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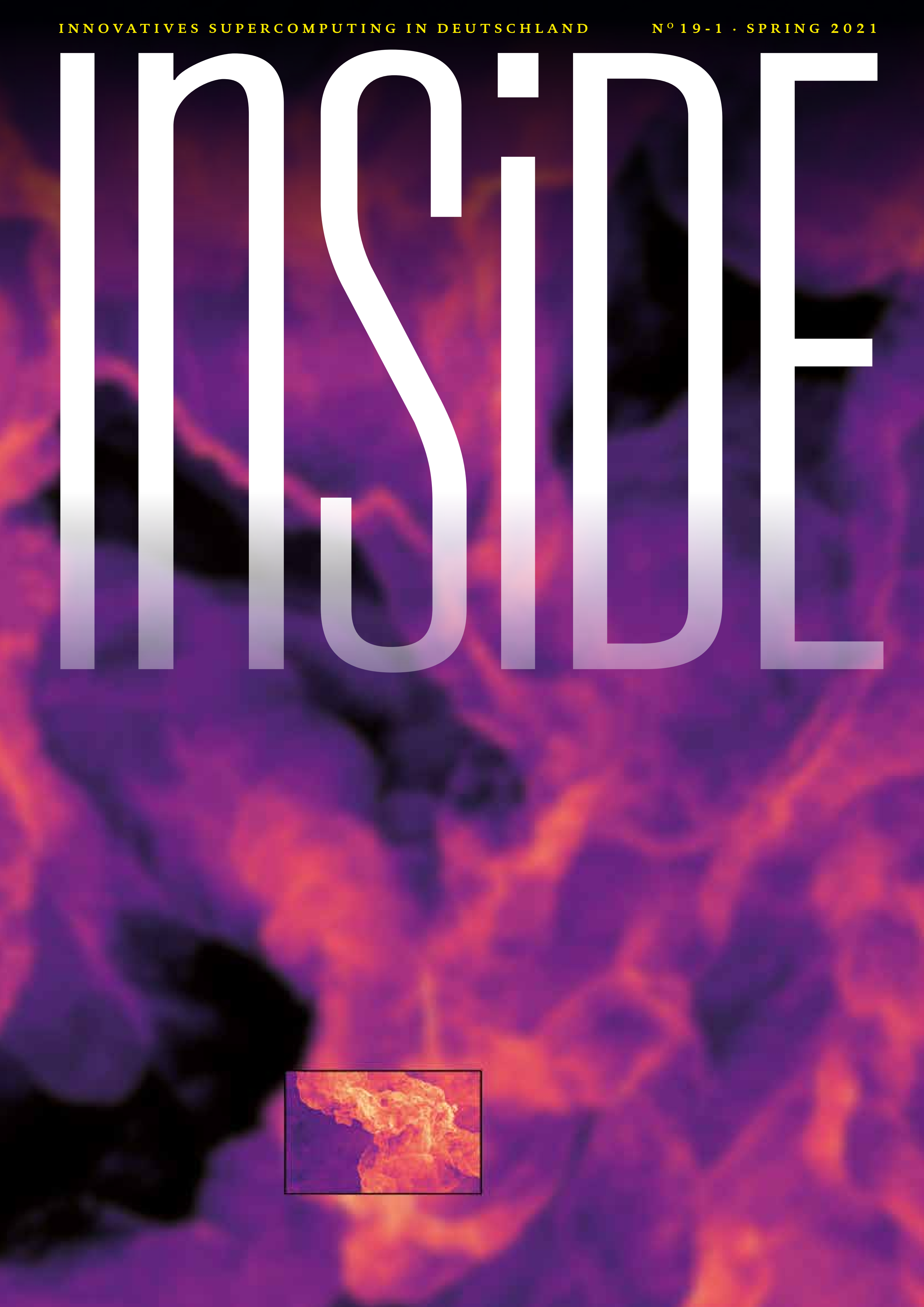

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Gauss Centre for Supercomputing

Welcome to the latest issue of InSiDE, the bi-annual Gauss Centre for Supercomputing magazine showcasing innovative supercomputing developments in Germany. While many of the centres' staffs have remained working from home to start 2021, the increasing global vaccination rates leave us hopeful that the latter half of the year can bring a return to in-person education and training as well as other events at our centres. We look forward to welcoming our staff, supporters, and research collaborators back as soon as conditions allow.

The latest issue of InSiDE is also looking forward. In Garching, the Leibniz Supercomputing Centre announced its latest addition to the GCS HPC family—SuperMUC-NG Phase 2 is being developed with partners at Intel and Lenovo (Page 4). The centre also inaugurated its Quantum Integration Centre during the first half of the year, looking to take another meaningful step forward in scaling up the exciting potential hidden in quantum computers (Page 26). In that same vein, HLRS is participating in the SEQUOIA project, funded by the Baden-Württemberg Ministry of Economic Affairs, Labor, and Housing to support bringing the promise of quantum computing to industrial researchers, and JSC is continuing to extend its Jülich UNified Infrastructure for Quantum computing, JUNIQ, co-funded by the German Federal Ministry of Education and Research (BMBF) and the Ministry of Culture and Science of the State of North Rhine-Westphalia.

While all three of our centres aim to embrace new technologies and equip our users with the skills needed to make the most of them, our users are embracing our current generation of systems for groundbreaking research findings. Staff at JSC partnered with researchers at the University of Wuppertal to run unprecedented simulations of tiny subatomic muons in the search for cracks in the standard model of physics. The work accompanies major findings released as part of the "muon g-2" collaboration earlier this year (Page 9). Researchers are using HLRS computing resources to develop more efficient methods for storing energy with hydrogen, a potential game-changing technology for storing renewable energy more efficiently (Page 14).

We are still committed to making our resources available to researchers focused on getting the world beyond the COVID-19 pandemic. These last 18 months have provided unprecedented challenges to people all over the world, and the pandemic has left us with new questions about how to govern certain aspects of our lives moving forward. GCS has a long history of embracing new challenges and helping pave the way toward solutions. In 2021, our commitment to this work is as strong as ever.

Prof. Dieter Kranzlmüller
Prof. Thomas Lippert
Prof. Michael Resch

NEWS FEATURES

LRZ TO EXPAND ITS FLAGSHIP SUPERCOMPUTING SYSTEM TO INTEGRATE HPC AND AI

Together with its partners Intel and Lenovo, the Leibniz Supercomputing Centre is designing the second phase of its flagship supercomputer to ensure that users focused on data-intensive applications and emerging technologies can take full advantage of the new system.

Together with its partners Intel and Lenovo, the Leibniz Supercomputing Centre (LRZ)—one of the three HPC centres in the Gauss Centre for Supercomputing (GCS)—will expand its current flagship HPC system SuperMUC-NG. In addition to top performance in simulation and modeling, phase 2 of SuperMUC-NG will integrate and advance artificial intelligence (AI) methods of computation.

For this purpose, the system will be equipped with next-generation Intel Xeon Scalable processors (codenamed Sapphire Rapids) and "Ponte Vecchio", Intel's upcoming GPU based on the Xe-HPC micro-architecture for high-performance computing and AI. The storage system will feature distributed asynchronous object storage (DAOS), and leverage 3rd Gen Intel Xeon Scalable processors and Intel Optane persistent memory to accelerate access to large amounts of data.

As with Phase 1, SuperMUC-NG Phase 2 will be jointly funded by the Free State of Bavaria and the Federal Ministry of Education and Research (BMBF) through GCS. The computing capacities are made available to specially qualified research projects nationwide in a scientific selection process.

New research tasks for supercomputing

"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." This requires not only computing power, but different computer architectures and configurations as well as more flexible data storage.

"We're continuously pushing the boundaries of hardware and software technology to deliver an easy and scalable compute stack in the data center for a wide range of diverse and emerging workloads in HPC and AI," said Raja Koduri, SVP, chief architect, and general manager of Architecture, Graphics, and Software at Intel. "We are thrilled that LRZ has chosen to partner with Intel in bringing their SuperMUC system to market based on Intel's XPU product portfolio, advanced packaging and memory technologies, and the unified oneAPI software stack to power the next generation of high-performance computing."

Practical experience with using artificial intelligence methods is increasingly becoming a key capability in science. This is attracting new user groups to LRZ: Until now, it was mostly experts from physics, engineering and the natural sciences who relied on high-performance computing. With AI techniques becoming more widely used, demand in HPC and AI resources is now increasing in the fields of medicine, life and environmental sciences, as well and the humanities. For example, practitioners use automated image, speech, or pattern recognition in earth observation or climate data from satellites, anonymized medical imagery and health records, or data demographics. The more complex these neural networks and the desired functions, the higher the demand for computing and fast memory performance.

SuperMUC-NG already offers enormous computing power, but will now be upgraded for more diverse tasks with this expansion: Some of the new technology is currently being tested in the LRZ test environment BEAST (Bavarian, Energy, Architecture, Software Testbed) to better understand its capability in a future large-scale HPC system. 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, and connected to the DAOS storage system via a high-speed network. Its capacity is 1 petabyte of data storage, but more importantly, this technology enables fast throughput of large data volumes. This system architecture is particularly well-suited then for highly scalable, compute- and data-intensive workloads and artificial intelligence applications.

"The Leibniz Supercomputing Centre has been a thought leader in new technologies for many years, setting standards for research and development and being an important innovation partner for Lenovo. For example, LRZ has already installed warm water cooling and is planning to implement an integrated system for artificial intelligence and deep learning - all from Lenovo," emphasizes Noam Rosen, EMEA Director, HPC & AI, ISG at Lenovo. "Sustainability has also been important for LRZ in its infrastructure projects. That's why we are pleased to play a part in this initiative too, as the Lenovo components for SuperMUC-NG phase 2 will be manufactured in our new production facility in Hungary—rather than in our American or Asian production facilities—further improving the eco-footprint of our supply chain."

SuperMUC-NG already offers enormous computing power, but will now be upgraded for more diverse tasks with this expansion. © LRZ

Consulting and training

While the DAOS storage system is expected to arrive in Garching in the fall of 2021, the compute system will follow in the spring of 2022. The LRZ is working with its user community in preparation: Researchers already have access to GPU systems specialized on AI applications and LRZ's HPC and Big Data teams consult and support the users in adapting and optimizing their codes and AI algorithms. The LRZ training program also offers a wide variety of machine and deep learning courses where students and researchers learn how to adapt existing algorithms or develop and train their own.

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INSIDE · NO 19-1 · SPRING 2021

HAWK EXPANSION WILL ACCELERATE RESEARCH COMBINING SIMULATION AND ARTIFICIAL INTELLIGENCE

The addition of HPE Apollo systems with NVIDIA graphic processing units (GPUs) to HLRS's flagship supercomputer will enhance the center's capacity for deep learning applications and enable new kinds of hybrid computing workflows that integrate HPC with Big Data methods.

HLRS and HPE at the contact signing. (l-r) Heiko Meyer (Chief Sales Officer, Hewlett Packard Enterprise), Prof. Michael Resch (Director, HLRS), Aron Precht (VP Channels & Ecosystem DACH, HPE), Jan Gerken (Chancellor, University of Stuttgart). © HLRS

Hawk, a Hewlett Packard Enterprise (HPE) Apollo system installed in 2020, is already one of Europe's most powerful high-performance computing (HPC) systems. In November it placed 16th in its debut on the Top500 list of the world's fastest supercomputers, based on the High-Performance Linpack (HPL) benchmark.

Through an agreement signed with HPE in December, HLRS will soon expand this world-class CPU-based computing system by adding 24 HPE Apollo 6500 Gen10 Plus systems with 192 NVIDIA A100 GPUs based on the NVIDIA Ampere architecture. The addition of 120 petaflops of AI performance will not only dramatically expand HLRS's ability to support applications of deep learning, high-performance data analytics, and artificial intelligence (AI), but also enable new kinds of hybrid computing workflows that combine traditional simulation methods with Big Data approaches.

The expansion also offers a new AI platform with three times the number of NVIDIA processors found in HLRS's Cray CS-Storm system, its current go-to system for AI applications. It will enable larger-scale deep learning projects and expand the amount of computing power for AI that is available to HLRS's user community.

"At HLRS our mission has always been to provide systems that address the most important needs of our key user community, which is largely focused on computational engineering," explained HLRS Director Prof. Michael Resch. "For many years this has meant basing our flagship systems on CPUs to support codes used in computationally intensive simulation. Recently, however, we have seen growing interest in deep learning and artificial intelligence, which run much more efficiently on GPUs. Adding this second key type of processor to Hawk's architecture will improve our ability to support scientists in academia and industry who are working at the forefront of computational research."

Two approaches to computational research: simulation vs. deep learning

In the past, HLRS's flagship supercomputers — Hawk, and previously Hazel Hen — have been based exclusively on central processing units. This is because CPUs offer the best architecture for many codes used in fields such as computational fluid dynamics, molecular dynamics, climate modeling, and other research areas in which HLRS's users are most active. Because the outcomes of simulations are often applied in the real world (for example, in replacing automobile crash tests), simulation algorithms must be as accurate as possible, and are thus based on fundamental scientific principles. At the same time, however, such methods require large numbers of computing cores and long computing times, generate enormous amounts of data, and require specialized programming expertise to run efficiently.

In recent years, researchers have begun exploring how deep learning, high-performance data analytics, and artificial intelligence could accelerate and simplify such research. As opposed to simulation, in which a complex system is modelled in a "top-down" way based on scientific principles, these newer methods use a "bottom-up" approach. Here, deep learning algorithms identify patterns in large amounts of data, and then create a computational model that approximates the behavior of the actual data. The "trained" model can then be used to predict how other systems that are similar to those in the original dataset will behave. Although such models are not guaranteed to be as precise as simulations based on first principles, they often provide approximations that are close enough to be useful in practice, complementing or sometimes even replacing more computationally intensive approaches.

For technical reasons, such deep learning approaches do not run efficiently on CPU processors, but benefit from a different type of accelerator called a graphic processing unit. Originally designed to rapidly re-render screens in action-packed video games, GPUs are also capable of analyzing the large matrices of data required for algorithms using neural networks.

Whereas CPUs are best suited for diverse calculations, GPUs are better at flying through repetitive tasks in parallel. In deep learning and AI this can mean simultaneously comparing hundreds of thousands of parameters in millions of large datasets, identifying meaningful differences in them, and producing a model that describes them.

