one day process gigantic amounts of data, controlled by algorithms or statistical methods for classifying data. In order for quantum computers to recognize images and find patterns in them, they are now trained in a similar way to artificially intelligent systems or neural networks. The methods do not differ significantly, on the contrary - Henderson observes that some training steps already anticipate quantum technology, although they were actually developed for conventional computers. He concludes that quantum computing and quantum-suitable algorithms could enrich the machine learning of supercomputers and conventional computers and lead to alternative solution strategies.

New Business in Prospect



Discussions around quantum computers at the "Reclaim the Future - Can Europe become a Leader in Quantum Computing" event at BMW-Welt at the end of June focused on the practical development and advancement of the technology as well as its impact to academia, society, industry, and the regional economy. The first research institutes are already working on OpenSuperQ, a quantum computer with up to 100 qubits, which is to start work next year in Juelich. The recent federal stimulus package calls for the placement of two additional quantum computers in Germany research facilities. Garching is a highly competitive option for such a system. "We have everything that a successful ecosystem needs here. There is hardly any other place in the world where you can find this," says LRZ director Kranzlmueller promoting the location. Companies such as BMW and Allianz are gradually recognizing the opportunities offered

by the new computer technology that is already being researched and developed in the area around Munich. With IQM, an early start-up has already emerged from the environment of Munich's universities and the Walter-Meissner-Institute for low temperature measurement. IQM focuses on building European quantum computers and processors. Others will follow: "The hardware is only a beginning, a complete ecosystem for quantum computing is needed" says Kranzlmueller. Quantum computing will also stimulate new services. If Europe and Germany contribute and realize their own ideas to the new technology, the current dependence on computer technology made in the USA, Japan or China could decrease.

Coming Up: BQCX and LRZ will be parts in the Munich Conference of Quantum Science and Technology on 6 - 8 July. LRZ will be involved in the Science meets Industry session on Tuesday, July 7 from 12:00 to 14:30. Luigi Iapichino (Lead of Quantum at LRZ) will give a talk on LRZ activities in quantum computing on the virtual stage B and will then participate to a panel discussion on quantum technologies. On July 29, the BQCX will hold a special working group with Bavarian quantum computing specialists on the quantum resource and service needs of the community. On August 12th BQCX welcomes Dr. Philip Makotyn of Honeywell to discuss their recent developments building trapped ion quantum computers. Additionally, the Quantum Up-and-Comers session will highlight Bavarian quantum computing students' work and projects: They will have the opportunity to discuss their quantum computing projects with specialists, interested parties and potential partners. **(vs)**

Back to Content

Learning Library for Three-Dimensional Animal Models

What do you do with nearly 600 sensitive animal preparations? At the Faculty of Veterinary Medicine of the Ludwig-Maximilians-University Munich (LMU) researchers had already purchased a hand scanner (Artec Space Spider) to convert bones, teeth and organs into digital objects of interest. In the long term, this should have resulted in a database that students can use to learn. Then came the corona lockdown and the digital semester: And all of a sudden everything had to happen very quickly. "The Leibniz Supercomputing Centre (LRZ) has been a great help to us and has shown us ways to make the scans available to students quickly," says lecturer Sven Reese. The veterinary surgeon with a doctorate in veterinary medicine sought advice from the Centre for Virtual Reality and Visualisation (V2C) at the LRZ: "Presenting 3D data via the Internet is not so easy. In the meantime, almost 300 of the specimens have been scanned, about 40 of which can be accessed via the faculty's Moodle learning platform or at Sketchfab for study purposes. With the university library, the veterinarians are now planning a platform for three-dimensional objects. An interview with 3D specialists Lea Weil and Kristian Weinand from LRZ' V2C on how digitization and innovative visualization are changing research and teaching.

When and how did the cooperation with the veterinary faculty begin?

