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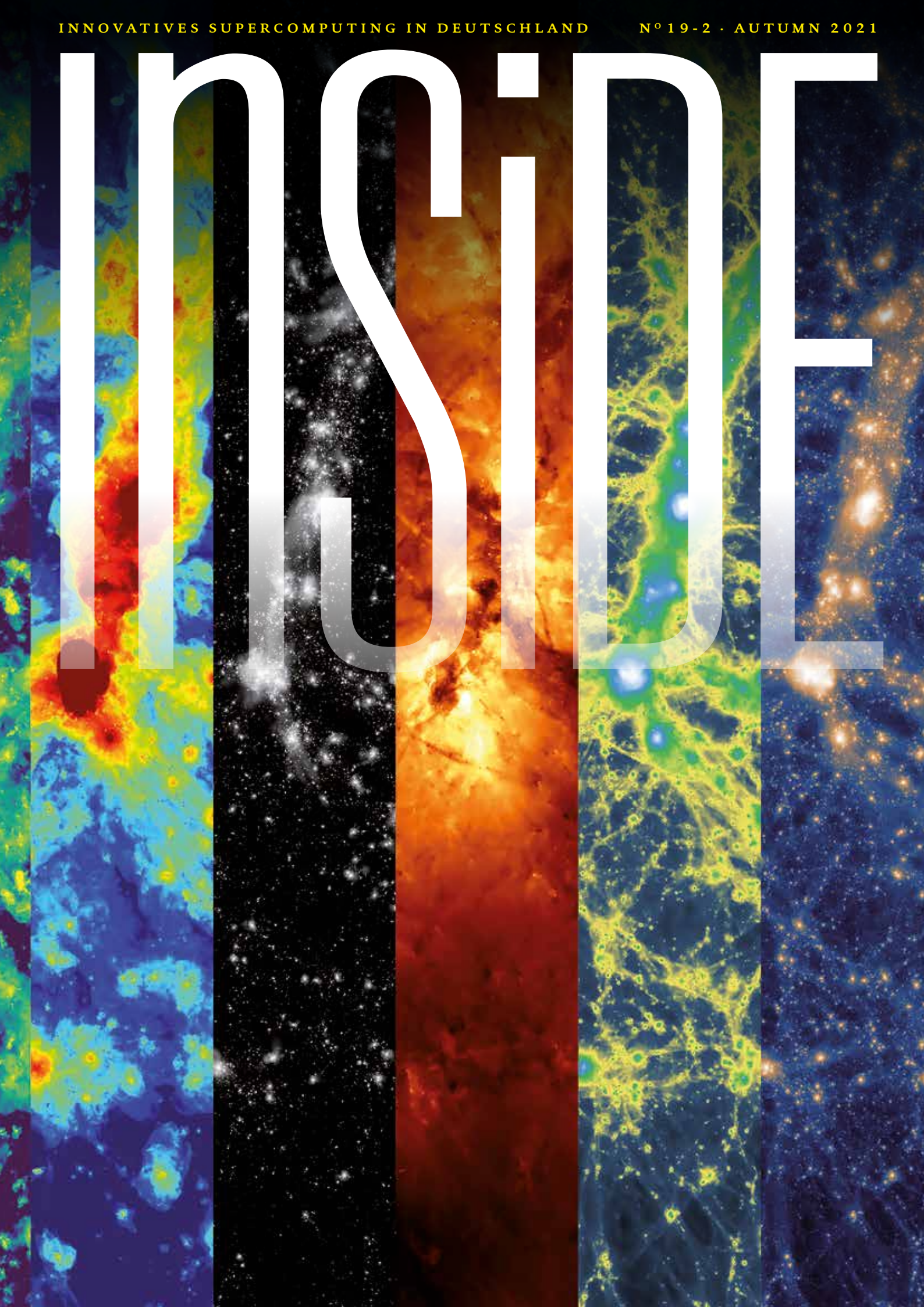

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GCS
Gauss Centre for Supercomputing

Welcome to the latest issue of InSiDE, the bi-annual Gauss Centre for Supercomputing magazine showcasing innovative supercomputing developments in Germany. In this issue, we at GCS are highlighting both where we have been and where we, as Germany's most powerful supercomputing infrastructure, plan to go.

In our news features, you will find a summary of the High-Performance Computing Center Stuttgart's (HLRS's) 25th anniversary celebration (Page 9). With precursor organizations dating even farther back, HLRS was named Germany's first national high-performance computing (HPC) centre in 1996. The event provided a chance for researchers and administrators alike to highlight science breakthroughs over the last quarter century and talk about where the organization is headed.

At the same time, all three GCS centres are playing active roles in Germany's National Research Data Infrastructure (NFDI) initiatives (Page 4), laying the groundwork for more seamlessly and efficiently sharing data across research groups and organizations. As Germany, and indeed the international scientific community, continues to embrace data-intensive artificial intelligence applications, we view these investments of resources and energy as essential infrastructure for science moving forward.

Another key component of forward-looking science is closer collaborations between scientific partners. The Jülich Supercomputing Centre (JSC) just finished up the PPI4HPC project (Page 22), which resulted in the European Union's first successful joint procurement of next-generation HPC resources for the continent. The Leibniz Supercomputing Centre (LRZ) has been supporting researchers from the Technical University of Munich in their quest to provide medical professionals better diagnostic tools for making decisions when using artificial respiration on patients with acute lung diseases or damage (Page 14). As the world still grapples with the COVID-19 pandemic, it is clearer than ever that our centres' resources need to be available for non-traditional use cases, and our staffs and researchers must be equipped to provide essential support to get the most out of these invaluable resources.

Our centres are no strangers to both being at the cutting edge of science and understanding that science and technology evolve rapidly. In 1996, HLRS's flagship Cray T3E system was capable of 461 gigaflops, and JSC's JUWELS Booster today is capable of 70 petaflops. Rather than resting on our laurels, we will continue to do what we've always done—look forward to the next scientific horizon and provide our users the best technology and support possible along the way.

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

GCS CENTRES PLAY MAJOR ROLE IN GERMAN NATIONAL DATA INFRASTRUCTURE INITIATIVES

Several new German Research Foundation consortia aim to standardize and streamline data storage and access for specific scientific disciplines. As Germany's leading HPC institutions, the three GCS centres will play important roles in the development of a findable, accessible, interoperable, and reusable data infrastructure for the German research community.

In recent decades, advancements in high-performance computing (HPC) technology have enabled researchers to take on increasingly difficult scientific challenges. Early in this development, computational power outpaced data storage in such a way that it was often cheaper to recalculate data than find ways to transfer it across long physical distances.

But as scientists' and engineers' research goals have grown, so too has the volume of data being produced in simulations. These goals have also grown increasingly complex and interdisciplinary, necessitating closer collaboration between theorists and experimentalists as well as the sharing of simulation and experimental data in rapid, iterative ways.