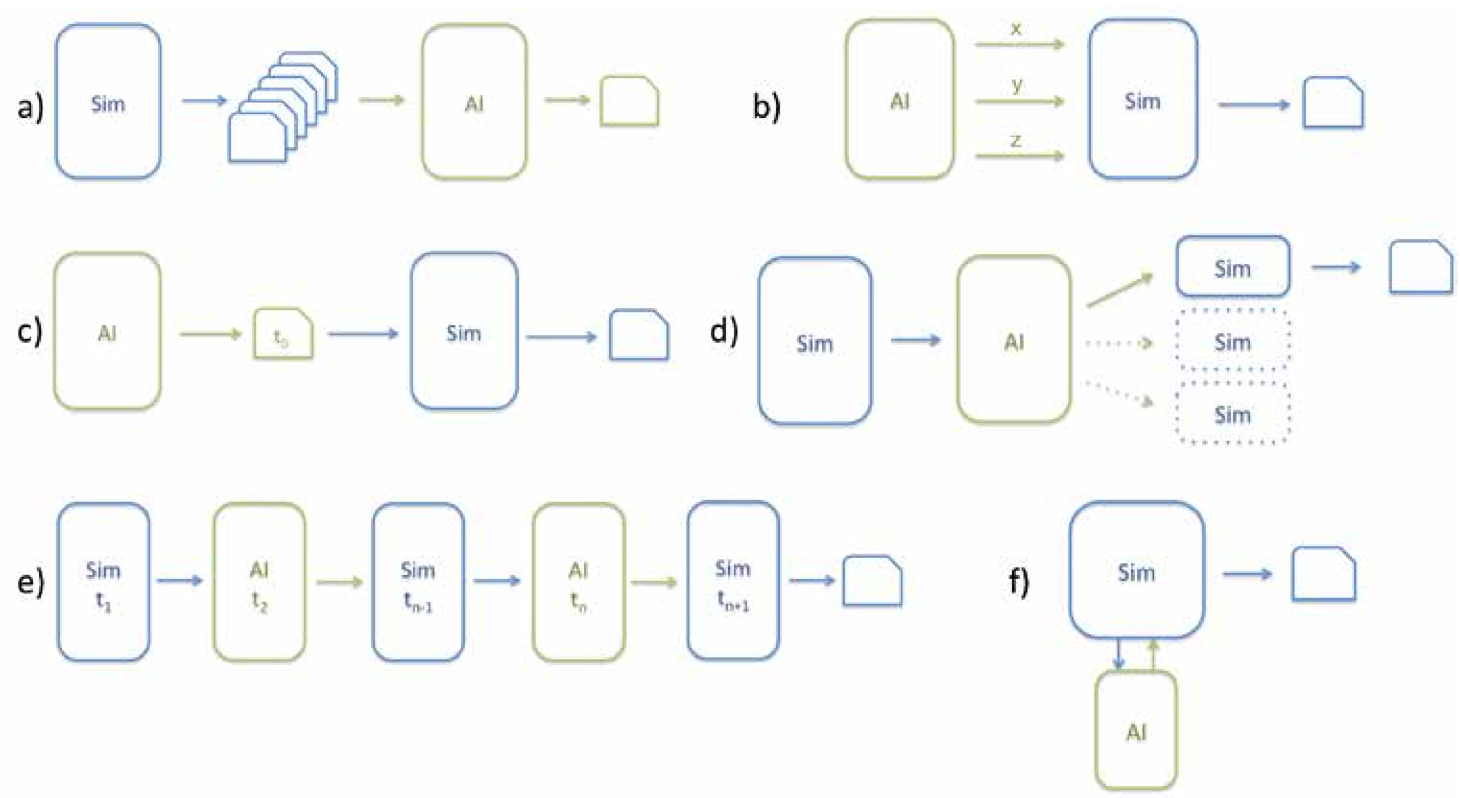
Hybrid methods that integrate HPC and AI can accelerate computational engineering

Although some have speculated that AI could eventually replace high-performance computing altogether, the truth is that some of the most interesting research methods right now lie in combining these bottom-up and top-down approaches.

Deep learning algorithms typically require enormous amounts of training data in order to produce statistically robust models — a task that is perfectly suited to high-performance computers. At the same time, models created using deep learning on GPU-based systems can inform and accelerate researchers' use of simulation. Learning algorithms can, for example, reveal key parameters in data, generate hypotheses that can guide simulation in a more directed way, or deliver surrogate models that substitute for compute-intensive functions. New research methods have begun integrating these approaches, often in a circular, iterative manner.

Examples of interactions between HPC and AI

In 2019 HLRS made a significant leap into the world of deep learning and artificial intelligence by installing an NVIDIA GPU-based Cray CS-Storm system. The addition has been well received by HLRS's user community, and is currently being used at near capacity.



Various interaction patterns between AI and simulations: a) generation of data for AI training from simulations; b) finding simulation parameters by AI; c) generation of initial solutions by AI; d) choosing the right path by AI; e) replacing iterations in simulation by AI; f) replacing specific functions/equations by AI.

Although the Cray CS-Storm system is well suited for both standard machine learning and deep learning projects, the experience has nevertheless revealed limitations in using two separate systems for research involving hybrid workflows. Hawk and the Cray CS-Storm system use separate file systems, meaning data must be moved from one system to the other when training an AI algorithm or using the results of an AI model to accelerate a simulation. These transfers require time and workflow interruptions and that users master the ability to program two very different systems.

"Once NVIDIA GPUs are integrated into Hawk, hybrid workflows combining HPC and AI will become much more efficient," said Dennis Hoppe, who leads artificial intelligence operations at HLRS. "Losses of time that occur because of data transfer and the need to run different parts of the workflows in separate stages will practically disappear. Users will be able to stay on the computing cores they are using, run an AI algorithm, and integrate the results immediately."

HLRS users will also be able to leverage the NVIDIA NGC™ catalog to access GPU-optimized software for deep learning, machine learning, and high-performance computing that accelerates development-to-deployment workflows. Furthermore, the combination of the new GPUs with the In-Networking Computing acceleration engines of the HDR NVIDIA Mellanox InfiniBand network enables leading performance for the most demanding scientific workloads.

Hoppe also anticipates that in the future the new GPUs could be more easily used to run certain kinds of traditional simulation applications more quickly. *cw*

GERMAN NATIONAL SUPERCOMPUTING CENTRE PROVIDES COMPUTATIONAL MUSCLE TO LOOK FOR CRACKS IN THE STANDARD MODEL OF PHYSICS

Physicists have spent 20 years trying to more precisely measure the so-called "magnetic moment" of subatomic particles called muons. Findings call into question long-standing assumptions of particle physics.

Physicists have spent 20 years trying to more precisely measure the so-called "magnetic moment" of subatomic particles called muons. Findings call into question long-standing assumptions of particle physics.

Since the 1970s, the Standard Model of Physics has served as the basis from which particle physics are investigated. Both experimentalists and theoretical physicists have tested the Standard Model's accuracy, and it has remained the law of the land when it comes to understanding how the subatomic world behaves.

Recently, cracks formed in that foundational set of assumptions. Researchers of the "Muon g-2" collaboration from the Fermi National Accelerator Laboratory (FNAL) in the United States published further experimental findings that show that muons—heavy subatomic relatives of electrons—may have a larger magnetic moment than earlier Standard Model estimates had predicted, indicating that an unknown particle or force might be influencing the muon. The work builds on anomalous results first uncovered 20 years ago at Brookhaven National Laboratory (BNL), and calls into question whether the Standard Model needs to be rewritten.

Meanwhile, researchers in Germany have used Europe's most powerful high-performance computing (HPC) infrastructure to run new and more precise lattice quantum chromodynamics (lattice QCD) calculations of muons in a magnetic field. The team found a different value for the Standard Model prediction of muon behavior than what was previously accepted. The new theoretical value is in agreement with the FNAL experiment, suggesting that a revision of the Standard Model is not needed. The results are now published in *Nature* (https://doi.org/10.1038/s41586-021-03418-1).

The team primarily used the supercomputer JUWELS at the Jülich Supercomputing Centre (JSC), with the computational time provided by the Gauss Centre for Supercomputing (GCS) as well at JSC's JURECA system, along with extensive computations performed at the other two GCS sites—on Hawk at the High-Performance Computing Center Stuttgart (HLRS) and on SuperMUC-NG at the Leibniz Supercomputing Centre (LRZ).

Both the experimentalists and theoretical physicists agreed that further research must be done to verify the results published this week. One thing is clear, however: the HPC resources provided by GCS were essential for the scientists to achieve the precision necessary to get these groundbreaking results.

"For the first time, lattice QCD results have a precision comparable to these experiments. Interestingly our result is consistent with the new FNAL experiment, as opposed to previous theory results, that are in strong disagreement with it," said Prof. Kalman Szabo, leader of the Helmholtz research group, "Relativistic Quantum Field Theory" at JSC and co-author of the *Nature* publication. "Before deciding the fate of the Standard Model, one has to understand the theoretical differences, and new lattice QCD computations are inevitable for that."

Minor discrepancies, major implications

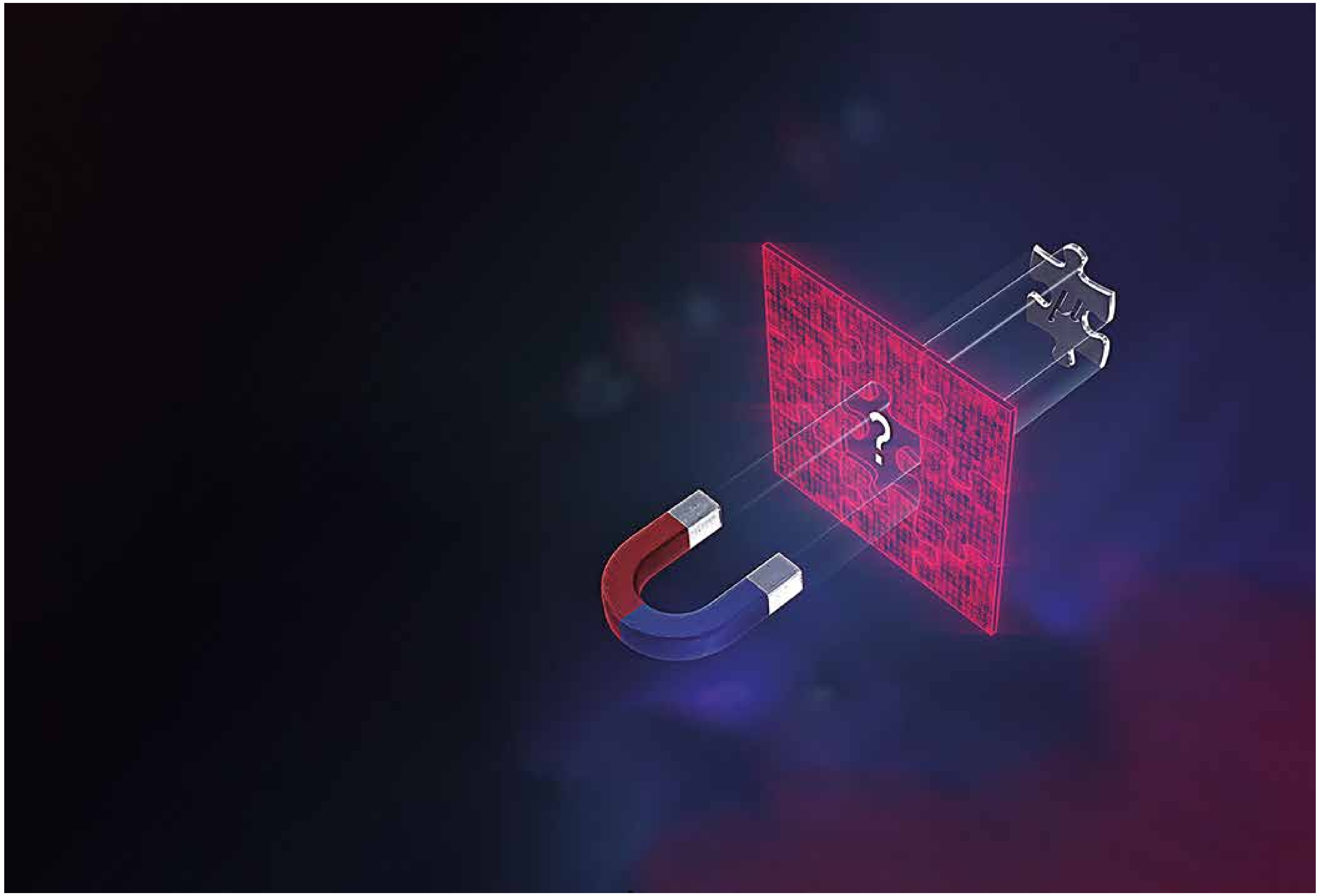
When BNL researchers recorded unexplained muon behavior in 2001, the finding left physicists at a loss—the muon, a subatomic particle 200 times heavier than an electron, showed stronger magnetic properties than predicted by the Standard Model of Physics. While the initial finding suggested that muons may be interacting with previously unknown subatomic particles, the results were still not accurate enough to definitely claim a new finding.

Over the next 20 years, heavy investments in new, hyper-sensitive experiments done at particle accelerator facilities as well as increasingly sophisticated approaches based in theory have sought to confirm or refute the BNL group's findings. During this time, a research group led by the University of Wuppertal's Prof. Zoltan Fodor, another co-author of the *Nature* paper, was progressing with big steps in lattice QCD simulations on the supercomputers provided by GCS. "Though our results on the muon g-2 are new, and have to be thoroughly scrutinized by other groups, we have a long record of computing various physical phenomena in quantum chromodynamics." said Fodor. "Our previous major achievements were computing the mass of the proton, the proton-neutron mass difference, the phase diagram of the early universe and a possible solution for the dark matter problem. These paved the way to our most recent result."

Lattice QCD calculations allow researchers to accurately plot subatomic particle movements and interactions with extremely fine time resolution. However, they are only as precise as computational power allows—in order to perform these calculations in a timely manner, researchers have had to limit some combination of simulation size, resolution, or time. As computational resources have gotten more powerful, researchers have been able to do more precise simulations.

"This foundational work shows that Germany's world-class HPC infrastructure is essential for doing world-class science in Europe", said Prof. Thomas Lippert, Director of the Jülich Supercomputing Centre, Professor for Quantum Computing and Modular Supercomputing at Goethe University Frankfurt, current Chairman of the GCS Board of Directors, and also co-author of the *Nature* paper. "The computational resources of GCS not only play a central role in deepening the discourse on muon measurements, but they help European scientists and engineers become leaders in many scientific, industrial, and societal research areas."

While Fodor, Lippert, Szabo, and the team who published the *Nature* paper currently use their calculations to cool the claims of physics beyond the Standard Model, the researchers are also excited to continue working with international colleagues to definitively solve the mystery surrounding muon magnetism. The team anticipates that even more powerful HPC systems will be necessary to prove the existence of physics beyond the Standard Model. "The FNAL experiment will increase the precision by a factor of four in two years. We theorists have to keep up with this pace if we want to fully exploit the new physics discovery potential of muons." Szabo said. *eg*



Does the magnetic moment of muons fit into our understanding of the laws governing the physical world around us?
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RESEARCHERS USE LRZ HPC RESOURCES TO PERFORM LARGEST-EVER SUPERSONIC TURBULENCE SIMULATION

A multi-institution team from Australia and Germany simulates turbulence happening on both sides of the so-called "sonic scale," opening the door for more detailed and realistic galaxy formation simulations.

Through the centuries, scientists and non-scientists alike have looked at the night sky and felt excitement, intrigue, and overwhelming mystery while pondering questions about how our universe came to be, and how humanity developed and thrived in this exact place and time. Early astronomers painstakingly studied stars' subtle movements in the night sky to try and determine how our planet moves in relation to other celestial bodies. As technology has increased, so too has our understanding of how the universe works and our relative position within it.

What remains a mystery, however, is a more detailed understanding of how stars and planets formed in the first place. Astrophysicists and cosmologists understand that the movement of materials across the interstellar medium (ISM) helped form planets and stars, but how this complex mixture of gas and dust—the fuel for star formation—moves across the universe is even more mysterious.

To help better understand this mystery, researchers have turned to the power of high-performance computing (HPC) to develop high-resolution recreations of galactic phenomena. Much like several terrestrial challenges in engineering and fluid dynamics research, astrophysicists are focused on developing a better understanding of the role of turbulence in helping shape our universe.

Over the last several years, a multi-institution collaboration being led by Australian National University Associate Professor Christoph Federrath and Heidelberg University Professor Ralf Klessen has been using HPC resources at the Leibniz Supercomputing Centre (LRZ) in Garching near Munich to study turbulence's influence on galaxy formation. The team recently revealed the so-called "sonic scale" of astrophysical turbulence—marking the transition moving from supersonic to subsonic speeds (faster or slower than the speed of sound, respectively)—creating the largest-ever simulation of supersonic turbulence in the process. The team published its research in *Nature Astronomy* (https://doi.org/10.1038/s41550-020-01282-z).