Lea Weil: Last winter, Sven Reese contacted us and asked how to visualize preparations in 3D. A scanner, which displays colours and textures of skin and bones, had already been purchased, but there was uncertainty about how the virtual preparations could be made available to the students. A smartphone app first appeared to be the got-to solution for rapid provision. Enriched with augmented reality functions the specimens would have appeared even more lifelike. However, many students use smartphones based on different operating systems and versions, which could have led to problems with installation and display. On an online platform, the preparations can be accessed via a 3D viewer using a computer, notebook, tablet or smartphone - in this case the best way.

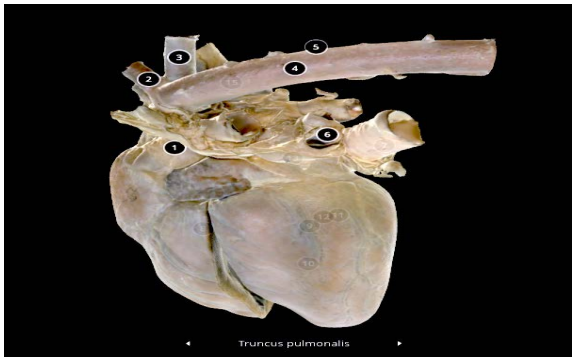
How do you find such tools?

Kristian Weinand: On the Internet, at museums, universities and other specialists. We looked at tools like Verge 3D, Blend4Web, Sketchfab, and the viewer used by the Smithsonian National Museum of Natural History in Washington and experimented with scans from the Veterinary School. The presentation and interaction with the objects are similar, all of them allow you to rotate and turn the objects. For the evaluation, we therefore looked at the quality of view and user-friendliness as well as the

costs of use. Criteria such as the limitation of access rights, data security and data storage also played a role. Because the corona lockdown had to make things go faster, we recommended Sketchfab. The platform is well established, the tool is easy to use, uploading is fast and straightforward. Sketchfab offers a website with an integrated viewer and many functions, such as captions or annotations. Many universities and museums publish their exhibits there. However: Sketchfab stores the data in the USA, with the free version everyone can download everything. The Faculty of Veterinary Medicine has decided to opt for a subscription to limit access.
Weil: In the long term, a separate platform would be more practical, but the development should not be underestimated financially, especially if it is to grow with the requirements and wishes of the students. Then it can also be determined where the data will be stored. Bavarikon, the Internet portal of the Free State of Bavaria, uses its own 3D viewer to make art, cultural and knowledge treasures accessible in 3D.

Scanning and uploading - does it work just like that?

Weinand: Not quite, if you want the visuals to be loaded quickly. 3D scans produce large amounts of data that need to be optimized if users want to access them online and with mobile devices. The scans consist of a fine grid that can be reduced to a coarse resolution to minimize file size and complexity. However, this results in the loss of details that can be projected and preserved using textures. But this requires some more work steps and additional software. In this case we have recommended Blender - a free open source program. It combines many functionalities, which could make the optimization of 3D models more difficult. For an uncomplicated standard work-flow we have therefore created a video tutorial. It worked just fine, and everyone got along well with it



Now the preparations are available at Sketchfab, what else could you do with them?

Weil: Integrated in augmented or virtual reality apps, the individual preparations could be presented in an even more impressive and playful way and enriched with additional information. They convey an immersive impression, as if the three-dimensional model were on the table and one could interact with it naturally. This clarifies the real proportions, shows the similarities and differences of, for example, pelvic bones of different animals. In such apps, preparations can also be assembled virtually, for example the teeth with the jaw bones. The visual objects look lifelike, which is also a great advantage for learning. Combined with animations, complex relationships could be illustrated. A whole lot is conceivable.

Not only veterinarians have spatial visualization objects, in which fields could sketchfab and 3D-viewer support teaching?