Additionally, the increasing use of machine learning applications has made large datasets all the more valuable, as they can be reused for training algorithms or other applications. Ultimately, simply recalculating datasets is no longer a viable way to move research forward, and scientists and engineers using HPC centres have to find ways to efficiently manage this relatively recent data deluge.

While HPC centres regularly expand the amount of data storage available and continue to innovate in the realm of data management and storage technologies, there are still major challenges in making sure that the ever-increasing data deluge is organized, secure, and is accessible to scientists whose research can benefit from it, whether that is 2 days or 2 years later.

As more research groups gain access to HPC resources, the need for standardizing how that data is organized with metadata is also becoming an increasing challenge. Despite many research communities ostensibly producing publicly available data, other researchers who want to verify or attempt to reproduce simulation results often find that between lack of standardized nomenclatures and frameworks and data being hosted in multiple locations, gaining access to datasets can be a nebulous, challenging process.

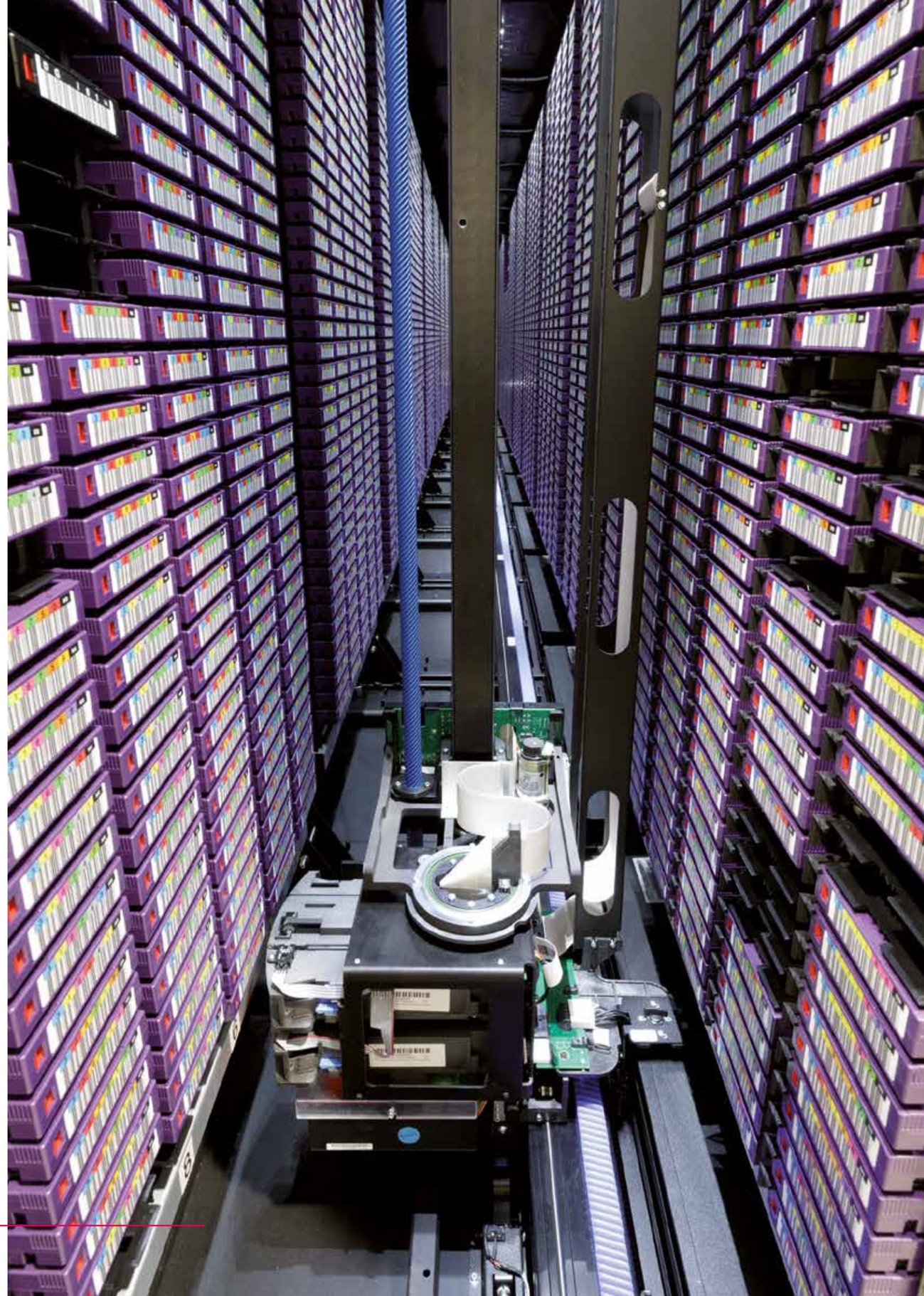
Recognizing the growing need for a standardized, uniform path forward, German federal and state-level government officials in 2018 came together to fund the National Research Data Infrastructure (German: nationale Forschungsdateninfrastruktur, NFDI). While the various consortia supported through NFDI funding all focus on specific research communities' needs, they all share a common goal—ensuring that the data infrastructure for German researchers adheres to the FAIR principles of data management—that is, that data is findable, accessible, interoperable, and reusable.

The program formally began in 2019, and spawned subprojects dedicated to developing research community-specific standards. As Germany's leading HPC organization, the Gauss Centre for Supercomputing (GCS) was a natural partner in several growing NFDIs. The three GCS centres—the High-Performance Computing Center Stuttgart (HLRS), the Jülich Supercomputing Centre (JSC), and the Leibniz Supercomputing Centre (LRZ)—are playing pivotal roles in multiple NFDI projects.

JSC focuses on users' strengths with PUNCH4NFDI, FAIRmat, and Text+

For decades, researchers have used state-of-the-art computing power at JSC to make new discoveries across multiple physics-related research fields. From studying the formation of galaxies to uncovering the behaviours of and interactions between the foundational building blocks of matter, physics researchers have always had a reliable partner in JSC staff.

Over time, distinct areas of physics research have started to overlap, creating more need for interdisciplinary teams to work together to solve increasingly complex problems. Furthermore, despite differences in scientific focus, astrophysicists and particle physicists are both dealing with a similar problem—they are in fields already dealing with rapidly increasing amounts of data. To address these needs, researchers from 20 German research institutes joined together to successfully launch the PUNCH4NFDI consortium.



As computational science has become more data-intensive, HPC centres have expanded their long-term tape storage capacities. JSC's TS4500 tape library plays a major role in managing JSC users' datasets. **© Forschungszentrum Jülich/Ralf-Uwe Limbach**

NEWS FEATURES

Lofar: JSC already plays a major role in managing data for the LOFAR low-frequency array.
© Forschungszentrum Jülich / Manfred Eckers

"These are the communities that have to really struggle to get the most out of enormously growing amounts of data," said Prof. Dr. Susanne Pfalzner, an astrophysicist at JSC who also serves as the centre's coordinator for the PUNCH4NFDI. "On the particle physics side, you have large experimental facilities like CERN in Switzerland that put out a ton of data, and on the astrophysics side, you have large-scale, international telescopes such as the low-frequency array LOFAR, whose data archive JSC is also involved in hosting. These demands are only getting bigger, and this is a big aspect binding these communities and inspired this joint NFDI project."