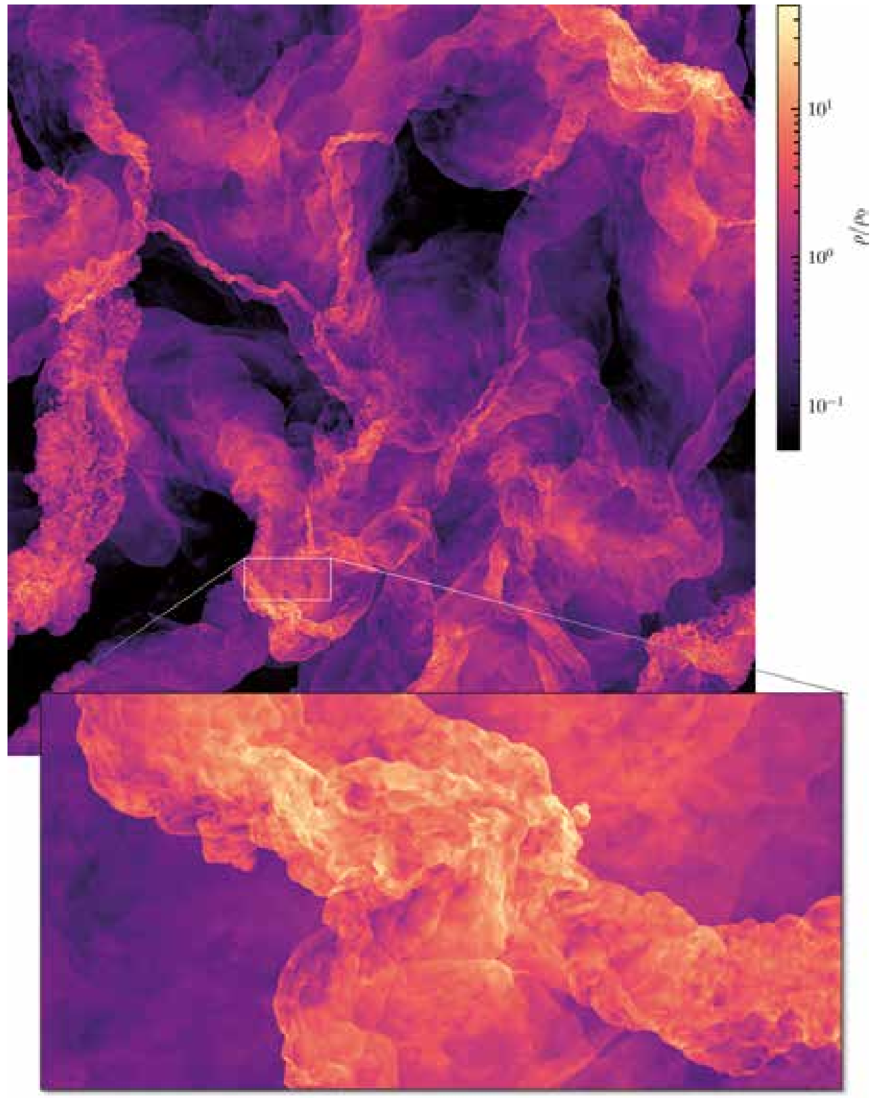
Many scales in a simulation

To simulate turbulence in their research, Federrath and his collaborators needed to solve the complex equations of gas dynamics representing a wide variety of scales. Specifically, the team needed to simulate turbulent dynamics on both sides of the sonic scale in the complex, gaseous mixture travelling across the ISM. This meant having a sufficiently large simulation to capture these large-scale phenomena happening faster than the speed of sound, while also advancing the simulation slowly and with enough detail to accurately model the smaller, slower dynamics taking place at subsonic speeds.

"Turbulent flows only occur on scales far away from the energy source that drives on large scales, and also far away from the so-called dissipation (where the kinetic energy of the turbulence turns into heat) on small scales" Federrath said. "For our particular simulation, in which we want to resolve both the supersonic and the subsonic cascade of turbulence with the sonic scale in between, this requires at least four orders of magnitude in spatial scales to be resolved."

In addition to scale, the complexity of the simulations is another major computational challenge. While turbulence on Earth is one of the last major unsolved mysteries of physics, researchers who are studying terrestrial turbulence have one major advantage—the majority of these fluids are incompressible or only mildly compressible, meaning that the density of terrestrial fluids stays close to constant. In the ISM, though, the gaseous mix of elements is highly compressible, meaning researchers not only have to account for the large range of scales that influences turbulence, they also have to solve equations throughout the simulation to know the gases' density before proceeding.

Understanding the influence that density near the sonic scale plays in star formation is important for Federrath and his collaborators, because modern theories of star formation suggest that the sonic scale itself serves as a "Goldilocks zone" for star formation. Astrophysicists have long used similar terms to discuss how a planet's proximity to a star determines its ability to host life, but for star formation itself, the sonic scale strikes a balance between the forces of turbulence and gravity, creating the conditions for stars to more easily form. Scales larger than the sonic scale tend to have too much turbulence, leading to sparse star formation, while in smaller, subsonic regions, gravity wins the day and leads to localized clusters of stars forming.



Turbulence shaping the interstellar medium. The image shows a slice through the turbulent gas in the world's highest-resolution simulation of turbulence published in Nature Astronomy. Turbulence produces strong density contrasts, so-called shocks (see zoom-in). The interaction of these shocks is believed to play a key role in the formation of stars. © Federrath et al. (2021). NatureAstronomy.DOI:10.1038/s41550-020-01282-z

In order to accurately simulate the sonic scale and the supersonic and subsonic scales on either side, the team worked with LRZ to scale its application to more than 65,000 compute cores on the SuperMUC HPC system. Having so many compute cores available allowed the team to create a simulation with more than 1 trillion resolution elements, making it the largest-ever simulation of its kind.

"With this simulation, we were able to resolve the sonic scale for the first time," Federrath said. "We found its location was close to theoretical predictions, but with certain modifications that will hopefully lead to more refined star formation models and more accurate predictions of star formation rates of molecular clouds in the universe. The formation of stars powers the evolution of galaxies on large scales and sets the initial conditions for planet formation on small scales, and turbulence is playing a big role in all of this. We ultimately hope that this simulation advances our understanding of the different types of turbulence on Earth and in space."

Cosmological collaborations and computational advancements

While the team is proud of its record-breaking simulation, it is already turning its attention to adding more details into its simulations, leading toward an even more accurate picture of star formation. Federrath indicated that the team planned to start incorporating the effects of magnetic fields on the simulation, leading to a substantial increase in memory for a simulation that already requires significant memory and computing power as well as multiple petabytes of storage—the current simulation requires 131 terabytes of memory and 23 terabytes of disk space per snapshot, with the whole simulation consisting of more than 100 snapshots.

Since he was working on his doctoral degree at the University of Heidelberg, Federrath has collaborated with staff at LRZ's AstroLab to help scale his simulations to take full advantage of modern HPC systems. Running the largest-ever simulation of its type serves as validation of the merits of this long-running collaboration. During this period, Federrath has worked closely with LRZ's Dr. Luigi Iapichino, Head of LRZ's AstroLab, who was a co-author on the *Nature Astronomy* publication.

"I see our mission as being the interface between the ever-increasing complexity of the HPC architectures, which is a burden on the application developers, and the scientists, which don't always have the right skill set for using HPC resource in the most effective way," Iapichino said. "From this viewpoint, collaborating with Christoph was quite simple because he is very skilled in programming for HPC performance. I am glad that in this kind of collaborations, application specialists are often full-fledged partners of researchers, because it stresses the key role centres' staffs play in the evolving HPC framework." *eg*

HPC HELPS SCIENTISTS IN QUEST FOR ADVANCING HYDROGEN-BASED ENERGY STORAGE

Researchers are working to identify materials and methods to improve water electrolysis, a promising approach that could more efficiently store energy generated from renewable sources.

Advances in renewable energy technologies continue to move humanity closer to being able to power our lives using cleaner, safer methods. Whether it is wind turbines or solar panels, researchers have made great strides in making these sources more efficient.

One major issue remains, though, and it is unlikely to go away any time soon—humans have no influence over when the wind blows or the sun shines. This means that in order to use renewable energy on a global scale, researchers must also devise methods for efficiently storing excess energy generated during "boom" times so there is ample power stores for moments when renewables are not keeping up with demand.

Among the promising contenders for storing excess energy, hydrogen is among the most popular. In a process called water electrolysis, scientists can create chemical reactions to break down the molecular bonds of water molecules so they become their constituent parts—hydrogen and oxygen. The resulting hydrogen molecules must then be compressed into storage containers where they can be used as replacements for dirtier energy sources coming from fossil fuels.

While researchers have made some progress identifying ways to do electrolysis at an industrial scale, there is still one major hurdle to clear—currently, iridium is the only catalyst proven to remain both active and stable enough to facilitate water oxidation, a key step in water electrolysis. Unfortunately, natural sources of iridium are vanishingly rare on the Earth's surface. Without having the technology to drill down to the Earth's core or harvest iridium from passing meteors, researchers must search for either an entirely new material or develop metal alloys—mixes of two or more different metals that retain certain characteristics from their constituent materials—in order to scale up water electrolysis to the point where it can make a meaningful contribution to global energy storage requirements.

Recently, researchers from the Fritz Haber Institute in Berlin have been using high-performance computing (HPC) resources at the High-Performance Computing Center Stuttgart (HLRS) to model the complex chemical reactions that take place during electrolysis at a molecular level. The team hopes that by using both cutting-edge experimental techniques and world-class supercomputers for simulation, they can gain a greater insight into what makes iridium so effective in order to develop an efficient method for using hydrogen to store energy on a global scale.

"It really is a million-dollar question about why iridium is so special," said Dr. Travis Jones, Fritz Haber Institute scientist and a researcher on the project. "There are a lot of ideas out there, and many of them revolve around the idea that the absorption energy of different intermediates in the reaction is ideally balanced. That said, a deep understanding is lacking, so we can't just look at the periodic table and say iridium works for electrolysis because of how many electrons it has. We would love to know what it is about iridium makes it work so well in this context."

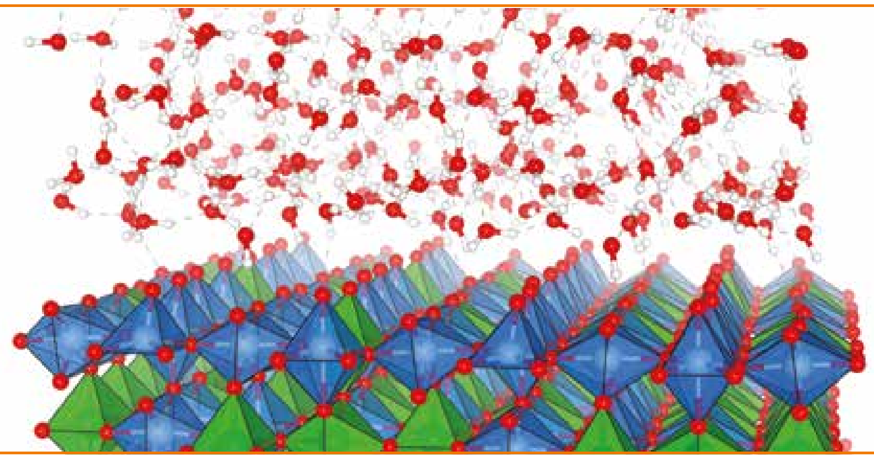
Viewing fine-grained interactions through two different lenses

Gaining a more fundamental view into how molecules behave during electrolysis requires both world-class computing resources and high-end experimental facilities. Scientists need to observe these chemical reactions at the atomic level, charting the paths of electrons for individual atoms while watching several hundreds of these atoms interacting with one another. Moreover, they would like to study these phenomena under a variety of conditions, an approach that would be impossible experimentally but can be done using computational modeling. Computational scientists then share these models with experimentalists, providing further insights into spectroscopic experiments that use focused light to illuminate atomic-level behaviors in a chemical reaction.

This is only the first point when HPC plays an important role, though. "Simulating the electrons by solving Schrödinger's equation is the first step. Here, we are basically guessing what we have in the system by uncovering the atomic structure of the catalysts during experiments," Jones said. "What the experiments can't tell us, however, is how the reaction mechanism works at the atomic level, but the simulations can."

In essence, the first phase of modeling and experimental work allows the researchers to get accurate, atomic-level detail of water atoms on the surface of the catalyst. Once the researchers feel confident that they have an accurate picture, they begin the second phase, which allows them to make slight modifications to inputs and model how the reaction proceeds under different conditions. This rapid-fire approach to modeling allows the researchers to observe how the reaction changes under the influence of small changes in voltage or of variations in the composition of metal alloys being used as the catalyst, among other inputs.

Through its work, the team identified a particular alloy, iridium oxide mixed with niobium ($Ir_{60}Nb_{40}Ox$) that behaves nearly as stably as pure iridium, but requires 40 percent less of the precious metal. While the team knows that much more work needs to be done to identify other materials that might be suitable as an electrocatalyst, it feels confident that the two-pronged approach of spectroscopic experiments and large-scale simulations is the ideal method for moving the research forward. The results were published in *ACS Appl. Mater. Interfaces.* (https://doi.org/10.1021/acsami.0c12609)



The solid-liquid interface at the iridium rich surface of an Ir-Nb mixed oxide water oxidation catalyst. Iridium atoms are shown as blue, niobium as green, oxygen as red and hydrogen as white. **© Travis Jones**

Today's supercomputers focused on tomorrow's reimagined energy grid

Like many researchers in his field, Jones indicated that being able to scale up electrolysis to the point it can function on a global level still faces many challenges. But the promise of using clean hydrogen gas to spin turbines in power plants or developing new fuel cells that could supplant combustion-based automotive engines has scientists focused on finding ways to make the process more efficient.

Through a large, international effort, the code used by Jones and his collaborators was recently modified to run on hybrid supercomputing architectures—machines that use graphics processing units (GPUs) in addition to traditional CPUs. The team also began working on scaling its application to take full advantage of increasingly powerful architectures such as those made available by GCS at its three centres.

While Jones indicated that faster, larger computers make it possible for the team to study larger molecular systems or more permutations of a given system, the investigators are still limited in the number of atoms they can simulate during each run. Next-generation systems will help address some of these computational hurdles. At the same time, however, simulating ever larger systems will introduce a new problem: his team will primarily be limited by system memory availability—an increasingly common challenge for researchers at the forefront of computational science in many research domains.

Despite more technical hurdles to overcome, the team feels confident that using HPC to accelerate experimental efforts will prove indispensable moving forward. While water electrolysis may not immediately become the dominant method for changing the world's energy grid, Jones feels confident that hydrogen will prove to be a game-changer in electrical energy storage and conversion. Whether scientists wind up finding a cheaper, more readily available replacement for iridium or developing alloys that can use iridium in sparing amounts, the promise of clean energy storage motivates the team to keep searching.

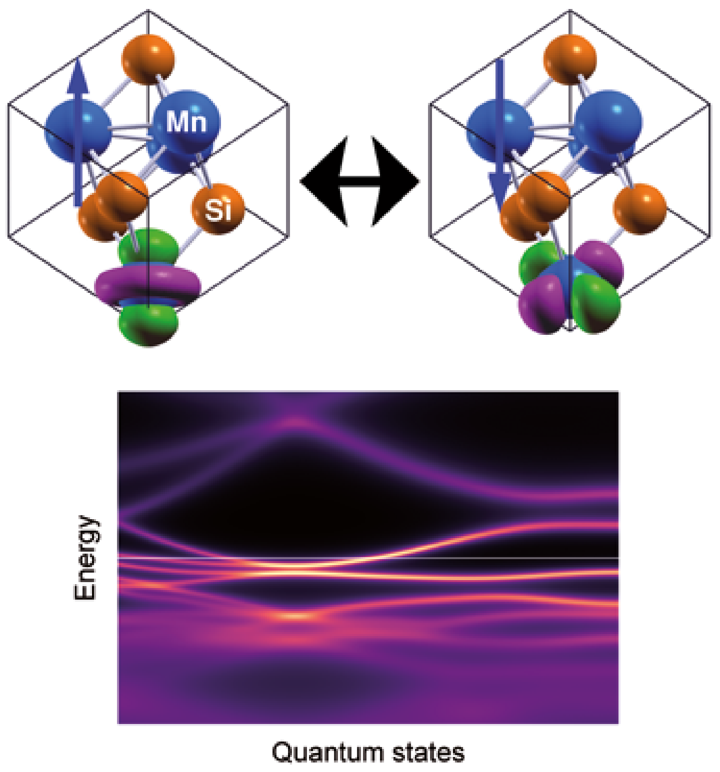
"Electrolytic water splitting links the electrical and chemical sectors, and when we think about going climate-neutral by 2050, that link becomes critical," Jones said. "It is not just energy storage that we have to worry about; it is also sustainable chemical production. Green hydrogen could help solve both of these issues." *eg*

RESEARCHERS USE THE POWER OF HPC TO ELUCIDATE HUND METAL CHARACTERISTICS

A cross-disciplinary, international research consortium is working on understanding a novel state of matter that may have implications for advanced electronics and data storage.