Weinand: They are already being used in archaeology and art history. Architecture, mechanical engineering, biology and quite a few more science domains also work with three-dimensional models and benefit from spatial representation. In the long term, an online platform for three-dimensional objects is to be developed at the LMU and the university library. This will open up many opportunities for the exchange of information between universities, students and researchers and interested experts worldwide. Rare and sensitive specimens, which are otherwise well protected in universities or museums, will thus become publicly accessible, worldwide. That is great.
Weil: I am sure that augmented, virtual and mixed reality applications or platforms for 3D views, which we also develop at the Leibniz Supercomputing Centre, will enrich research and teaching enormously. The corona lockdown has pushed the digitization of learning content. Hopefully, the experience gained will be taken into account when the situation recovers. Then it will not be long before soon-to-be physicians will be able to spatially explore organs, bones and tissue of humans or animals with the help of data glasses and an AR app. This will make learning more sustainable, more impressive. **(vs)**

Back to Content

Poll Data per App

Almost three million people in Bavaria are expecting spring and summer with mixed feelings: When alder, hazelnut and

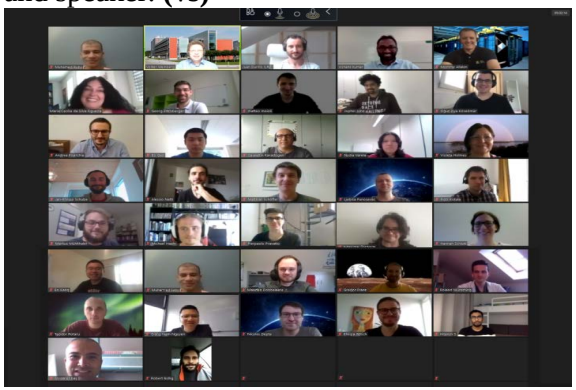
other plants begin to blossom, their noses tingle, their eyes water and they have dificulties breathing. "We are observing allergies in many people, nature is reacting to climate change", says Caroline Herr from the Bavarian State Office for Health and Food Safety in Erlangen. "If people suffering from allergies know when which pollen is flying, they can take timely precautions." That's why ePIN, the first fully automated pollen information network, came into operation a good year ago. It provides daily updated data on air pollution with pollen from mugwort, birch, alder, ash, grasses, hazelnut, rye and ragweed - the most important allergens in Bavaria. The data can be accessed online and recently even via app

For ePIN, the Bavarian State Health Office cooperates with the the Center of Allergy and Environment (Zaum) of the TUM and the German Research Center for Environmental Health - an Helmholtz institute. The Leibniz Supercomputing Center (LRZ) supports the research project in building and operating the research infrastructure and provides the data strorage.At eight locations in Bavaria, ePIN measures the pollen concentration in the air. These are immediately evaluated and published using image recognition and artificial intelligence. Thousands of photos are taken for each sample at the eight measuring points - over the course of a year, terabytes of data are collected. They are sent online and via radio to the LRZ, where they are stored and made publicly accessible: for allergy sufferers and doctors as well as for researchers from all over the world. In May 2020, around 10,000 users accessed the ePIN website of the Bavarian State Health Office. It is hoped that also commercial weather and app providers will discover and use the treasure trove of data on pollen flight. **(vs)**

Back to Content

Figures of the month

This is an interesting side effect of the digitization of workshops and seminars: The online courses offered by the Leibniz Supercomputing Centre (LRZ) and its partners PRACE, the scientific computing centres in Erlangen, Ostrava, Stuttgart, Vienna and the technology companies NVIDIA and Intel have proven to be export hits since the corona lockdown. Until mid-June, **241 interested researchers** from **24 countries** participated in **13 training days**. The courses reached people from **4 continents** - next to Europe participants virtually joined from Argentina, Canada, Saudi Arabia, Egypt. **17 speakers** among them Carla Guillen Carias, Momme Allalen, Juan Durillo Barrinuevo, Gerald Mathias and Volker Weinberg from the LRZ, showed the participants how to program processors or how to optimize codes and algorithms. "For two weeks there was something going on almost every day," said Volker Weinberg, coordinator of the training programs. "I really enjoyed the last two weeks as a presenter and speaker. **(vs)**