Pfalzner indicated that JSC staff is actively participating in multiple task areas associated with PUNCH4NFDI, and despite the project primarily focusing on astrophysics and particle physics data, partners are investing in developing solutions that will be transferable to other fields. This includes fields with additional data security concerns beyond what astrophysicists and particle physicists typically encounter.

"Today, the name of the game is the reproducibility of the results," Pfalzner said. "Research groups often put their codes up on GitHub or the like, but without the input data and results, it does not help in the realm of reproducibility. If we want to trust simulations, the data has to be there. We didn't think carefully enough about how to address data challenges during this transition in science—it used to be that you do an experiment, measure a curve, or the like, but today, we have simulations and other data science products at the end."

JSC is not just involved in PUNCH4NFDI, though. The centre is also a project partner in the FAIRmat and Text+ NFDI projects. FAIRmat is focused on supporting data needs of researchers working in condensed matter physics and chemical physics of solids. As the name indicates, the project is focused on making sure research data is managed according to the FAIR principles of data science (a common thread throughout the NFDI initiatives)—data must be findable, accessible, interoperable, and reusable. Text+ is also focused on implementing FAIR principles, but more specifically for text and language archives. The project is focused on large digital collections and lexical resources, and other digital archives. Although a wealth of data has been digitalized and preserved in literature archives, these collections are scattered around the globe, and are organized and indexed using different systems and nomenclature. With Text+, as with the other NFDI initiatives, the goal is to design an automated process that will also create more uniform standards for organizing and accessing data.

LRZ applies its IT-service experience to seven NFDIs

In addition to being one of Germany's leading HPC centres, LRZ has also long served as the IT provider for Munich and Bavaria universities. As a result, the centre has a broad mix of expertise in not only data science, but also networking and infrastructure. This fact was not lost on organizations applying for new NFDI projects and has resulted in LRZ becoming a valuable partner in 7 consortia funded through the initiative.

"The LRZ has gained a lot of experience in dealing with big data in a wide variety of areas over the past few years," said LRZ researcher Stephan Hachinger. "We have built up our very large high-performance storage facilities, and together with researchers we offer and optimise AI-based and classical methods for top-notch data analysis. To continue to progress in this area, we absolutely needed an initiative like NFDI—we store enormous volumes of world-class scientific results every year, and we also have to enable scientific communities to make most of the data by making them Findable, Accessible, Interopreable and Reusable, the original FAIR idea. Within the NFDI consortia and together with JSC and HLRS, we are developing a research data management strategy, and in particular a research data management service on top of LRZ storage. This service is planned to offer metadata storage, data search, persistent identifiers and data publication to search engines."

LRZ is part of the PUNCH4NFDI, FAIRmat, and Text+ consortia alongside JSC. It is also involved in several other consortia:

- BERD@NFDI applies NDFI principles to the emergent fields of artificial intelligence and machine learning, fields where the FAIR principles have even greater value, as the training of machine learning applications benefits from larger, more detailed datasets.
- NFDI4Earth focuses on Earth system sciences, fields in which LRZ has a vibrant user base.
- The German Human Genome-Phenome Archive (GHGA), led by the German Cancer Research Institute, focuses on organizing medical and genetic data while strictly adhering to privacy laws surrounding patients' medical records.
- NFDI4Ing applies the NFDI initiative's principles to a wide ranging of engineering research, centrally involving also GCS computing resources.

In this collaborative context and within GCS, LRZ contributes and evolves its data management concepts for users to make their big datasets at LRZ "FAIR" and publish them appropriately. Within NFDI initiatives, LRZ develops solutions complementary to high-performance storage and high-speed data transfer. "Researchers at institution A should be able to easily find, access, and reference the data sets of institution B and, if possible, already be able to evaluate them via cloud services using initial analysis procedures," LRZ researcher Hachinger said.

In its commitment to more centralized data access adhering to FAIR principles, LRZ is participating in the terrabyte project with the German Aerospace agency to make roughly 50 petabytes of Earth observation readily available with a rapid 10 gigabit-per-second transfer speed (for more information about terrabyte, please visit page 12).

Additionally, LRZ staff members are involved in the LEXIS project, a pan-European effort to further integrate big data

and high-performance computing. One of the main project objectives centres around developing a heterogeneous distributed data storage platform integrated with EUDAT services (which, in turn, JSC has been traditionally involved).

HLRS lends its data expertise to the world of catalysis research

In 2020, HLRS became a member of the NFDI4CAT consortium, led by the non-profit chemical society DECHEMA. (Editor's note: A more detailed description of the NFDI4CAT project can be found on page 21 of the autumn 2020 issue of InSiDE).

This NFDI project includes 16 partners who are pursuing strategies for better organizing and sharing catalysis research data. Catalysis, the process of making chemical reactions go faster or slower by introducing materials called catalysts, is a fundamental process in chemistry, and has broad implications for industrial firms working in fields ranging from biochemistry and pharmaceutical development to combustion. HLRS was tasked with creating and hosting a data repository for catalysis-related research, including a portal for sharing and accessing data stored at multiple locations. In addition, HLRS is playing a significant role in establishing standardized metadata and ontologies for catalysis research to ensure compatibility among different data sets, increasing their usability and amplifying their potential impact for scientific progress.

"We are very pleased that HLRS is participating in the development of a National Research Data Infrastructure," said HLRS Director Prof. Dr.-Ing. Michael Resch. "Working together with partners in the catalysis research community, this project should offer outstanding opportunities to accelerate research in a field that is not only of great economic importance, but that also holds keys to addressing some of our greatest global challenges."

Data-driven science: the natural progression for research at the intersection of theory and experiment

The NFDI initiative was born out of the need to better organize and share data across Germany's robust, interdisciplinary research landscape, but it also serves as a key component for shaping the future of German science and engineering. Through modelling and simulation, HPC has helped experimentalists gain insights into previous intractable scientific challenges. Experimentalists are still among the first to find gaps in computer simulations, and the iterative feedback loop of hypothesising, testing, and verifying only gets more important the more complex a scientific challenge becomes. Accordingly, developing standardised data access and organisation frameworks are essential to ensure that these iterative processes happens as efficiently as possible.

Additionally, next-generation computing technologies are poised to further complicate this picture, as much of the promise of machine learning and other artificial intelligence applications rests in the quality and volume of training data. While the GCS centres have served as Germany's official federal HPC centres for more than a decade, they have also played a pioneering role when it comes to emergent technologies like these. All three GCS centres have experience in embracing disruptive technologies, and the centres have built out expansive, fast data storage capabilities that will continue to play an essential role in hosting NFDI-related data.