In the last 100 years, materials science, condensed matter physics, and elementary particle physics research became one of the largest new frontiers for scientists. In order to study materials at a fundamental level, scientists focused on technological advancements, building neutron research facilities that allow researchers to shoot individual neutrons at a variety of sensitive experimental tools. These facilities, among other technical innovations, allow researchers to gain more insight into the atomic and subatomic worlds.

Even with the most advanced experimental methods, though, researchers still encounter difficulties in studying particle interactions under certain conditions—atomic particles can interact with one another in extremely short-lived ways that can still have a major influence on a material, or only display novel properties when in extreme temperature or pressure environments.



The top image describes the fluctuation of orbital (green/violet lobes) and spin (blue arrows) character that takes place when electrons move between sites in the MnSi crystal.
The bottom image provides a view of the electronic energy spectrum in such a material for its various quantum states. The white line refers to the energy for which the electrons are on the move through the system. © Frank Lechermann

With the advent of high-performance computing (HPC), many researchers started to pair experimental research with computationally intensive modeling and simulation. Taken together, these two approaches have helped scientists uncover new materials, modify existing materials at the atomic level in order to impart specific properties, and generally advance our understanding of materials' atomic interactions under a variety of conditions.

Among these materials is manganese monosilicide (MnSi), a compound that, at first glance, seems to behave similarly to many other metals. When brought down to extremely cold temperatures, however, MnSi shifts from behaving like a run-of-the-mill metal to something subtler and more mysterious.

In order to better understand MnSi, a research team led by University of Hamburg researcher Dr. Frank Lechermann partnered with experimentalists to record and confirm aspects of this material's relatively hidden behavior. The team published its results in *Nature Communications*. (https://doi.org/10.1038/s41467-020-16868-4).

"Many people studied this material, and it is for instance known that if you apply pressure, you can reach different phases, phases of transport, and even stranger magnetic phases. Very intriguing physics pop up with this material," Lechermann said.

The search to define Hund metal physics

Growing up, most people play with magnets in elementary science classrooms or on their home refrigerator. Despite their nearly ubiquitous nature in our daily lives, magnets and magnetism are less straight-forward than just identifying a magnetic material and shaping it into a refrigerator magnet.

Materials can display a variety of characteristics when it comes to either conducting for or insulating against electric charges. Through extensive trial and error, humans have learned that things like iron can reliably conduct electricity and act as magnets under the right environmental circumstances. Our ability to zoom in and look at the atomic and subatomic interactions of materials ushered in a new era of advancement, with silicon-based semiconductors playing a central role in commercializing computers and other telecommunication technologies.

With a greater understanding of more exotic materials, or how certain materials behave under more radical temperature and pressure settings, researchers hope to discover cheaper, more effective alternatives for manufacturing technologies.

MnSi is a good example—while the material exhibits many typical characteristics common to metals, such as serving as a conductor and demonstrating ordered magnetism in its naturally occurring state at cold temperature, researchers uncovered that MnSi acts as a "Hund's metal;" that is, it shows unusual transport and magnetic properties at temperatures above magnetic ordering some of the time, while still behaving as typical metal at other moments.

Much like cuprates—copper-infused metals that can serve as lossless superconductors under the right circumstances—Hund's metals present possibilities for researchers to develop new electronics and other technologies. In order to exploit Hund's metals unique characteristics, though, researchers first need to have a fundamental understanding of how the material works at the atomic level.

To that end, researchers developed a two-pronged approach involving both supercomputing simulations as well as experiments at neutron sources. Experiments done at neutron sources are expensive, however, and considering that researchers are still trying to develop a more comprehensive list of characteristics for Hund's metals, HPC simulations play an essential role in discovery.

"For this material, it was incredible to have access to supercomputing facilities," Lechermann said. "The problem is really demanding. We can, of course, do simpler, standard theories that you can run on your own machine, but when you want to understand the correlation effects—interactions that are more sophisticated, with interacting electrons, so it is a many-body problem—that becomes very complicated."

Fuzzy focus on electron motion

In order to understand how materials' behaviors change under different circumstances, researchers must focus on electrons' motions and interactions in a given system. For a material to be magnetic, serve as a conductor, an insulator, or any other number of properties, its electrons must often act in a specific manner. Depending on the material in question, in an atomic system, negatively charged electrons starting off from a certain position, or a certain atomic orbital and with a certain quantum rotation ('spin'), may have an easier or more difficult time moving to another position.

Moving electrons in MnSi behave as "quasiparticles," which basically means that the motion of an individual electron always also affects the state of other electrons nearby, because electrons interact with each other. In a second step, this correlated flow gives rise to a new entity: the given particle and its attached cloud of interactions with other particles along a given path.

"Assume you go to a concert, and you see that the band is about to play, so you want to go to the stage," Lechermann said. "You know what happens, some people step aside, other people stand in your way, and behind you some people follow you because you're making a path, etc. That is what it is like for a quasiparticle—one particle is moving, but many other particles are affected because of this movement. Such a quasiparticle has a certain level of coherence—meaning it can see a path to move toward to the stage—but if you raise the temperature, it is like the band is now playing and everyone is hopping around, making it much more difficult to chart a coherent path because of all the shaking in the environment."

In its investigations, the team found that unlike other correlated metals that have relatively large windows for forming these coherent paths, MnSi as a specific Hund's metal only showed these properties in a much narrower window. The actual dependence on the electrons' orbital and spin character is at the root of this restraint.

Frontier life

Having completed an initial investigation into MnSi, the team feels confident in its two-pronged approach. Further, working with JSC staff ensured that the team was able to efficiently install its code on JSC's current flagship computer, JUWELS. Lechermann indicated that he and his collaborators were interested in developing a more comprehensive understanding of which materials demonstrate Hund's metal properties, and under which conditions they are most likely to occur. Other silicides and certain novel iron compounds show many of the same Hund's metal characteristics as MnSi, but it is too early to tell if those would behave the same under a wider variety of conditions.

For Lechermann and his collaborators, the most exciting part of this work is knowing that their research sits on the true frontier of scientific discovery, and that by leveraging both HPC resources and state-of-the-art experimental facilities, they help illuminate more about material interactions on an atomic level and help set the stage for a new era of technological advancement. *eg*

SEQUOIA PROJECT TO BRING QUANTUM COMPUTING TO INDUSTRY

HLRS will help develop new software for quantum computers and investigate ways to integrate them with conventional systems for high-performance computing and artificial intelligence.

For certain kinds of problems, quantum computing promises to offer advantages over even the fastest supercomputers. Because the technology is only now moving from theoretical research into practical use, however, there is an urgent need to identify which kinds of applications would benefit most from quantum computing, particularly in industry. At the same time, research is needed to develop the software, algorithms, and IT infrastructure that will be necessary to take full advantage of the power that quantum computing could offer.

The High-Performance Computing Center Stuttgart (HLRS) aims to help fulfill these ambitious goals in a newly announced project called SEQUOIA (Software Engineering for Industrial Hybrid Quantum Applications and Algorithms). Working together with the Fraunhofer Institute for Industrial Engineering (Fraunhofer IAO) and five additional partners, HLRS will conduct research to improve the performance of algorithms for quantum computing. Additionally, HLRS will focus on developing hybrid approaches that integrate quantum computing with existing high-performance computing (HPC) and artificial intelligence (AI) methods. By pursuing this research in the context of collaboration with industry partners, the results should lead to quantum computing applications that both resolve current challenges facing HPC and AI, and demonstrate the potential benefits of quantum computing for industry.

SEQUOIA is one of six new projects funded through grants totaling 19 million Euro from the Baden-Württemberg Ministry of Economic Affairs, Labor, and Housing. Fraunhofer IAO will lead the project, which will operate in coordination with the national Competence Center "Quantum Computing Baden-Württemberg." The competence center is managing the testing and use of an IBM Q System One quantum computer, installed in early 2021 in Ehningen, a small town just south of Stuttgart.

"The access to Germany's first IBM quantum computer will make Stuttgart and the State of Baden-Württemberg a European center for research and development in the field of quantum computing," said HLRS Director Michael Resch. "As is the case with HLRS's high-performance computing systems, however, it is important that we ensure that researchers in the industrial high-tech community across our region who could benefit from this new technology also have access to the necessary solutions and expertise. SEQUOIA will investigate fundamental problems that will need to be addressed to achieve this goal."

New software for quantum computing

The excitement surrounding quantum computers results from the fact that they are substantially different from other kinds of high-performance computing systems. Based on principles of quantum physics, they have already begun to demonstrate the possibility of "quantum supremacy," an accomplishment in which quantum computers perform calculations faster than supercomputers running on more traditional architectures.

This fundamental difference in the technology, however, means that software and algorithms designed for traditional high-performance computing and artificial intelligence applications cannot simply be ported onto a quantum computer.

For this reason, researchers at HLRS will investigate questions that are important for the programming of quantum computing systems and their usage in real-world scenarios. This will include evaluating how well existing algorithms for simulation and artificial intelligence perform on quantum systems and optimizing them in ways that make them run more efficiently. This algorithm and software development will take place in the context of demonstration projects investigating their potential to improve industrial applications.

Integrating quantum computing into hybrid workflows

Although quantum computers promise to be faster at running certain applications, researchers expect them to have the most impact for future research by integrating them into hybrid workflows that optimally combine quantum computing with HPC, AI, and other more established approaches. In order to make such workflows operate efficiently, however, research is necessary to develop the software interfaces between quantum computers and classical computing platforms.

Looking at potential applications of quantum computing in industry, HLRS will develop, evaluate, and test a variety of hybrid approaches involving quantum computers. Specifically, researchers at HLRS will investigate hybrid applications for commonly encountered problems in the fields of optimization, machine learning, and linear algebra.

Potential applications of quantum computing in industry

Close cooperation with industry will be important to the success of SEQUOIA. The exact applications that the project will investigate are still to be determined, but the team currently plans to look at the relevance of quantum computing for industries such as manufacturing, robotics, logistics, energy, engineering, finance, and healthcare.

"We expect to identify applications of quantum computing that offer clear opportunities to increase productivity in comparison with more traditional approaches," said Dennis Hoppe, who will oversee HLRS's activities in SEQUOIA. "At the same time, gaining a better understanding of the possibilities of quantum computing and demonstrating real-world applications of hybrid scenarios that combine the power of HPC and quantum computers will be a valuable outcome of this project." *cw*

SEQUOIA

Funding:
Baden-Württemberg Ministry of Economic Affairs, Labor, and Housing

Funding amount:
6,162,226 Euro

Runtime:
01.01.2021 – 31.12.2022

Partners:
Fraunhofer-Institut für Arbeitswirtschaft und Organisation (IAO)
Fraunhofer-Institut für Produktionstechnik und Automatisierung (IPA)
Fraunhofer-Institut für Angewandte Festkörperphysik (IAF)
FZI Forschungszentrum Informatik (FZI)
Universität Stuttgart, Institut für Architektur von Anwendungssystemen (US-IAAS)
Universität Stuttgart, Höchstleistungsrechenzentrum Stuttgart (US-HLRS)
Eberhard Karls Universität Tübingen, wLehrstuhl Eingebettete Systeme (EKUT)

PROJECTS

DEEP-SEA AND REGALE HELP BOLSTER DYNAMIC SOFTWARE FOR EXASCALE

Future exascale high-performance computers require a new kind of software that allows dynamic workloads to run with maximum energy efficiency on the best-suited hardware available in the system. The Technical University of Munich (TUM) and the Leibniz Supercomputing Centre (LRZ) are working together to create a production-ready software stack to enable low-energy, high-performance exascale systems.

Prof. Martin Schulz **© Andreas Heddergott / TU Muenchen**

Exascale supercomputers are knocking at the door. They might be a game-changer to the way we design and use high-performance computing (HPC) systems. As exascale performance drives more HPC systems toward heterogenous architectures that mix traditional CPUs with accelerators like GPUs and FPGAs, computational scientists will have to design more dynamic applications and workloads in order to get massive performance increases in their applications.

The question is: How will applications leverage these different technologies efficiently and effectively? Power management and dynamic resource allocation will become the most important aspects of this new area of HPC. Stated more simply: how do HPC centres ensure that users are getting the most science per Joule?

Optimization is challenging

Optimizing application performance on heterogeneous systems under power and energy constraints poses some challenges. Some are quite sophisticated, like the dynamic phase behavior of applications. And some are basic hardware issues like the variability of processors: Due to manufacturing limitations, low-power operation of CPUs can cause a wide variety of frequencies across the cores. Adding to these is the ever-growing complexity and heterogeneity on node-level.

A software stack for such heterogeneous exascale systems will have to meet some specific demands. It has to be dynamic, work with highly heterogeneous integrated systems, and adapt to existing hardware. The Technical University of Munich and the Leibniz Supercomputing Centre are working closely together to build a software stack based on existing and proven solutions. Among others, MPI and its various implementations, SLURM, PMIx or DCDB are well-known parts of this Munich Software Stack.

“The basic stack is already running on the SuperMUC-NG supercomputer at the LRZ”, says Martin Schulz, Chair for Computer Architecture and Parallel Systems at the Technical University of Munich and Director at the Leibniz Supercomputing Centre. “Right now, we are engaged in two European research projects for further development of this stack on more heterogeneous, deeper integrated and dynamic systems, as they will become commonplace in the exascale era: REGALE and DEEP-SEA.” One of the foundations for the next generation of this software stack is the HPC PowerStack, an initiative, with TUM as one of the co-founders, for better standardization and homogenization of approaches for power and energy optimized systems.

EU projects address the questions

REGALE aims to define an open architecture, build a prototype system, and incorporate in this system appropriate sophistication in order to equip supercomputing systems with the mechanisms and policies for effective resource utilization and execution of complex applications. DEEP-SEA will deliver the programming environment for future European exascale systems, capable of adapting at all levels of the software stack. While the basic technologies will be implemented and used in DEEP-SEA, the control chain will play a major role in REGALE.

Both projects are focused on making existing codes more dynamic so they can leverage existing accelerators: Many codes today are static and might only be partially ready for more dynamic systems. This will require some refactoring, and in some cases, complete rewrites of certain parts of the codes. But it will also require novel and elaborate scheduling methods that must be developed by HPC centres themselves. Part of the upcoming research in DEEP-SEA and REGALE will be to find ways to determine, where targeted efforts on top of an existing software stack can yield the greatest result. To this end, agile development approaches will play a role: Continuous Integration with elaborate testing and automation are being established on BEAST (Bavarian Energy-, Architecture- and Software-Testbed) at the LRZ, the testbed for the Munich Software Stack.