Back to Content

Workshops and Events

Deep Learning and Programming with OpenACC

Train neural networks and efficiently describe images, video clips or content and accelerate scientific applications with OpenAcc: The online workshop of the LRZ, the Stuttgart HRLS and Nvidia from **14 to 17 July** combines lectures on deep learning, data types and supercomputing with practical exercises and programming aids. These will be performed on a GPU-accelerated workstation in the cloud. The last day will be dedicated to the preparation of data for supercomputers, in particular HLRS systems. Login and Registration

Back to Content

Iterative Linear Solvers and Parallelization

The focus of this five-day compact course from August 31 to September 4 is on iterative and parallel solvers, the parallel programming models MPI and OpenMP as well as the parallel middleware PETSc. Based on real applications, different modern Krylov subspace methods (CG, GMRES, BiCGSTAB ...) and highly efficient preconditioning techniques are presented. Participants can test and understand solutions in exercises. Knowledge of the programming languages C and Fortran is required. The online course is organized by the University of Kassel, the High Performance Computing Centre Stuttgart (HLRS), the LRZ and the IAG. Login and Registration

Back to Content

Deep Learning and Programming

The workshop from September 7th to 10th deals with the basics of deep learning, computer vision and programming of multi-GPU. Lectures and practical exercises with the programs Open ACC and the programming languages CUDA C / C ++ will deepen the theory. All exercises are performed on a fully configured GPU-accelerated workstation and on Jupyter notebooks in the cloud. For the workshop PRACE, CSC (Finland), IT4Innovations and LRZ cooperate with Nvidia. Login and Registration

Back to Content

Fortran for Advanced Students

Scientists who want to extend their knowledge in Fortran will learn in this four-day course Objects, Interfaces and object-based programming. Lectures and exercises also cover IEEE functions and floating point exceptions, interoperability with C and Fortran 2003 E, and the advantages of OO design patterns or co-arrays. Login and Registration

Back to Content

C++ for Software Development

C++ for advanced users: The three-day training course from November 18th to 20th, 2020, deals with object-oriented (OO) software design. Principles, concepts and good application examples will be discussed and tried out in practical exercises. Specialized applications, such as the Template Meta Programming (TMP), will be discussed, as well as the quirks and curiosities of C ++. Participants learn the tricks they can use to develop mature, robust code for their applications. Login and Registration

Back to Content

Job Opportunities

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 LRZ or send an unsolicited application. We are LRZ - and curious about you!

- IT Specialist for the management of MAC-Devices
- IT-Specialist for the management of Windows-Clients
- Student Assistant for the support of HPC-users
- Student Assistant for web backend and app development
- Student Assistant for Web - Java Script - Type Script
- Student Assistants for the Serviceesk

Back to Content

More to Read

Here you will find links to the latest information from the German and European supercomputing community and our cooperation partners:

- Publications of the Gauss Centre for Supercomputing (GCS): GCS-News and Inside
- Infoletters of the Gauss-Allianz
- Publications of PRACE: PRACE Digest, Annual Report

Back to Content

Informations about the

Informations about the LRZ-Newsletter

- 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 short description of your problem to <NewsletterRedaktion_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.

Back to Content

Imprint

Editor:
Leibniz-Supercomputing Centre of the Bavarian Academy of Science and Humanties
Boltzmannstr 1
D-85748 Garching
Phone:
+49-89-35831-8000
Telefax:
+49-89-35831-9700
E-Mail:
newsletter_AT_lrz.de, pr-team_AT_lrz.de
Twitter: LRZ_DE
LinkedIn: Leibniz Supercomnputing Centre
Editorial Office:
PR Team
Photos, Graphics:
Volker Weinberg/LRZ, Dawid Zawila/Unsplash, Ibrahim Boran/Unsplash, Joshua Sortino/Unsplash, 1E9, Cray/HPE

Back to Content