"GCS has never just focused on high-performance computing; we want to support the whole ecosystem that exists around HPC to enable world-class research breakthroughs," said Dr. Claus-Axel Müller, Managing Director of GCS. "The NFDI program is a perfect example of how HPC serves not only a variety of scientific disciplines, but also acts as a linchpin technology in bringing disparate research groups together to solve the world's great research challenges."

More information about the NFDI initiative can be found here: https://www.nfdi.de/ *eg*

HLRS CELEBRATES 25 YEARS OF INNOVATION

At a special anniversary celebration, friends from across the HLRS community gathered to reflect on milestones in the center's history and the challenges that will shape its evolution over the coming decade.

Prof. Dr. Michael Resch, Director of HLRS, welcomes attendees to the 25th anniversary celebration. **© HLRS**

Founded in 1996 as Germany's first national high-performance computing (HPC) centre, the High-Performance Computing Center Stuttgart (HLRS) has grown to become not just a key facility of the University of Stuttgart but also an internationally prominent research center. At a hybrid online/offline event held at the center on October 6, HLRS marked the 25th anniversary of its creation. The gathering offered a wide range of perspectives on HLRS's role in powering scientific discovery, supporting industrial competitiveness, driving technical evolution, and meeting global challenges.

In a press release, Prof. Wolfram Ressel, Rector of the University of Stuttgart, congratulated HLRS on its anniversary, remarking, "The high-performance computing center is a prominent example of the University of Stuttgart's excellent research infrastructure. For more than a quarter century Stuttgart's supercomputing has stood at the pinnacle of scientific and technological progress and is synonymous with visionary research and education, as well as for technology transfer in support of prosperity in industry and society. On the occasion of its anniversary celebration I congratulate all of the researchers who on a daily basis contribute to these exciting efforts for their internationally recognized achievements."

German Federal Minister of Education and Research Anja Karliczek also extended her congratulations on the anniversary: "High-performance computing is an important cornerstone for building technological sovereignty in Germany and Europe. By making reliable investments in the research and development of digital technologies we are ensuring our competitiveness. HLRS has been engaged at the intersection of science and industry for more than 25 years, and again and again its supercomputers have enabled ground-breaking achievements, for example in the simulation of more energy efficient airfoils. The high level of commitment of the staff at HLRS is crucial to this great success: thanks to them, algorithms and supercomputers are transformed into excellent research and innovation."

"The High-Performance Computing Center at the University of Stuttgart is among the largest and most important facilities for supercomputing worldwide," said

The 25th anniversary celebration was a hybrid in-person/virtual event. © HLRS

Baden-Württemberg Minister of Science Theresia Bauer. "The past 25 years at HLRS have been a remarkable success story and its international visibility is of upmost importance for the state as a center for research. In its role as a competence center, HLRS is active in almost all areas of research, from engineering to the digital humanities, and makes essential contributions to key political fields such as the transition underway in the energy sector and the development of more environmentally sustainable mobility solutions."

Reflecting on HLRS's accomplishments and future

The anniversary celebration brought together close partners from across the HLRS community to consider the center's accomplishments and contributions to science and industrial R&D. In the first half of the day, four panel discussions considered key aspects of HLRS's history and activities. HLRS Director Prof. Michael Resch, together with several of HLRS's "founding fathers" reflected on factors that led to the center's establishment, as well as how its technical infrastructure and expertise have grown in relevance for an expanding range of applications. SICOS BW Managing Director Dr. Andreas Wierse led a conversation focusing on how supercomputing supports industry and how models for technology transfer developed at HLRS promote competitiveness both for individual companies and for Europe as a whole. In a session moderated by HLRS Steering Committee Chair Prof. Wolfgang Nagel, long-time scientific users of HLRS's systems explained why HPC is essential for their work, what opportunities increased computing power could offer, and future challenges resulting from the need to manage and analyze increasingly massive data sets. Finally, HLRS Department of Philosophy Chair Prof. Andreas Kaminski spoke with former HLRS staff members, who reflected on their experience of completing PhD's at the center and their career development since then.

A more formal anniversary ceremony took place in the late afternoon. Guests of honor (either present or delivering greetings online) included University of Stuttgart Rector Prof. Wolfram Ressel, Federal Minister of Education and Research Anja Karliczek, and Baden-Württemberg Ministry of Science, Research, and Art Ministerial Director Dr. Hans Reiter. Representatives of the European Union, including Gustav Kalbe from the European Commission Directorate-General for Communications Networks, Content, and Technology (CNECT), and EuroHPC Joint Undertaking Managing Director Anders Dam Jensen recognized HLRS's contributions to supercomputing at the European level. The ceremony was capped by short lectures by senior representatives of several of HLRS's international partners, focusing on questions that the HPC community will address in the coming years. These included Prof. Dr. Jesus Labarta (Barcelona Supercomputing Center, Spain), Prof. Horst Simon (Lawrence Berkeley National Laboratory, USA), and Prof. Dr. Hiroaki Kobayashi (Tohoku University, Japan).

New technologies and environmental considerations present key challenges

Looking toward HLRS's future, Michael Resch suggested that the demand for larger supercomputers, the emergence of new technologies like artificial intelligence and quantum computing, and the urgent need to make HPC more environmentally sustainable are three key factors that will drive HLRS's continuing evolution over the coming decade.

"As HLRS plans for its next-generation supercomputer, which we hope to inaugurate in 2026, we will face the twin challenges of constructing a new building and developing a new energy infrastructure that will meet the new supercomputer's significantly larger power requirements," Resch said in the pre-event press release. "A focus on maximizing efficiency will be particularly important as HLRS builds on its recent EMAS and Blue Angel certifications for environmental and energy management, and works toward the goal of becoming carbon neutral by 2032." Considering the role that simulation and data analysis have played in the global response to the ongoing Covid-19 pandemic, HLRS is also focused on addressing a growing need for urgent supercomputing resources that can be deployed quickly in crisis situations.

"Today is a day to look back with pride at what HLRS and its many partners have accomplished over the last 25 years," Resch said. "At the same time we look forward to continuing to provide new kinds of resources and solutions that will help scientists, technology creators, public administrators, and others across our society to address the many challenges that we face." *cw*

HLRS Director Prof. Dr. Michael Resch (right) participates in a discussion with University of Stuttgart Rector Prof. Dr. Wolfram Ressel (centre), and Dr. Alfred Geiger (left), Head of Scientific Computing at T-Systems and Managing Director of hww. © HLRS

NEWS FEATURES

LIFTING A TREASURE TROVE OF DATA FOR ENVIRONMENTAL SCIENCES

The innovative high-performance data platform, terrabyte, grew from a collaboration between the German Aerospace Center (DLR) and the Leibniz Supercomputing Centre (LRZ) of the Bavarian Academy of Sciences and Humanities. The platform makes Earth observation data accessible for research and offers practical tools for analytics.

Extreme weather, droughts, melting glaciers, coastal erosion, even the development of cities over time: Currently, eight satellites, including the Copernicus Sentinel, the US Landsat, and the radar satellites of the German Aerospace Center send approximately 19 terrabytes of data per day about the current state of planet Earth.