Need for holistic approach

“Most research in the field of power and energy management today is done site-specific,” Schulz said. “We see little integration of the components; we have a lack of standardized interfaces that work on all layers of the software stack. In the end, this leads to suboptimal performance of the applications and increases the power needed by the system. With the Munich Software Stack, TUM and LRZ are working on an open, holistic, and scalable approach to an integrated power and energy management in order to get the most out of supercomputers to come.” *js*

DEEP-SEA & REGALE

Runtime:
2021 – 2024

Funding Source:
EuroHPC Programmes + involved member states under grant agreement numbers 955606 (DEEP-SEA) and 956560 (REGALE)

Funding:
15 Mio Euro (DEEP-SEA) & 7,5 Mio Euro (REGALE)

German Partners:
Leibniz Supercomputing Centre
Technical University of Munich
Jülich Supercomputing Centre
TWT GmbH Science & Innovation
Technical University Darmstadt
Fraunhofer Gesellschaft

ADVANCING AI TECHNOLOGIES TOWARDS EXASCALE COMPUTING

CoE RAISE receives funding from the European Commission

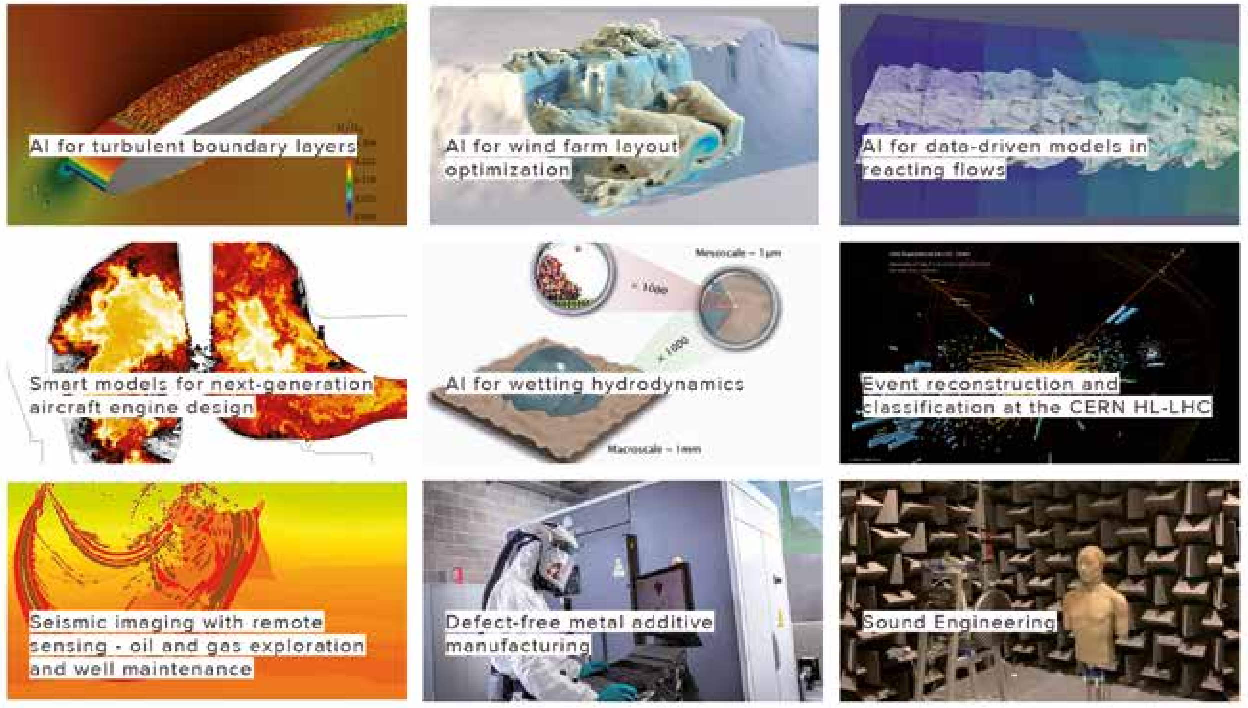


Fig. 1: Compute- and data-driven use cases of CoE RAISE. © CoE RAISE

Since the beginning of 2021, a group of experts in high-performance computing (HPC), artificial intelligence (AI), engineering, and natural sciences has received funding from the European Commission (EC) to form the European Center of Excellence in Exascale Computing "Research on AI- and Simulation-Based Engineering at Exascale" (CoE RAISE). The project has been awarded a grant of roughly 5 million Euro and is led by the Jülich Supercomputing Centre (JSC) at Forschungszentrum Jülich. In CoE RAISE, researchers representing academia and industry from 10 different European countries are focused on developing novel AI technologies towards exascale along various use cases of societal importance. The 11 full partners and two additional third parties of the project join the other 15 CoEs funded by the EC and cover the continuously emerging field of AI, with a special focus on efficiently utilizing future HPC hardware.

CoE RAISE converges traditional HPC and innovative AI techniques, working to further accelerate scientific discovery by leveraging ever more powerful and complex hardware infrastructures. This complexity, often in the form or heterogeneous HPC architectures or stemming from the application workflow itself, must be taken into account. To cover a broad spectrum of applications, several compute-driven and data-driven use cases have been selected (see Fig. 1). For the compute-driven cases, CoE RAISE develops HPC codes and workflows that deal with solving multi-physics, multi-scale problems at large scale. The project places a special emphasis on the development of "full loops," where traditional workflows — comprised of input, simulation, and output processes — are advanced to workflows that have recurrent and optimizing components (see Fig. 2). In contrast, the data-driven use cases have a strong focus on processing big data in efficient workflows.

Fig. 2: Full loop model optimization. © CoE RAISE

The HPC, AI, and application domain developments are tightly intertwined in a co-design sense. AI methodologies relevant for the use cases will be generalized for universal application in a functional and versatile software infrastructure ready to scale for enormous quantities of data. This means that a unique AI framework according to the workflow shown in Fig. 3 is developed. This framework addresses the needs of a broad range of HPC workloads that are intertwined with complementary advanced AI algorithms such as gated recurrent units, residual networks, deep belief networks, stacked auto-encoders, data augmentation techniques, pre-trained neural networks, transfer learning, or neural architecture search techniques driven by reinforcement learning and evolutionary computation methods.

The developments are performed on novel hardware technologies, such as modular supercomputing architectures, quantum annealing systems, and HPC prototypes, to explore a yet-unachieved performance increase in data processing and to establish exascale readiness. CoE RAISE's European network will develop and provide best practices, support, and education for industry, small and medium-sized enterprises (SMEs), academia, and HPC centers. This is closely linked to the development of a business providing new services to various user communities. That is, to reach self-sustainability beyond of the funding horizon, CoE RAISE will establish a business providing support and training on the unique AI framework as well as infrastructures, platforms, and software as services to increase the uptake of exascale and AI among various stakeholders from industry and academia.

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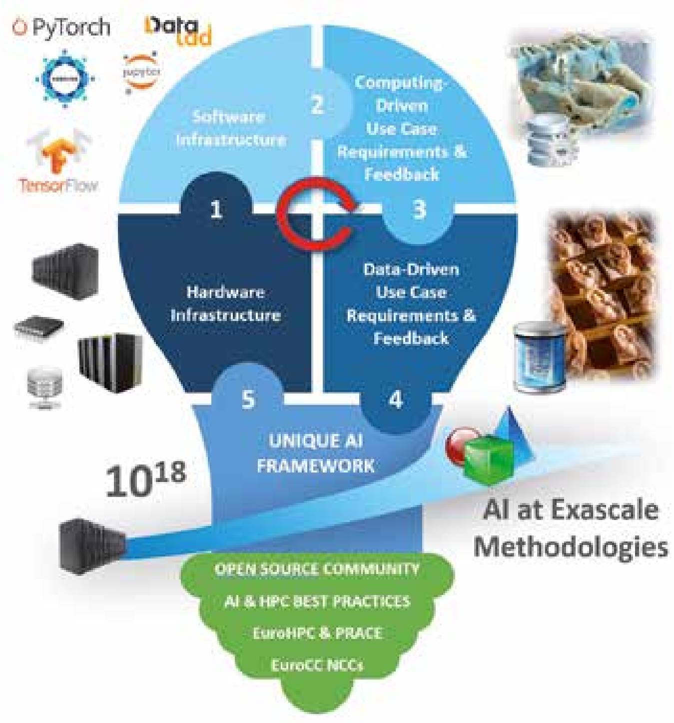

Fig. 3: Development of a unique AI framework within CoE RAISE. © CoE RAISE

RAISE

Runtime (funding period):
2021 – 2023

Funding Source:
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4.97 million Euro

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Forschungszentrum Jülich GmbH (DE), University of Iceland (IS), The Cyprus Institute (CY), RWTH Aachen University (DE), Barcelona Supercomputing (ES), Center Conseil Européen pour la Recherche Nucléaire (CH), Centre Européen de Recherche et de Formation Avancée en Calcul Scientifique (FR), Bull SAS (FR), Rigas Tehniska Universitate (LV), Flanders Make VZW (BE), Safran HE (FR), ParTec AG (DE), Technische Universiteit Delft (NL)

JUWELS BOOSTER EARLY DAYS HELP USERS MAKE THE MOST OF JSC'S GPU-ACCELERATED MODULE

Multi-day event focuses on giving users a deeper introduction to the newest JUWELS module.

In November 2020, the JUWELS Booster module at the Jülich Supercomputing Centre (JSC) was officially put into production. When it came online and made publicly available, it became Europe's fastest supercomputer. Prior to its commissioning, the system had already been put through its paces for several months by a selected number of application teams and their codes within the JUWELS Booster Early Access Program (EA Program). The program allowed the participating teams to prepare and optimize their applications for the new hardware and software stack, while also providing JSC system administrators important insights to the behavior of the system.

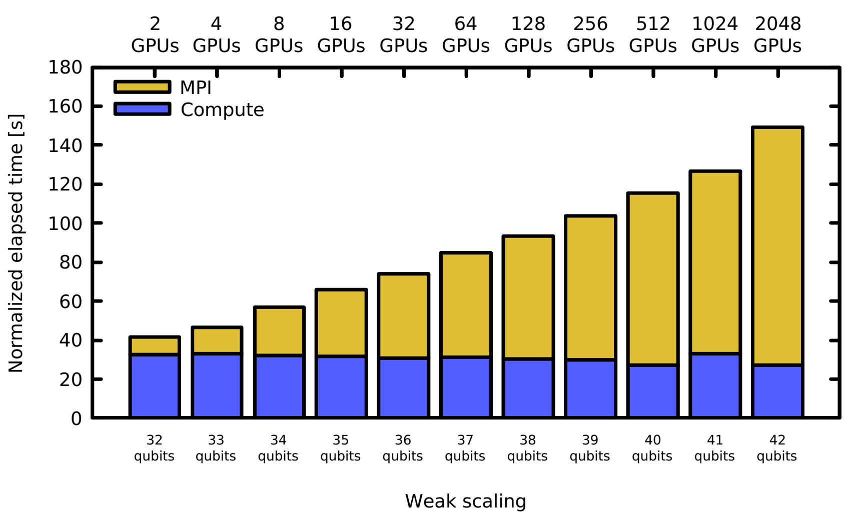
In order to present the first scientific results, performance measurements, and lessons learned obtained during these early days of JUWELS Booster, JSC staff organized the JUWELS Booster Early Access Colloquium in January 2021 (online). The colloquium was the preceding event to the first JUWELS Booster Porting Workshop, aiming at supporting researchers with a jump-start on JUWELS Booster.

During the EA Colloquium, 11 EA Program participants from a diverse set of scientific domains presented their results. The majority reported good performance improvements. ParFlow, for example, a library for modeling hydrologic simulations, measured great performance improvements when comparing GPUs to CPUs in a Booster node. The new methods just built into ParFlow and tailor-made for GPUs proved successful, with up to 26-fold speed-up comparing GPUs to CPUs in a Booster node, consistent over hundreds of nodes.

The quantum simulator JUQCS saw good performance increase when comparing previous GPU architectures to the new A100 Tensorcore GPUs used in the JUWELS Booster. The InfiniBand-based high-bandwidth network made scaling for this communication-intensive application a breeze.

SOMA, an application modeling the kinetics of nanomaterial formation, saw improvements over previous GPU generations for different test benchmarks and new scientific cases. As part of their preparation, the team participated in the Helmholtz GPU Hackathon, during which they were able to analyze and tune their algorithms specifically for the new GPU.

An application from the theoretical particle physics community saw large reductions in times-to-solution for their simulations, utilizing the lower precision computing capabilities of the A100 extensively. At the same time, the application was able to deliver important input to the system operation: JSC staff and EA Program participants were able to trigger adoptions in the systems' hardware and software, resulting in improved overall performance.

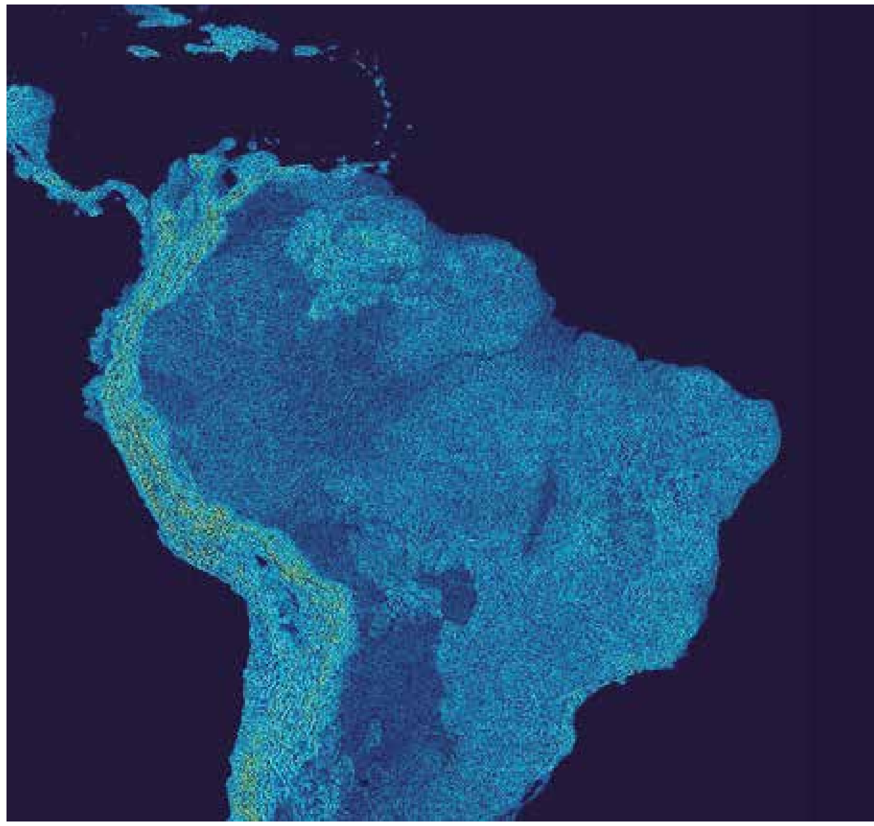


Weak scaling results for the simulation of quantum circuits with an increasing number of qubits. Shown is the normalized run time, split into the time spent on computation (blue, nearly constant) and MPI communication (yellow, increasing linearly). With every additional qubit (bottom axis), the number of GPUs is doubled (top axis) to beat the otherwise exponential increase in run time.

© JUQCS-G Developers, presented in pre-print https://arxiv.org/pdf/2104.03293.pdf

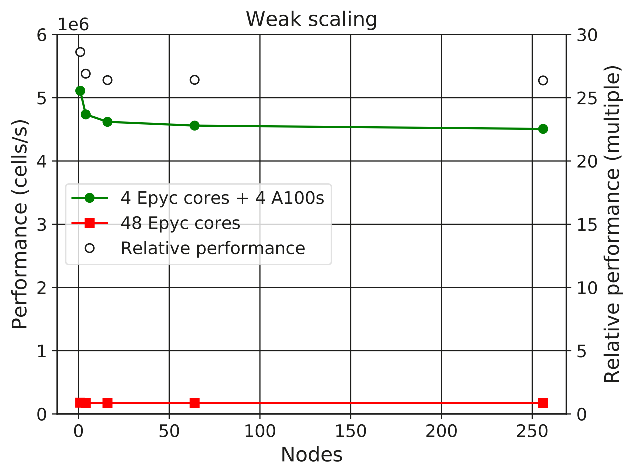
Most of the EA Colloquium participants either reported great results or were anticipating good, upcoming performance and a faster start to their research projects due to the early access. Users indicated they were satisfied with the EA Program, as they could use the 75-petaFLOPS module from the very first day for their challenging, new scientific endeavours, even though this meant preparing on a system that was still under construction. All EA Program participants re-quested compute time in the first GCS Large Scale Call for JUWELS Booster, attesting the sci-entific excellence of the involved projects.