To explore this gigantic treasure trove of historical and current earth observation data, DLR's large datasets can now be quickly transferred to the terrabyte High-Performance Data Analytics (HPDA) platform at LRZ. The system connects DLR's satellite data archive in Oberpfaffenhofen with new, intelligently managed online storage of around 50 petabytes and the supercomputers of the scientific computing centre in Garching via a 10 gigabit/s line.

Analysis of Earth observation data

"The terrabyte concept allows our scientists to evaluate huge amounts of data highly efficiently without running their algorithms in less protected environments," says Stefan Dech, Director of the German Remote Sensing Data Center (DFD) at DLR. "The data that satellites provide on urbanisation or the melting of glaciers and polar ice caps, for example, can be processed immediately in the future. This is a milestone for environmental research and remote sensing of the Earth. We expect an enormous leap in knowledge."

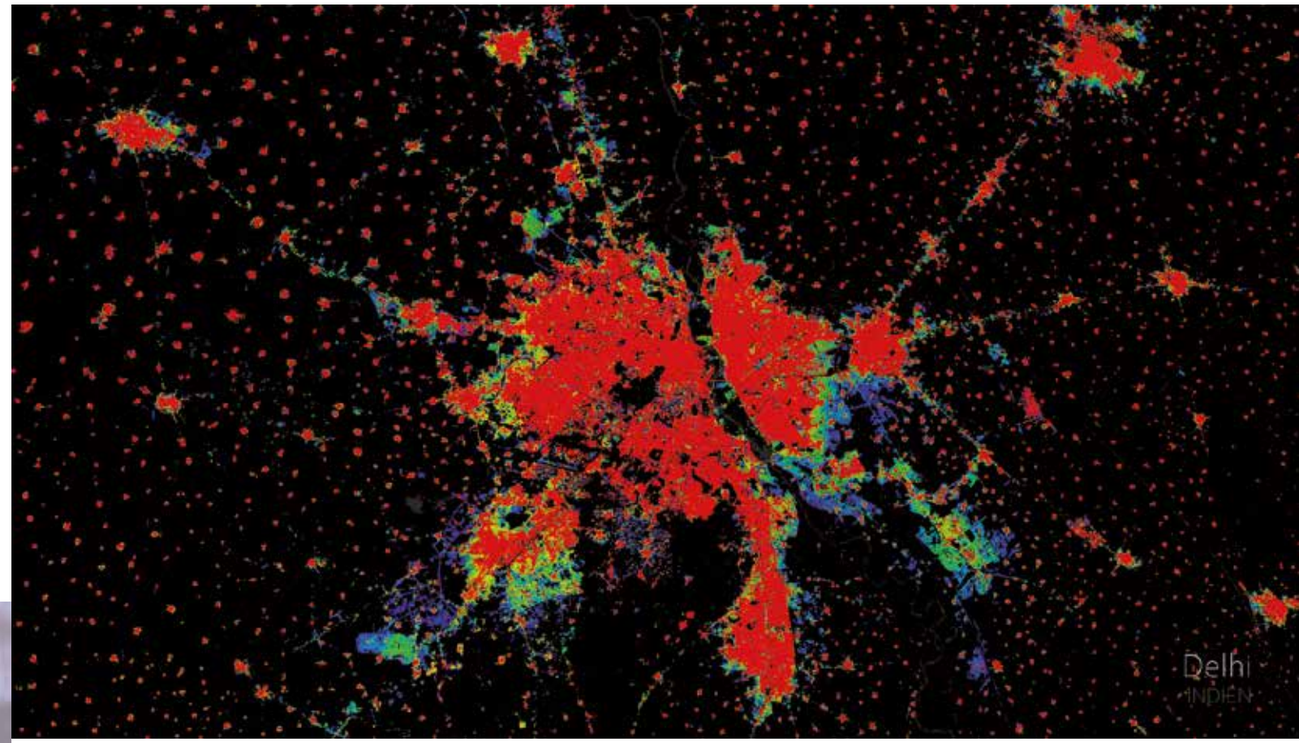
Environmental protection, the economy, and society at large should benefit from this development. For DLR, terrabyte also offers an alternative to the data clouds of commercial providers, because the platform meets all security and data protection requirements.

The core of the terrabyte platform is made up of 10 racks packed with ThinkSystem SR630 servers and variously sized DSS-G storage systems from Lenovo. Together they offer 49 petabytes of storage. The data is organised by IBM's Spectrum Scale file system, and the Infiniband network ensures extremely fast data transfers between storage and compute capacities. "Internally, we transfer the data at 300 gigabytes per second, which opens up new possibilities for their processing," says Dieter Kranzlmüller, Director of the LRZ. "The collaboration with DLR is a challenge that we gladly accept. terrabyte is not only about very large compute capacities, but above all about processing mass data. The platform also shows the growing importance of storage volumes for research. In more and more scientific fields, data should be easily accessible and ideally processed on site." To be able to check research results or process them further, open access is increasingly in demand. terrabyte is the technical implementation the high-performance analytics platform, and therefore also serves LRZ as a model for further storage and compute offerings in other research areas.

Understanding the environment better

In 2020, DLR invested 8 million Euros on the procurement of the storage part of the terrabyte platform. The LRZ in turn supports and maintains the HPDA system. With further funding from DLR, terrabyte is now being expanded to include its own compute capacities that will enable data processing and analyses, with a special focus on using artificial intelligence methods. DLR's satellite data is to be used widely in the future; in addition to DLR, Munich and Bavarian universities will soon also have access to terrabyte.

The core of the terrabyte platform is made up of 10 racks packed with ThinkSystem SR630 servers and DSS-G storage systems from Lenovo. Together they offer 49 petabytes of storage. © LRZ



This image, taken from satellite imagery, shows the development of Delhi over the last 3 decades. © DLR/EOC

Xiaoxang Zhu, chair at the Technical University of Munich and head of department at DLR's Earth Observation Center (EOC), has been working with satellite data for years. The engineer has developed a wide variety of algorithms to depict mega-cities three-dimensionally and with the highest accuracy. Today, her models can be used to optimise spatial and urban planning or disaster control. Easily accessible earth observation data also advance environmental and climate research, simplify the construction of mobile phone and IT networks or provide evidence for the calculation of subsidies.

Another EOC team led by Thomas Esch also uses this data to create the "World Settlement Footprint" (WSF), a quasi-comparative and control instrument for urbanisation: for this purpose, information on the extent, structure, and development of settlement areas as well as on population density and distribution is automatically evaluated. The WSF provides valuable information for science, politics and business, enabling them to react to the impoverishment of city districts, weather changes, or the loss of biodiversity. *sv*

RESEARCHERS USE SUPERCOMPUTERS IN AN EFFORT TO DEVELOP SAFER, MORE PERSONALIZED MEDICAL PROCEDURES FOR RESPIRATORY ILLNESSES

Using a combination of CT-scans, other available patient data, and simulations, researchers are forging a path toward personalizing medicine and improving outcomes for patients with acute respiratory illnesses. In collaboration with the Leibniz Supercomputing Centre, researchers from the Technical University of Munich are developing new computational methods to put insights from more accurate modelling and simulation into the hands of medical professionals.