The EA Colloquium was followed by the first JUWELS Booster Porting Workshop, with participants from fifteen teams covering a wide range of scientific topics. The 4-day online workshop consisted of lectures in the morning, introducing the system architecture and its program-ming, followed by generous amounts of hands-on time for the remainder of the days. While the first two days were more general, the last two days focused on advanced topics during the lectures and additional hands-on time.



Surface drainage in South America, simulated with ParFlow on JUWELS Booster (1-kilometre resolution).

© J. Hokkanen, S. Kollet, B. Naz



Weak scaling behavior of ParFlow on JUWELS Booster after implementing support for GPUs, comparing CPUs and GPUs of different numbers of nodes. Right axis: Relative speedup. © J. Hokkanen, S. Kollet, https://doi.org/10.1007/s10596-021-10051-4

This approach got new users up to speed quickly, allowing them to get started on porting their applications to JUWELS Booster and its GPUs. During the intensive hands-on sessions, teams worked on their codes and had in-depth discussions, making progress on their way to GPU-accelerated applications. All of this was done under expert instruction by the mentors each team was assigned at the beginning as well as additional experts from JSC and NVIDIA that were available throughout the course of the workshop, giving advice and providing professional support.

The JUWELS Booster got off to a strong start. Both new and long-time users alike are showing interest in making full use of the machine, and the center staff is already looking forward to seeing what new scientific outcomes the machine will enable. *ah*

LRZ STEPS INTO THE QUANTUM AGE

With the inauguration of LRZ's quantum integration centre, the centre demonstrates its commitment to architectural diversity and an embrace of emerging technologies.

"This is the warp drive for the research of the future. We enable research in new dimensions with a quantum district in Bavaria. What Silicon Valley is today, Munich Quantum Valley will be in the future," Bavarian Minister President Söder (left) underlines at the QIC opening. Right: State Minister for Science and the Arts Bernd Silber **© LRZ**

In mid-March, 2021 Bavaria's Minister President Markus Söder opened the new Quantum Integration Centre (QIC) at the Leibniz Supercomputing Centre (LRZ). During the virtual event, "On Heisenberg's Shoulders: The Future of Quantum Computing in Bavaria," the Bavarian Minister President, along with the Bavarian Minister of Science, Bernd Sibler, led a lively discussion with LRZ quantum experts as well as researchers and scientists from the Bavarian quantum computing community on the hopes and challenges associated with this disruptive but exciting new technology.

With the QIC, the LRZ is pursuing three ambitious goals and making an important contribution to supporting the Bavarian Hightech Agenda:

- Establish and expand quantum computing resources and services for research scientists in a reliable, secure, and flexible manner.
- Research and development towards integrating quantum acceleration into future high-performance computing (HPC) systems, including developing the necessary hybrid software stack.
- Exchange with the local and international quantum community for collaboration, networking, assessing emerging technology and identifying current and coming end-user needs.

"The LRZ Quantum Integration Centre really is where we bundle our quantum computing activities and drive them forward with our partners in the Munich Quantum Valley under the umbrella of the Bavarian Hightech Agenda," explains Prof. Dieter Kranzlmüller, Director of the LRZ. While the opening of the QIC symbolizes this integration, efforts in the area of quantum computing had already started some years back: Intel's quantum simulator had already been installed and running on SuperMUC-NG since summer 2019 and provides researchers with the computing power of up to 42 qubits.

To best fit offerings with needs, LRZ founded the Bavarian Quantum Computing eXchange (BQCX) in 2019 to serve as a strong channel with and for both the local and international quantum communities. Through the BQCX, researchers from academia and industry are connected with emerging technologies, one another for research collaborations, and hardware and software providers for education and training opportunities. In addition to ideas for initial seminars and workshops, early BQCX meetings facilitated LRZ's quantum strategy to establish the QIC. "This is the time to get into the field, to be part of this quantum era, and to help stir the future and direction forward," said Laura Schulz, Head of Strategic Development and Partnerships at LRZ. Schulz largely influenced

"Munich is to become one of the leading hotspots in the field of quantum technologies with funding from the Hightech Agenda Bavaria. The Quantum Integration Centre is the novel prototype of a pioneering experiment for combining quantum and supercomputing. It is located in the perfect place with the LRZ as one of the world's most powerful computing centres."

Bavarian Minister of Science Bernd Sibler

the LRZ quantum strategy, and feels confident that LRZ is embracing an important emerging technology early in its development.

With the QIC opening, quantum activities have picked up speed: The Atos Quantum Learning Machine (QLM), offering up to 38 qubits, has been installed at LRZ and LRZ staff just hosted a first training workshop on the topic. Together with the Finnish-German start-up IQM, Technical University of Munich (TUM), Freie Universität Berlin, Forschungszentrum Jülich, and chip manufacturer Infineon, LRZ will develop a robust quantum processing unit (QPU) in the next few years and put it into operation in its high-performance computer architectures.

In another recent development, the "Digital-Analogue Quantum Computing" (DAQC), a project funded by the Federal Ministry of Education and Research (BMBF) that combines the technology of analogue circuits with that of digital-universal computing units, allowing researchers to essentially get the best of both worlds in using the flexibility of digital QPUs and the powerful but less universal analogue QPUs. The resulting QPU will, among other things, help to accelerate high-performance computers at LRZ and make other services possible. Supporting the research and development on the software side of things, LRZ is partnering with the two Munich universities and various Fraunhofer institutes in the Bavarian Competence Centre for Quantum Security and Data Science (BayQS), led by

"As a leading international computing centre, we are already working on setting up quantum computing hardware on site and making it available to researchers integrated in our HPC systems or through the cloud. In addition, our course programme offers training for todays and future quantum computing experts." said Prof. Dieter Kranzlmüller, Director of the LRZ.

the Fraunhofer AISEC in Garching. This project evaluates prototypes for quantum computing and the foundations for reliable use of the technology in business and society.

Along the way, the QIC is preparing to add additional resources and services to its portfolio and to advance its research efforts for future capability development. *sts and sv*

Read on: Dr. Luigi Iapichino and Dr. Stefan Huber from LRZ's Quantum Computing Group talk about concrete next steps for QIC in this interview: https://www.lrz.de/presse/ereignisse/2021-04-30-Quantum-Computing/

The recording of the one-hour live-streaming event, can be watched online: https://www.youtube.com/watch?v=-16tw-VKbtg

EVENTS

SAS WORKSHOP CONSIDER HISTORY OF IMITATION, ADAPTION, AND DECEPTION

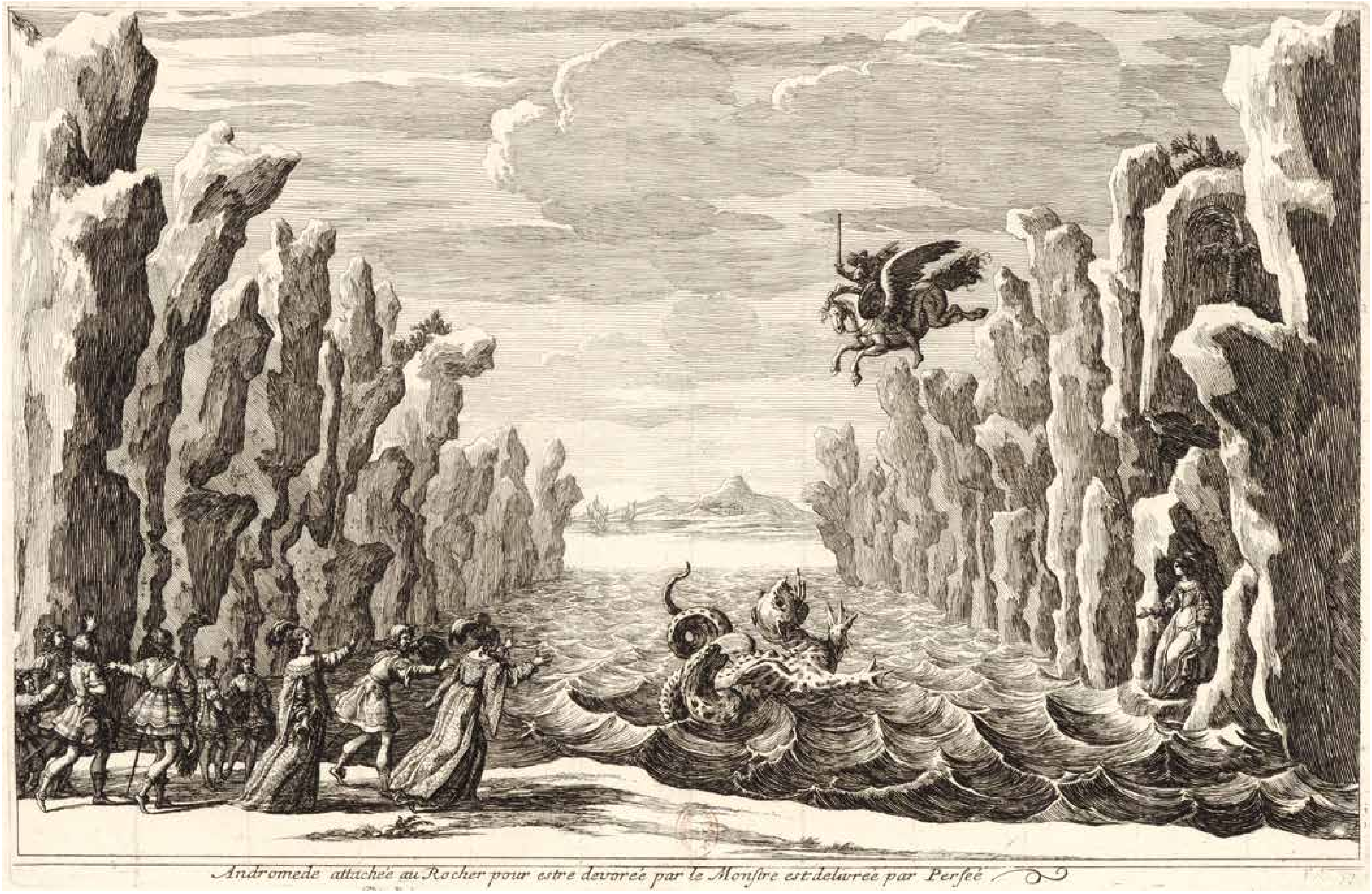
In this multidisciplinary meeting, scholars exchanged perspectives on how these related practices have emerged and changed over time.

Illusions, scams, counterfeits, self-delusion — deception can take many forms. And although the growing influence of artificial intelligence (AI) and disinformation campaigns in social media might suggest that our current digital era faces unique threats, the potential to deceive others or to be deceived is perhaps as old as human cognition.

On February 16-17, 2021, the sixth Science and Art of Simulation (SAS) workshop at the High-Performance Computing Center Stuttgart (HLRS) looked at the history of deception from many perspectives, with a particular focus on deception's relationship to imitation and adaptation. Held online due to the ongoing COVID-19 pandemic, the event gathered scholars from literary studies, computer sciences, philosophy, the digital humanities, sociology, art history, psychology, and pedagogy to look closely at uses of technology for deception and illusion both in the past and in the context of today's digital media and computational research.

The meeting, which included researchers from the University of Stuttgart, University of Tübingen, University of Cologne, and the VDE, was organized by Michael Resch (Director, HLRS), Kirsten Dickhaut (Professor of Romance Literatures, University of Stuttgart), and Andreas Kaminski (Leader, HLRS Department of Philosophy of Computational Science).

Throughout modern history, imitation, illusion, and deception using technology have been used both for entertainment and to manipulate others in more malicious ways. For this reason, lectures at the SAS workshop considered examples of such practices from the past, including in the design of church altars, Renaissance-era gardens, and theater sets. As Prof. Dickhaut explained, "Many of the contributions focused on the theater, which offers a useful model for considering an interest that participants shared related to cognition, specifically for understanding both how deception and illusion arise frontstage and what is actually possible on a technical level backstage."



Insights derived from these studies were brought into dialogue with presentations focusing on contemporary instances of illusion and deception such as deepfakes, AI language models, and scientific simulation. Talks also considered deception from a psychological perspective, including questions about how accurately we interpret not only the world around us but even our personal capabilities and motivations.

Despite this wide diversity of topics, the studies often sought to understand forms of deception in their anthropological contexts, particularly with respect to changing social and cultural assumptions of what it means to be human.

"Concepts and technologies used in deception are often associated with a specific perception of humans (Menschenbild) that provides a foundation for predicting how a person could be brought into a state of confusion," remarked Andreas Kaminski. "By studying historical examples of deception and questions related to trustworthiness we can not only learn how these conceptions have changed over time, but also gain a better understanding of contemporary forms of such phenomena. Perhaps what appears new to us today might in some ways actually turn out not to be new at all."

cw

Theatrical illusion: Set design for Act 3 of Pierre Corneille's "Andromède" as first performed on February, 1 1650 by the Troupe Royale at the Petit-Bourbon in Paris. © Wikimedia Commons

PROF. DR. PETER BASTIAN RE-ELECTED AS HEAD OF THE LRZ STEERING COMMITTEE

Prof. Dr. Peter Bastian of Heidelberg University continues as chairman of the steering committee at LRZ. At the last steering committee meeting, Bastian, who heads the "Parallel Computing" working group at the Interdisciplinary Center for Scientific Computing (IWR), was elected to the position for the third time. His deputy is Prof. Dr. Gerhard Wellein from the Friedrich-Alexander Universität of Erlangen-Nuremberg, who is also the spokesperson for the Competence Network Technical Scientific High Performance Computing in Bavaria (KONWIHR). The LRZ Steering Committee is elected every two years and consists of a total of 15 scientists representing the LRZ, the Bavarian Academy of Sciences and Humanities (BADW) and the German Research Foundation (DFG). The LRZ Steering Committee allocates computing time and evaluates the scientific merit of simulation projects that are applied for locally at LRZ. Last year, this amounted to about 70 applications.

MUNICH'S QUANTUM VALLEY

The Bavarian Academy of Sciences and Humanities (BAdW), the Fraunhofer Gesellschaft, the Max Planck Society, and both Munich universities pooled their expertise in a Memorandum of Understanding at the beginning of the year to jointly establish the Munich Quantum Valley (MQV). Science, research, and private industry big and small will find a stimulating environment and opportunities for cooperation and exchange in order to develop quantum technologies and quantum computing and bring them to market. As an institute of BAdW, the LRZ supports this technology cluster. As a Bavarian initiative, the Munich Quantum Valley is to be a pillar in a national and European quantum strategy and is to compete with international technology centers. To this end, the Free State of Bavaria will be investing 120 million euros over the next two years. In addition, the Munich Quantum Valley will receive funding from the federal government, which is providing some two billion euros for quantum technologies.

GUIDING SUSTAINABLE DIGITALIZATION IN BADEN-WÜRTTEMBERG

As coordinating center for a new project called ENRICH (Energie, Nachhaltigkeit, Ressourceneffizienz in IT und Rechenzentren), HLRS will lead a collaborative effort to investigate the future of digitalization across the state of Baden-Württemberg, and to identify opportunities to make the IT sector more sustainable. Following a study of long-term megatrends that will drive ongoing digitalization, the project will develop recommendations for sustainable procurement and supply chain management, as well as energy efficiency in computing centers and the IT sector. At the conclusion of the project, ENRICH will produce a "digital atlas" for Baden-Württemberg that provides a geographic overview of relevant facts, numerical data, and projections. The atlas will provide a guide to digitalization for stakeholders from industry, politics, government, and citizen groups, and could help to identify symbioses in which waste heat produced by the IT sector could be recycled for building heating. The project is funded by the Baden-Württemberg Ministry of the Environment, Climate Protection and the Energy Sector.