Since March, 2020, the world has confronted a cold reality long known to epidemiologists and other public health experts—viruses that cause novel respiratory illnesses are among our greatest microbial foes. Viruses that attack human lungs can spread easily and leave lasting damage in their wake. The novel SARS-CoV-2 virus, for instance, unleashed the COVID-19 pandemic and has infected hundreds of millions of people, leaving more than 5 million dead.

Part of what makes viruses such as SARS-CoV-2 so dangerous (and so terrifying) is the organ they attack. Zoom in to view human lungs at the micro level, and you see a delicate, sponge-like organ with very thin, flexible and sensitive structures that allow a direct connection to the human circulatory system. The novel virus attacks these vulnerable parts and heavily increases the number of patients suffering from Acute Respiratory Distress Syndrome (ARDS) – a disease that so far has been caused by sepsis, pneumonia, traumata, smoke or toxic gas inhalation, among other causes, and strongly lowers the chances for survival of a person.

Modern approaches for supporting patients fighting off acute respiratory illness, such as inserting a tube into a person's trachea and using a machine to mechanically assist with breathing, have helped stave off death for COVID patients as well as others with lung damage or injury, but these methods also come with their own risks. In essence, ventilators add stress to an already damaged organ, and prolonged use can lead to complications, other health problems, and frequently even lead to death themselves.

Over the last 15 years, a team of researchers from the Technical University of Munich (TUM) has worked on novel approaches for developing strategies to better assess risks associated with machine ventilation and other invasive health procedures to combat respiratory illness. In the last five years this was supported via collaboration with staff at the Leibniz Supercomputing Centre (LRZ) in Garching near Munich. With the advent of the COVID-19 pandemic, the team's work became even more essential.

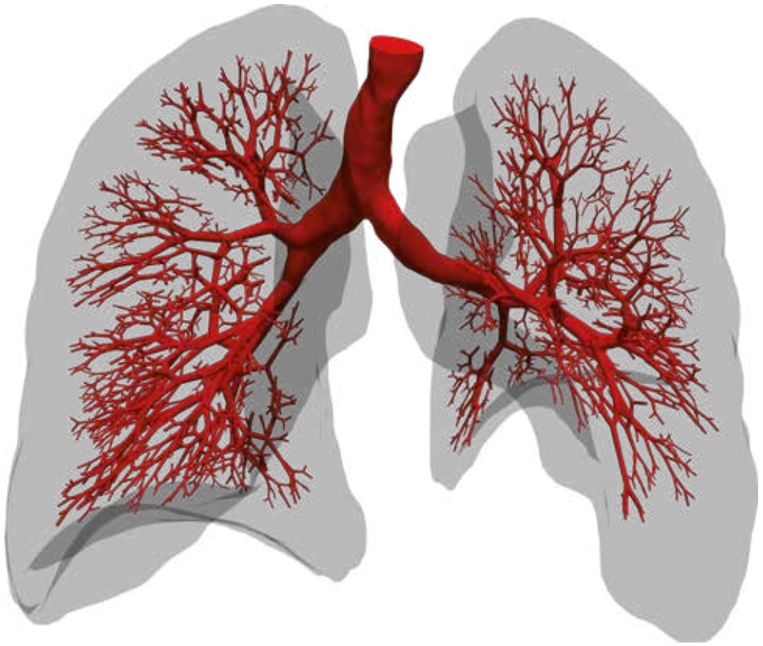
"For the research in our group, COVID-19 didn't change our focus, per se, because we were working on this issue already," said Prof. Dr. Wolfgang Wall, Professor of Computational Mechanics and Director of the Institute for Computational Mechanics at TUM as well as the principal investigator on this project. "Of course, the pandemic became something that raised awareness of this issue, and these acute lung injuries are one of the major complications that have led to people dying when having COVID, but the mortality rate for patients with ARDS requiring respirators was already high. In that sense, COVID became a bit of added motivation and visibility for us."

Using the SuperMUC-NG supercomputer at LRZ and closely collaborating with the centre's computational experts, the team mixed relatively new computational approaches with modified classical computational fluid dynamics (CFD) techniques, achieving a significant performance boost when doing high-resolution lung modelling. In the coming years, the team will take this approach to design both more accurate as well as novel reduced-order models that could be used by medical professionals to inform how to best mechanically respirate patients. The team presented its research at the SC21 computing conference this November.

Smorgasbord of simulation techniques

Researchers across multiple scientific and engineering disciplines use CFD simulations to help solve difficult problems. From modelling air flow around a wind turbine to gaining increased insight into the physics and chemistry happening in a fuel injector during combustion, CFD allows researchers to gain insights into things either too diffuse or difficult to see experimentally.

The complications in a CFD simulation primarily stem from scales—both size and time. Researchers have to simulate features of a fluid flow at fine enough detail to capture realistic behaviour while simultaneously creating a large enough simulation to reflect how the system would behave in real-world conditions.



The section of the lung geometry (red) is fully resolved by three-dimensional simulations. From the smallest features in the illustration, the spongy network of the lung continues into even smaller structures where the flow is laminar. The researchers' current simulation practice applies a reduced model representing the effective mechanical response in terms of a boundary condition specific to each individual airway section. © Maximilian Bergbauer

The first step typically requires that researchers break up their simulations into a computational grid of small mesh cells. Researchers then solve equations for these individual grid spaces—a matrix, of sorts—that represent how "fluid particles" behave with one another. In order to capture these interactions accurately, though, researchers also need to advance their simulations with very small time steps, meaning that they must recalculate particles' positions and interactions at micro or nanosecond intervals. In order to do this, researchers need access to powerful enough processors to quickly solve these equations, but also a computer that has large amounts of memory that cores can continually access as well as fast connections between the individual computer cores so they may share their results with computer cores calculating the spaces nearby.

Modelling air moving in and out of the human lungs is, in principle, the same approach to modelling other fluid flows. Unfortunately, unlike modelling fluid flows in a uniform, stationary object like a fuel injector, lungs change shape while breathing, when air, the liquid that lines the inner surface of the lung, and tissue interact, and disperse inhaled air throughout increasingly smaller tubes before arriving at the alveoli where they can process the inhaled air into its constituent gases for use in the body.

To address these additional complications, the TUM team started to create novel models and develop more novel computational techniques. One of Wall's collaborators, Dr. Martin Kronbichler, has been focused on high performance in CFD modelling for more than a decade. He recognized that while processors have gotten more powerful every few years, the memory bandwidth for rapidly sharing information between processors has not kept pace.