HLRS CREATING DIGITAL TWIN OF HISTORIC LUDWIGSBURG PALACE THEATER

The baroque theater inside the Ludwigsburg Residential Palace is home to the world's oldest functioning stage machinery. In an effort towards digital preservation, members of the HLRS Visualization Department have been creating a digital twin of the theater. After using a 3D scanner to generate a point cloud of the facility, the researchers converted the data into an immersive virtual reality installation in HLRS's CAVE VR facility. Wearing 3D glasses, visitors can experience the illusion of moving through the theater, including backstage, as it might have looked in the 18th century. The digital twin also incorporates interactive animation of the stage machinery that will make it possible for the public and scholars to observe its design and function without the need to risk damage to the historic technology. Together with the University of Stuttgart's Institute for Literary Studies, additional discussions are underway with colleagues in France interested in using digital tools to research the Royal Opera at the Palace of Versailles.

RISC2: EU AND LATIN AMERICA COORDINATING HPC RESEARCH

The EU RISC2 project started January 1, 2021 as a network to support the coordination of HPC research between Europe and Latin America as well as encourage greater cooperation between the research and industrial communities surrounding both HPC applications and infrastructure deployment. The project brings together eight key European HPC stakeholders (including Atos, BSC, CINECA, INRIA, and JSC) and the main HPC actors from Brazil, Mexico, Argentina, Colombia, Uruguay, Costa Rica, and Chile. It runs for two and half years.

RISC2 will promote the exchange of best practices through workshops and trainings organized to coincide with major HPC events in Europe and Latin America. The main project deliverable will be a cooperation roadmap that identifies specific areas for collaboration in the realms of applications, HPC infrastructure, and policy requirements. The training activities will provide a boost to Latin American HPC, while the structured interaction between researchers and policymakers in both regions will help define a coordinated policy and a clear roadmap for the future.

PROF. DR. DR. THOMAS LIPPERT NAMED GCS CHAIRMAN OF THE BOARD OF DIRECTORS

As of April 8, 2021, Prof. Dr. Dr. Thomas Lippert of JSC is the new Chairman of the GCS Board of Directors. Lippert succeeds Prof. Dr. Dieter Kranzlmüller, Director of LRZ. In addition to his GCS position and having led JSC and its predecessor organization for 17 years, Lippert also serves as the Chair of Modular Supercomputing and Quantum Computing at Goethe University Frankfurt. Lippert takes over right after JSC finished installing its JUWELS Booster module, a GPU-accelerated component of JSC's modular supercomputer, JUWELS. The JUWELS Cluster and Booster modules together are capable of 85 petaflops, or 85 quadrillion calculations per second, making it the fastest supercomputer in Europe and one of the most energy-efficient in the world.

PROJECT DAQC: DIGITAL-ANALOG QUANTUM COMPUTING

February marked the start of the Digital-Analog Quantum Computing (DAQC) project, which is funded by BMBF. The DAQC project aims to combine the technology of analog, controllable systems with that of digital-universal quantum computers, whose computing power increases with each qubit. Step-by-step quantum processors will result with initially 5, 20, and then 54 qubits, as well as the methods and electronics to control them. These innovative control units will initially work in conjunction with the high-performance computing systems at LRZ and prove their reliability there. For this purpose, LRZ is procuring a cryostat, or cooling device for the low temperatures on which quantum computing is based. The project, coordinated by IQM Germany GmbH and involving not only LRZ but also the Jülich Supercomputing Centre (JSC) with various institute departments as well as the Freie Universität Berlin and the companies Infineon AG and Parity Quantum Computing GmbH, will run until 2025.

DEVELOP QUANTUM COMPUTING RELIABLY AND SECURELY

Processing even more data much faster—the hopes of science and industry are currently pinned on quantum computing. This technology of the future is still at the development stage. However, to ensure that it can soon be used by companies, the Bavarian Competence Center for Quantum Security and Data Science (BayQS) was established at the end of April. Together with the Fraunhofer Institutes for Applied and Integrated Security (AISEC), for Cognitive Systems (IKS) and for Integrated Circuits (IIS), as well as the two Munich universities, the LRZ will develop concepts and solutions for reliable quantum technology as well as for initial software and for security and data protection. The joint research and testing work will focus in particular on optimizing the first quantum processing units. The greatest challenge at present is to reliably control and monitor these processors so that computing power can be built up on them using the extremely unstable qubits, the smallest computing units, and sustained over the long term. The industry also needs trustworthy software to process data, as well as concepts on how to secure existing computer and IT systems. Quantum computers are already suspected of being able to quickly crack current encryption and security techniques.

DONATION TO SUPPORT COVID-RELATED RESEARCH AND URGENT COMPUTING ARRIVES AT HLRS

Computing hardware manufacturer AMD has donated 10 server systems to the High-Performance Computing Center Stuttgart that will be dedicated for research related to the SARS-CoV-2 pandemic. The donation, containing AMD EPYC™ processors and AMD Instinct™ accelerators, was part of the AMD COVID-19 High Performance Computing Fund. The new nodes will be used to support a collaboration between HLRS and the German Federal Institute for Population Research (Bundesinstitut für Bevölkerungsforschung) to implement a model for predicting demand for intensive care units across Germany up to eight weeks into the future. The daily "weather report," which will soon run on the newly donated infrastructure, could help health experts and government officials better anticipate when and where interventions such as lockdowns could become necessary — or be lifted — in response to changing stresses on hospitals' resources. The new resources will also support HLRS's activities in the field of Global Systems Science and expand the center's capacity to address future urgent computing needs.

SUPERMUC RESULTS BOOK PUBLISHED

Packed with excellent science, the new results report volume from LRZ describes 115 research projects computed on the HPC systems SuperMUC and its successor SuperMUC-NG from 2018 to 2020. Even at first glance, the work makes it clear that not only are data volumes constantly swelling in research, but also that increasingly more research fields require the performance of supercomputers. For example, simulations by LRZ systems helped to understand the formation of the Earth and the universe, to develop new vehicles and aircraft, and to explore earthquakes, floods and other consequences of climate change. The projects around COVID-19 show that this research not only satisfies scientific curiosity, but also benefits mankind.

HLRS AND INSTITUTE OF ADVANCED STUDIES, BRAZIL, (IEA) SIGN COLLABORATION AGREEMENT

The agreement will build on the complementary strengths of the two institutes related to the digital transformation of society, its political implications, and emerging e-cultures. The organizations plan to develop joint research programs, hold joint international conferences, develop joint continuing education programs, and engage in the exchange of researchers to promote the sharing of knowledge and expertise. Among the specific areas of collaboration, HLRS and the IEA will focus on topics related to the study of emerging e-cultures that use computer simulation and machine learning, the trustworthiness of information and the problems of disinformation, the history of adaptation and deception in technology and art, and the use of visualization in art. Leading the partnership are Lucia Maciel Barbosa de Oliveira and José Teixeira Coelho Netto of the IEA Study Group on Computational Humanities at the University of São Paulo, along with HLRS Director Michael Resch and Andreas Kaminski, leader of the HLRS Department of Philosophy of Science & Technology of Computer Simulation.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AI STRATEGY FOR EARTH SYSTEM DATA PROJECT KI:STE

Environmental data consists of large, heterogeneous datasets that encode spatio-temporal processes not yet fully understood. These datasets pose unique challenges to Earth scientists who decode natural processes to solve global environmental challenges. Recent advancements in algorithmic developments as well as the capabilities of artificial intelligence led to the first real-world applications using environmental data. Under JSC leadership, the KI:STE project aims to facilitate the application of large-scale machine learning on HPC systems for environmental data by using a sophisticated strategy that combines the development of an Earth-AI-Platform with a strong training and network concept. The Earth-AI-Platform will create the technical prerequisites to make high-performance AI applications on environmental data portable for future users and to establish environmental AI as a key technology.

DICE - DATA INFRASTRUCTURE CAPACITIES FOR EOSC

In January 2021, the European Commission launched projects aimed at increasing service offerings on the European Open Science Cloud (EOSC) Portal. As part of this effort, JSC is participating in the "Data Infrastructure Capacities for EOSC" (DICE) project that brings together a network of computing and data centers, research infrastructures, and data repositories. The network offers a European storage and data management infrastructure for EOSC, providing generic services and building blocks to store, find, access, and process data in a consistent, persistent way. 18 providers from 11 European countries are offering 14 state-of-the-art data management services with more than 50 petabytes of storage capacity.

JSC leads the activities focused on integrating the DICE services and resources with other platforms and infrastructures and offers B2DROP, a secure and trusted cloud storage, B2SAFE, a service for data replication and long-term preservation, and B2ACCESS, a federated cross-infrastructure authorization and authentication framework. The DICE project is funded under the grant agreement ID 101017207 with a duration form January 2021 to June 2023 and a total budget of approximately 7 million Euro.

LIFE FROM OUTER SPACE - FASCINATING VIDEO ON TV CHANNEL ARTE

We are all made up of stardust. When a massive star explodes as a supernova at the end of its existence, it creates and disperses out into space all the heavy elements that make up the Earth and all creatures on it. A documentary from the European TV station arte presents the theory that black holes heated the masses of gas orbiting around them at close to the speed of light, and eventually the resulting turbulence and magnetic fields mixed these gases and shot them far out into space as gigantic jets. In addition to extensive international experimental collaborations, new theoretical models and numerical simulations also played a decisive role. In the arte documentary, the supercomputer SuperMUC-NG at LRZ also makes a brief appearance, together with Prof. Dr. Volker Springel (from minute 33:50), at the MPI for Astrophysics in Garching. As a long-time intensive user of the GCS supercomputers, Professor Springel has already computed on all LRZ supercomputers and has ever since further developed his simulations. The film shows how experiment, theory, and simulation interact in an exemplary way to deepen our understanding of the world and the origin of life.

Moderator Eva Wolfangel with author Daniel Kehlmann and HLRS Director Michael Resch onstage at the Literaturhaus Stuttgart. **© Sebastian Wenzel**

FIRST STUTTGART "ZUKUNFTSREDE" EXPLORES THE BORDERS BETWEEN HUMANS AND COMPUTERS

For years, people have warned of the potential for artificial intelligence (AI) to take over activities traditionally considered to be uniquely and quintessentially human. At a time when machine learning and AI are rapidly gaining new capabilities and becoming increasingly present in our daily lives, how close have we come to this future? In the first Stuttgart "Zukunftsrede," bestselling novelist Daniel Kehlmann (Tyll, Measuring the World) read an essay in which he explored AI's ability to replicate one of humankind's greatest achievements: the ability to create and tell stories. Following the reading, HLRS Director Michael Resch joined Kehlmann for a nearly hour-long conversation moderated by journalist Eva Wolfangel that focused on how humans perceive and interact with AI, and on the differences between human and machine-based creativity. The event was broadcast online from the Literaturhaus Stuttgart on February 9, 2021.

COMPUTING POWER FOR ARTIFICIAL INTELLIGENCE

Artificial intelligence (AI) needs computing power. That is why LRZ and the Munich Centre for Machine Learning (MCML) are now bringing together knowledge and technology and jointly making availabile more computing power for basic research on AI. For this purpose, the cluster called MUNICH.ai (shortened for: MCML's UNIversal Cluster for High-performance AI) is based on 8 DGX-A100 nodes from NVIDIA with a total of 64 graphics processing units (GPUs). It has just been put into operation at LRZ. The system brings it to 40 AI petaflops. "The additional hardware installed represents state-of-the-art technology and guarantees a standard that only Germany's leading AI centers can offer," explains Professor Thomas Seidl, Chair of Database Systems and Data Mining at Ludwig-Maximilians-Universität (LMU), Director of MCML and LRZ.

STAFF SPOTLIGHT: REFLECTING ON 35 YEARS OF HPC, RECENTLY RETIRED APPLICATION SUPPORT GROUP LEADER REFLECTS ON HPC DEVELOPMENTS PAST AND PRESENT

Dr. Matthias Brehm, LRZ

In the late 80s, Dr. Matthias Brehm was a newly minted PhD graduate who had done research into vector computing during his education. He had spent some time collaborating with staff at the Leibniz Supercomputing Centre (LRZ) and wound up getting a position in the organization after finishing his degree, aiming to work with the emerging HPC technology.

That decision proved quite consequential—Brehm would spend the next 35 years working for the organization, using his skill set to help users make the best-possible use of cutting edge computing technologies for their respective applications and, in turn, growing with his colleagues to adapt to multiple generations of disruptive computing technologies. Brehm retired from LRZ at the end of 2020, but remains passionate about the world of computing and proud of his time at LRZ.

"I have seen a major increase in performance—something on the order of more than a million-fold since I started working," Brehm said. "But now I see that with accelerators and perhaps also quantum computing, it is again a disruption in the field, so the community must invest in some new things, rethink algorithms, and think about how to make good use of vectorization and parallelism in the machines."

During his time at LRZ, Brehm became increasingly involved in application support, becoming head of the APP group in 2000. In doing this essential work, Brehm sat on the front lines of making use of new and challenging technologies. While he came out of his studies with extensive knowledge of vector processors—processors that, unlike today's microprocessors, had a considerable compute balance—Brehm watched the usage of vector processors wane only a couple of years into his career. Despite that fact, Brehm still cites the Cray Y-MP supercomputer as his favorite among the many devices he worked with during his time at LRZ.

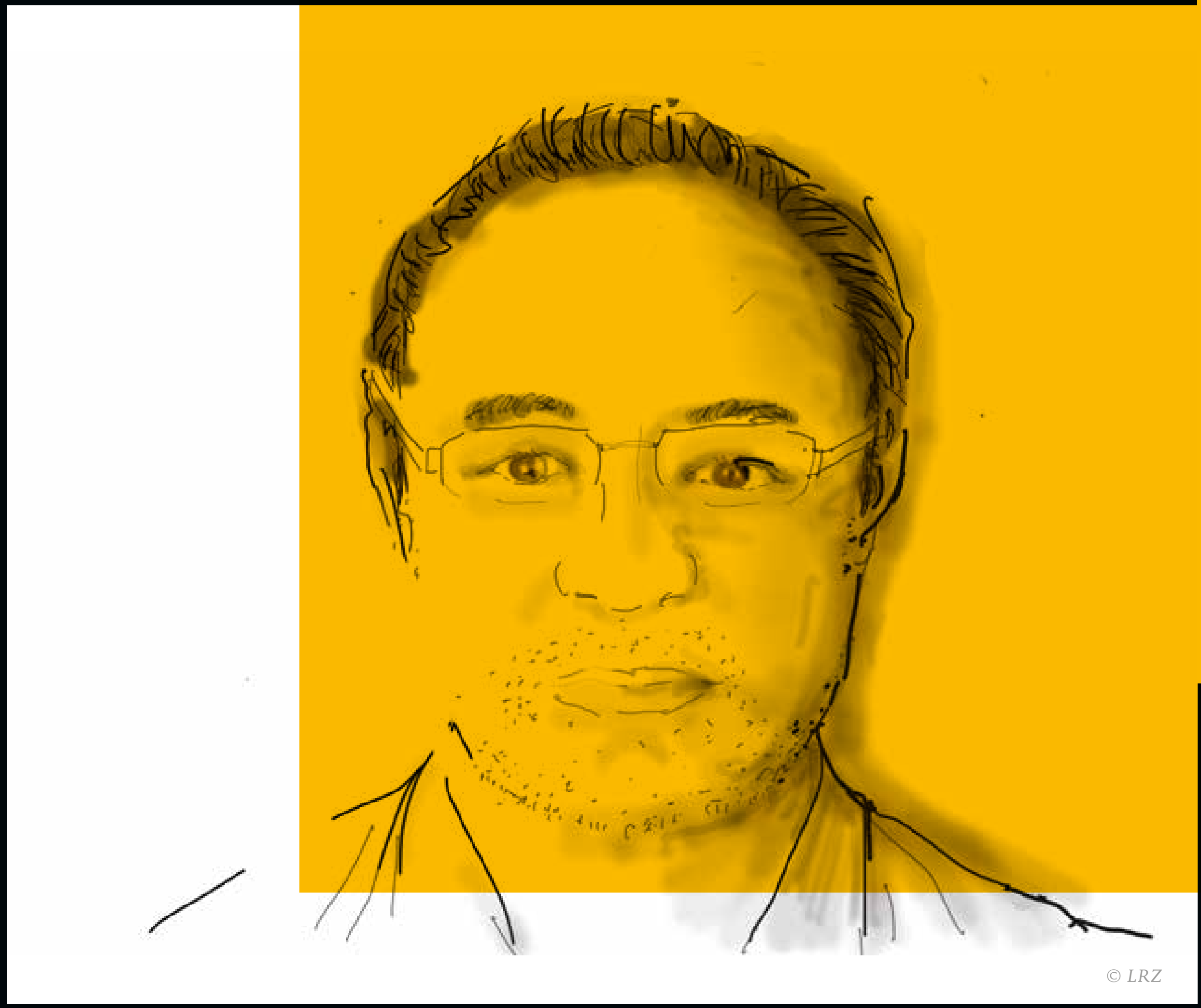
"The Y-MP machine had a huge memory bandwidth, relative to its performance, and it was easy to program," Brehm said. "Perhaps more importantly, it was quite clear what we had to do when it came to programming: namely, concentrate on vectorization. Today, you have so many things that you have to take into account and analyze. It makes it even harder for both users and centres' staffs to look closely for ways to improve performance."