"Nowadays, modern machines are so powerful at computing, but there is this bottleneck with transferring data from memory to the computer cores," he said. "So, we were observing that the movement is the expensive part, and we decided to try and use a so-called matrix-free algorithm, meaning that rather than saving information that we need for the next step then having to access it again, we're just re-computing this information. While it required us to

innovate and go away from how CFD software has traditionally been written, our new code ExaDG factors quicker because we can really utilize this method efficiently. So ultimately, we are computing more, but it is faster because you need to access less data."

The time steps themselves also present a computational hurdle, as the more frequently a code has to recalculate the area in question, the less total time can be captured in a simulation. The team has been working on another indirect method to create more efficient calculations by optimizing each time step, allowing for more expensive individual time steps move forward in time in wider intervals. To date, the team was able to optimize its simulations to require less than 0.1 second per time step, and is focused on continuing to optimize the myriad memory bandwidth and latency issues to improve performance further.

Collaborations and combinations set the stage for better patient outcomes

Despite significant performance gains and a stable of relatively novel computational models and methods that could be explored for further improvements, Wall and his collaborators recognize hospitals are not on the cusp of buying supercomputers for themselves, and even the best-performing simulations are not fast enough to support individual recommendations quick enough to help seriously ill patients.

Ultimately, the need to find balance between accuracy and efficiency is endemic across most areas of research in computational (bio) mechanics. Researchers who have access to world-class computational resources such as those at LRZ tend to run computationally expensive high-resolution simulations that calculate as many parameters as possible "from scratch." These simulations can then provide inputs for less computationally demanding simulations, making them more accurate and useful.

In the case of patients hospitalized with respiratory illnesses, every minute counts, and the team wants to use its computational work as the basis from which doctors could make more informed decisions about respirating a patient. Currently, doctors must use their background and training to predict what parameters to use for a ventilator, then modify and adjust on the fly based on whether the oxygen level in the blood is improving.

"In the coming years, we hope that our method can develop into providing a somewhat optimal ventilation strategy for each individual patient," Wall said. "Doctors primarily base these parameters on the oxygen level in the blood, which is of course very important, but the lung is a very heterogeneous and complex organ, and while you might be getting the patient more oxygen, you could risk damaging the lungs through the ventilation process itself. And doctors currently have no way to see this at the moment. We want to have models available that, with a combination of CT-scan data and recording of patients' breathing, can provide a suggestion for better ventilation parameters to use for that specific patient." Wall and his collaborators have spun off this work into a start-up company, Ebenbuild GmbH.

Part of the success of this plan hinges on the team further optimizing its work on cutting-edge HPC resources. The team's long-running collaboration with LRZ has not only provided the means to run simulations on a powerful supercomputer, but also resulted in regular exchange about the team's computational needs more broadly. The team has worked closely with Dr. Momme Allalen, Leader of LRZ's CFDLab team and user support specialist, as well as LRZ leadership. They have also had access to a variety of testbed systems at LRZ, most recently through its BEAST testbed.

"There are various levels of support we've received from LRZ," Kronbichler said. "We have a lot of interaction with Momme to tune our algorithms for the architecture at hand. When you go to a new machine, you start to see new bottlenecks, and while they were likely already there on the machine before, you don't notice them until you start leaving a lot of performance on the table. The collaboration with LRZ really helps us, because we have access to not just a single architecture, but multiple architectures."

Additionally, the team collaborates closely with Prof. Dr. Martin Schulz, who in addition to his role as leading TUM's Chair of Computer Architecture and Parallel Systems in the Informatics department, also works closely with LRZ and serves on the centre's Board of Directors. The team works closely with Schulz to explain their hardware and software limitations and requirements, and tries to provide details that can inform future computational investments from the centre.

While the team recognizes that running optimal and fully comprehensive individualized lung simulations is not yet around the corner, it knows that optimizing today's capabilities while planning improvements based on the promises of tomorrow's computing resources will ultimately help researchers and patients alike. *eg*

TAKING INSPIRATION FROM MICROORGANISMS, RESEARCHERS USE HPC TO PROPEL MAGNETOCAPILLARY SWIMMER RESEARCH

German-Research-Foundation-funded initiative supports research to better understand the movements of microorganisms in an effort to develop new environmental remediation efforts and drug delivery devices, among other applications.

When it comes to inspiration for innovations, humans have long looked to the natural world when designing new technologies. While birds and fish may have provided early strategies for new ways of transporting ourselves across air and sea, many researchers focused on new ways of transport have now set their sights lower—perhaps more accurately, they have set their sights smaller.

In an effort to design new ways to clean up pollutants in the environment or deliver drugs in a more targeted manner, for instance, scientists now study microorganisms like bacteria, algae, and sperm cells. By recording their behaviours and properties, scientists can gain insights for developing artificial microdevices that can effectively move with high precision in specific environments.

This research area has become so important, in fact, that the German Research Foundation (German: Deutsche Forschungsgemeinschaft, DFG) in 2014 funded an expansive initiative focused on better understanding "microswimmers," or microorganisms able to effectively propel themselves in liquids.

While experimental techniques have helped scientists to better understand and design artificial microdevices that can mimic their natural counterparts, researchers may not be able to observe some of the smallest-scale interactions between organism and environment that play a major role in effective movements.

As a result, a team led by Prof. Dr. Jens Harting at the Helmholtz Institute Erlangen-Nürnberg for Renewable Energy (HI ERN) has linked up with the experimental group of Prof. Nicolas Vandewalle at the University of Liege in Belgium as well as the "Physics underlying life science" group led by Prof. Ana-Sunčana Smith at the Friedrich-Alexander-Universität Erlangen-Nürnberg.

The researchers set out to combine experimental studies and theoretical modelling with state-of-the-art computer simulations to better understand a particular subset of artificial microswimmers called magnetocapillary swimmers. The HI ERN group looked to the power of high-performance Performance Computing Center Stuttgart (HLRS) and Jülich Supercomputing Centre (JSC).

"The motivation for our research was to create as highly complicated a system as numerically possible without multiple approximations and to study its dynamics close to the experimental conditions and parameters," Harting said. "Furthermore, our numerical method serves as an independent tool for verifying some theoretical predictions and open questions appearing in the experiments."

Surface-level sophistication

Simply put, magnetocapillary swimmers can be just a few micrometre-sized beads of magnetic material floating on the surface of water. While these relatively simple systems might seem straightforward to study, the challenge comes from the subtle changes they make to their immediate surroundings and, as a result, the influence they exert on one another.

For a clearer picture, think of pouring breakfast cereal in milk. While the individual flakes may be light enough to float "on top" of the milk, they are still deforming the surface of the milk by pushing it down. Anyone who has tried to sleep on an underinflated air mattress knows what happens next—this deformation creates a gradient of sorts that causes other flakes to drift toward one another and cluster, further deforming the surface area.