Brehm pointed out that as vector processors waned, the microprocessors waxed so rapidly that many scientists began to get major performance increases in their simulations even though many were becoming increasingly less aware of what was going on "under the hood" of the machines they were using to run those simulations. Additionally, public domain and vendor libraries and applications helped to overcome some of the performance obstacles.

"Many researchers say, 'I care about my scientific work, but I don't really care about the performance,'" Brehm said. "Because each generation of microprocessor offered such a significant performance increase, there weren't many researchers who were so interested in these kinds of analyses that help identify where to improve code performance. With vector processors, it was easy and clear to understand, but this has faded over time with microprocessors—you have hierarchies, larger latency issues with the data in different caches, then you have parallelization and parallel I/O. Taken together, it became a huge and complex programming environment to understand, and if something isn't clear, users are reluctant to spend time and efforts on an uncertain outcome. But if researchers successfully do so, they can get an advantage of several years over the scientific competitors."

Thankfully, Brehm feels confident that GCS's emphasis on support, education and training over the last decade continues to play the single largest role in addressing researchers' issues with making good use of GCS HPC resources. For Brehm, the key component of GCS's successful training program has been the diversity of expertise and hardware available at the three centres. "In GCS, we have a broad range of lectures and training programs," he said. "This is leading in Europe, and a big part of that has to do with one major point—we do not concentrate only on the top, but also the broad mass of users. In addition, though, you always have to give incentives to users, and this is where GCS does a good job of bringing together users from different domains or institutions."

The slowdown of conventional microprocessor technology, due to energy and thermal restrictions, corresponded with an increased interest and focus on emerging technologies again. Brehm pointed out that while the technologies in question have changed, the same basic truth about HPC centres remains true—each new generation of technology will challenge existing users to adapt, invite new users into the



© LRZ

dialogues happening between HPC centres' staff and the research communities they support, and call on HPC centres to ensure they are developing young talent to become experts in these disruptive of promising paradigm shifts.

Whether it is the increasing usage of artificial intelligence in HPC workflows, the promise of quantum computing technologies, or the increased focus on data analytics, the HPC centres of tomorrow cannot only provide a large computer for users; they must become agile, diversified partners for scientists and engineers to accelerate their research.

But those are the traits that Brehm looks back on fondly over 35 years of service at LRZ and thirteen of those years being a part of GCS. When he reflects on his years of taking hour-long bike commutes back and forth to LRZ, meeting colleagues to chat during coffee breaks, or watching users achieve breakthroughs in their research, Brehm feels confident that GCS has the tools in place to continue progressing for the next 35 years. "I just hope we continue to keep progressing, and that the centres keep working so well together" he said. "Today, we have far more people involved in user support and training, and that is good and important. Also, the three GCS centres and the European partners in PRACE are eager about sharing work and experience with one another. It is an exciting period, and that isn't even mentioning that we are also, of course, on the road to exascale."

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TRAINING CALENDAR
HPC COURSES AND TUTORIALS

Editor's Note
Due to the COVID-19 pandemic, the GCS centres provided many of their courses in the last year as online courses. Starting in autumn 2021, some of the courses may go back to the classrooms. These decisions are not yet finalized, so we have decided not to publish the training calendar as usual, as dates, locations, and plans may continue to change. For the most up-to-date information about GCS training courses, please visit:
https://www.gauss-centre.eu/trainingsworkshops

For a complete and updated list of all GCS courses, please visit:
https://www.gauss-centre.eu/training

The German HPC calendar (organized by the Gauss Allianz in cooperation with all German HPC centres) provides an extensive list of training all taking place German HPC centres. More information can be found at:
https://hpc-calendar.gauss-allianz.de/

Further training courses and events can be found on GCS member sites:
https://www.hlrs.de/training/
https://www.lrz.de/services/compute/courses/
https://www.fz-juelich.de/ias/jsc/events

The Rühle Saal at HLRS in Stuttgart © HLRS

JÜLICH SUPERCOMPUTING CENTRE
FORSCHUNGSZENTRUM JÜLICH

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The Jülich Supercomputing Centre (JSC) at Forschungszentrum Jülich is committed to enabling scientists and engineers to explore some of the most complex grand challenges facing science and society. Our research is performed through collaborative infrastructures, exploiting extreme-scale supercomputing, and federated data services.

Provision of supercomputer resources: JSC provides access to supercomputing resources of the highest performance for research projects coming from academia, research organizations, and industry. Users gain access for projects across the science and engineering spectrum in the fields of modeling and computer science.

Core tasks of JSC are:
- Supercomputer-oriented research and development in selected fields of physics and other natural sciences by research groups and in technology, e.g. by doing co-design together with leading HPC companies.
- Implementation of strategic support infrastructures including community-oriented simulation and data laboratories and cross-sectional teams, e.g. on mathematical methods and algorithms and parallel performance tools, enabling the effective usage of the supercomputer resources.
- Higher education for master and doctoral students in close coperation with neighbouring universities.

The Cluster module of JSC's Modular Supercomputer "JUWELS". **© Forschungszentrum Jülich**

Compute servers currently operated by JSC

System	Size	Peak Performance (TFlop/s)	Purpose	User Community
Modular Supercomputer "JUWELS"	Cluster (Atos): 10 cells, 2,567 nodes 122,768 cores Intel Skylake 224 NVIDIA V100 GPUs 275 TByte memory	12,266	Capability Computing	European (through PRACE) and German Universities and Research Institutes
	Booster (Atos): 39 racks, 936 nodes 44,928 cores AMD EPYC Rome 3,744 NVIDIA A100 GPUs 629 TByte memory	75,020		
Modular Supercomputer "JURECA"	Data-Centric Cluster (Atos): 768 nodes, 98,304 cores AMD EPYC Rome 768 NVIDIA A100 GPUs 443 TByte memory	18,515	Capacity and Capability Computing	European (only on the Data-Centric Cluster) and German Universities, Research Institutes and Industry
	Booster (Intel/Dell): 1,640 nodes 111,520 cores Intel Xeon Phi (KNL) 157 TByte memory	4,996		
Fujitsu Cluster "QPACE 3"	672 nodes, 43,008 cores Intel Xeon Phi (KNL) 48 TByte memory	1,789	Capability Computing	SFB TR55, Lattice QCD Applications
Atos Cluster "JUSUF"	205 nodes, 26,240 cores AMD EPYC Rome 61 NVIDIA V100 GPUs 52 TByte memory	1,372	Capacity Computing	European and German Universities and Rewsearch Institutes through PRACE and Human Brain Project
Modular Supercomputer "DEEP-EST" (Prototype)	Cluster: 50 nodes, 1,200 cores Intel Xeon Gold 6146 9.6 TByte memory + 25.6 TByte NVM	45	Capacity Computing (low-/medium-scalable code parts)	Partners of the "DEEP" and "SEA" EU-project series and interested users through Early Access Programme
	Booster: 75 nodes, 600 cores Intel Xeon Silver 4215 75 NVIDIA V100 GPUs 6 TByte memory	549	Capacity and Capability Computing (high-scalable code parts)	
	Data Analytics Module: 16 nodes, 768 cores Intel Xeon Platinum 8260 16 NVIDIA V100 GPUs 16 Intel Stratix10 FPGAs 7.1 TByte memory + 32 TByte NVM	170	Capacity and Capability Computing (data analytics codes)	

A detailed description can be found on JSC's web pages: https://www.fz-juelich.de/ias/jsc/systems

LEIBNIZ SUPERCOMPUTING CENTRE

Leibniz Supercomputing Centre
of the Bavarian Academy of Sciences and Humanities

For nearly six decades, the Leibniz Supercomputing Centre (Leibniz-Rechenzentrum, LRZ) has been at the forefront of its field as a world-class high performance computing centre dedicated to providing an optimal IT infrastructure to its clients throughout the scientific community–from students to postdocs to renowned scientists—and in a broad spectrum of disciplines–from astrophysics and engineering to life sciences and digital humanities.

Leadership in HPC and HPDA

Located on the research campus in Garching near Munich, the LRZ is a leadership-class HPC and HPDA facility delivering top-tier supercomputing resources and services on the national and European level. Top-notch specialists for HPC code portability and scalability support the LRZ' broad user base and ensure to run operations in the most energy-efficient way.

Future Computing at LRZ

The LRZ is leading the way forward in the field of Future Computing focusing on emerging technologies like quantum computing and integrating AI on large-scale HPC systems. A robust education program for HPC, machine learning, artificial intelligence and big data is complementing the LRZ offer.

IT backbone for Bavarian science

In addition to its role as national supercomputing centre, the LRZ is the IT service provider for all Munich universities as well as research organizations throughout Bavaria.

SuperMUC NG at the Leibniz Supercomputing Centre. © LRZ

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Compute servers currently operated by LRZ

System	Size	Peak Performance (TFlop/s)	Purpose	User Community
"SuperMUC-NG" Intel/Lenovo ThinkSystem	6,336 nodes, 304,128 cores, Skylake 608 TByte, Omni-Path 100G	26,300	Capability Computing	German universities and research institutes, PRACE (Tier-0 System)
	144 nodes, 8,192 cores Skylake 111 TByte, Omni-Path 100G	600	Capability Computing	
"CooLMUC-2" Lenovo Nextscale	384 nodes, 10,752 cores Haswell EP 24.6 TByte, FDR 14 IB	447	Capability computing	Bavarian Universities (Tier-2)
"CoolMUC-3" Megware Slide SX	148 nodes, 9,472 cores, Knights Landing, 17.2 TByte, Omnipath	459	Capability Computing	Bavarian Universities (Tier-2)
IvyMUC	Intel Xeon E5-2650 ("Ivy Bridge")	13	Capability Computing	Bavarian Universities (Tier-2)
Teramem	1 node, 96 cores, Intel Xeon E7-8890 v4 ("Broadwell"), 6 TByte RAM	13	Big Data	Bavarian Universities (Tier-2)
DGX-1, DGX-1v Machine Lerning Systems	2 nodes, Nvidia Tesla, 8 x P100, 8 x V100	1,130 (Mixed Precision)	Machine Learning	Bavarian Universities (Tier-2)
Compute Cloud for SuperMUC-NG	64 nodes, 3,072 cores, Intel Xeon ("Skylake"), 64 Nvidia V100	128, 8,000 (Mixed Precision)	Cloud	German Universities and Research Institutes, PRACE

A detailed description can be found on LRZ's web pages: https://doku.lrz.de/display/PUBLIC/Access+and+Overview+of+HPC+Systems

CENTRE DESCRIPTIONS

HIGH-PERFORMANCE COMPUTING CENTER STUTTGART

HLRS
High Performance Computing Center | Stuttgart

The High-Performance Computing Center Stuttgart (HLRS) was established in 1996 as the first German national high-performance computing center. A research institution affiliated with both GCS and the University of Stuttgart, HLRS provides infrastructure and services for HPC, data analytics, visualization, and artificial intelligence to academic users and industry across many scientific disciplines, with an emphasis on computational engineering and applied science.

Supercomputing for industry

Through a public-private joint venture called hww (Höchstleistungsrechner für Wissenschaft und Wirtschaft), HLRS ensures that industry always has access to state-of-the-art HPC technologies. HLRS also helped to found SICOS BW GmbH, which assists small and medium-sized enterprises in accessing HPC technologies and resources. Additionally, HLRS cofounded the Supercomputing-Akademie, a training program that addresses the unique needs of industrial HPC users.

Guiding the future of supercomputing

HLRS scientists participate in dozens of funded research projects, working closely with academic and industrial partners to address key problems facing the future of computing. Projects develop new technologies and address global challenges where supercomputing can provide practical solutions. With the support of the EuroHPC Joint Undertaking, HLRS is also currently coordinating efforts to build and integrate HPC competencies across Europe. The center is certified for environmental responsibility under the Blue Angel and EMAS labels.

Hawk at the High-Performance Computing Center Stuttgart. © Ben Derzian for HLRS

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Compute servers currently operated by HLRS

System	Size	Peak Performance (TFlop/s)	Purpose	User Community
HPE Apollo 9000 “Hawk”	5,632 nodes 720,896 cores 1.44 PB memory	26,000 TF	Capability Computing	German and European (PRACE) research organizations and industry
Hawk GPU Extension	24 nodes 192 NVIDIA A100 GPUs	120,000 TF AI performance	Machine Learning, Artificial Intelligence applications	German and European (PRACE) research organizations and industry
NEC Cluster (Vulcan, Vulcan 2)	662 nodes 18736 cores 119 TB memory	1,012 TF	Capacity Computing	German universities, research institutions, and industry
NEC SX-Aurora TSUBASA	64 nodes 512 cores 3072 GB memory	137.6 TF	Vector Computing	German universities, research institutions, and industry
Cray CS-Storm	8 nodes 64 GPUs 2,048 GB memory	499.2 TF	Machine Learning Deep Learning	German universities, research institutions, and industry
AMD COVID-19 System	10 nodes 80 AMD MI50 GPUs	530 TF	COVID-19 Research	German and European researchers focused on COVID-19 research

A detailed description can be found on HLRS' web pages: https://www.hlrs.de/systems

InSiDE magazine (German: Innovatives Supercomputing in Deutschland) is the bi-annual publication of the Gauss Centre for Supercomputing, showcasing recent highlights and scientific accomplishments from users at Germany's three national supercomputing centres. GCS was founded in 2007 as a partnership between the High-Performance Computing Center Stuttgart, Jülich Supercomputing Centre, and the Leibniz Supercomputing Centre. It is jointly funded by the German Ministry of Education and Science (Bundesministerium für Bildung und Forschung – BMBF) and the corresponding ministries of the three states of Baden-Württemberg, North Rhine-Westphalia, and Bavaria.

Cover image: Turbulence shaping the interstellar medium. The image shows a slice through the turbulent gas in the world's highest-resolution simulation of turbulence published in Nature Astronomy. For more information, visit page 13.

www.gauss-centre.eu

GCS
Gauss Centre for Supercomputing

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MINISTRY OF SCIENCE, RESEARCH AND ARTS

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