If the magnetocapillary swimmers' particles were just floating on water, a similar process would play out. Unlike cereal, though, these swimmers can be put under the influence of a magnetic field, and when properly configured, this magnetic field can not only oppose the particles' attraction to ultimately offset the water deformation, it can also guide a swimmer to travel where the researchers want it to go. Understanding how to efficiently and accurately guide swimmers' movements is a key component to developing artificial structures capable of assisting with precision tasks such as drug delivery.

When beginning their investigation, the researchers did not initially assume they would need some of Germany's most power computing resources to simulate these interactions—this relatively simple system moves slowly enough not to create large-scale turbulent motions in the water.

The swimmers' slow movements actually wound up being among the most computationally intensive challenges for the team's simulations, though.

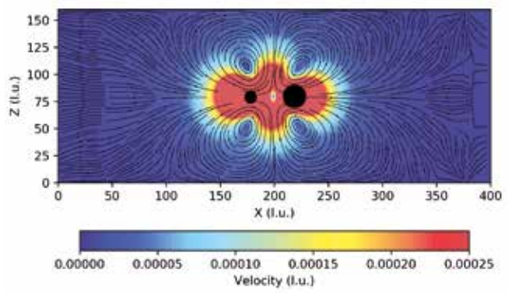
The swimmers are guided by the subtle oscillations of a magnetic field, so to accurately simulate this process, the researchers must ensure that individual oscillations are represented within the simulation, meaning that they must advance time in their computations very slowly while also modelling small-scale hydrodynamic interactions. And while these small particles are not moving fast enough to create large-scale turbulent motion in the liquid in which they are floating, the individual particles' movements still have subtle yet significant influence on other nearby particles' movements. Taken together, if the researchers want a realistic view of swimmers' movements and the constituent particles' interactions with one another, they must have a huge range of time and size scales in their simulations.

With access to GCS computing resources, the team is already capable of simulating these interactions at the level of detail necessary to help verify experimentalists' hypotheses. Unlike experiment, though, the researchers can also make slight modifications to inputs to speed-up the time-consuming, trial-and-error process necessary when designing these systems purely experimentally.

"Designing these materials is always an iterative process, but access to HPC resources allows us to speed up the iteration necessary to achieve desired outcomes significantly," Harting said.

Swimming and simulating toward the horizon

The team noted that current generation machines such as Hawk at HLRS and JUWELS at JSC have allowed them to push their simulations to a point where simply adding more computer cores no longer helps the team achieve its results any faster. "For our simulations in particular, we are already today able to reach sufficient system sizes," said Dr. Alexander Sukhov, a HI ERN researcher and collaborator on the project. "To further develop these simulations, we require faster cores in order to be able to achieve more time steps in less wall clock time."

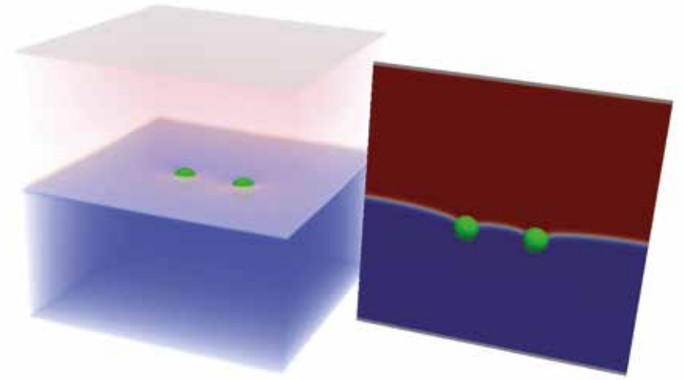


Flow fields upon the motion of a two-beads asymmetric micro-swimmer. **© Alexander Sukhov**

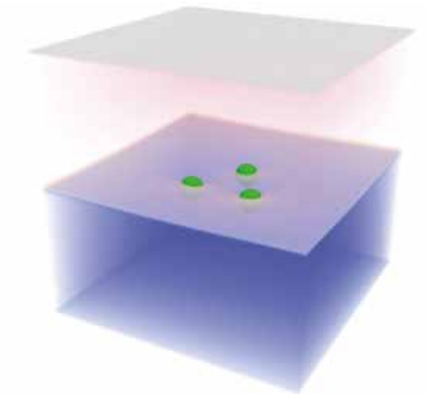
To achieve maximum performance on current generation compute cores, the team has worked closely with user support specialists at HLRS and JSC to address issues arising from how their code runs scripts on machines after updates as well as ensuring that they are getting the most out of the machine memory.

Moving forward, supercomputing resources will continue to play an increasingly important role in understanding the motion of magnetocapillary swimmers. In their interactions with experimentalists, Harting, Sukhov, and their collaborators already discovered that prior simulations did not fully account for the influence of particles on their nearby partners, and as the DFG Priority Programme continues, these types of exchanges between experimentalists and computational scientists will only become more essential.

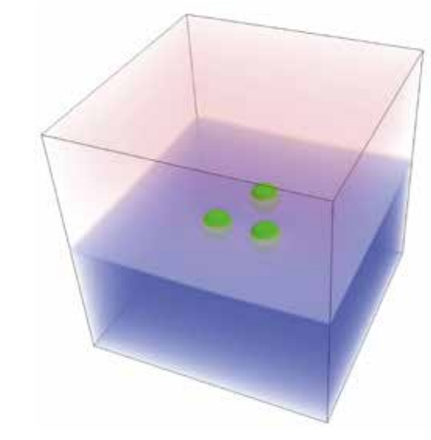
For researchers to fully understand the complex mechanisms that influence biological swimmers' motions, though, researchers will have to continue to focus on specific environmental and physics-based factors that play a role in propelling swimmers, whether that is light, gravity, chemical interactions, or other mechanisms. With the help of supercomputing resources, this cross-disciplinary collaboration aims to use HPC to take experimental data and run rapid-successions of simulations with slight modifications to input data, and ultimately design a new class of microdevices capable of helping clean up our environments and fight off illness. *eg*



Final state after relaxation of two particles at the fluid-fluid interface in 3D (left) and a cross-section of the interface (right). **© Alexander Sukhov**



Final state after relaxation of three particles at the fluid-fluid interface. **© Alexander Sukhov**



Magnetocapillary swimmer in motion modelled by lattice-Boltzmann simulations **© Alexander Sukhov**

USING JUWELS, RESEARCHERS WORK TO ADVANCE POLYMER-BASED FILTRATION PROCESSES

Separating and filtering complex mixtures is essential for many industrial and medical applications. In fact, industrial separation processes of chemicals account for roughly 10 percent of the world's energy consumption. Researchers are using a combination of simulation and experiments to deepen our understanding of how to make these essential processes more efficient.

Polymers are a broad class of materials made up of long chain molecules of repeating units —anything from biopolymers such as plant cellulose to a variety of synthetic materials, used in everyday applications such as packaging or car tires, among countless other applications. The polymer length and structure play significant roles in how polymers are able to mix (or phase separate) with other polymers.

Connecting two polymers into a single, long chain molecule, also called a diblock copolymer, gives rise to the "self-assembly" of these polymers at the molecular level, meaning that the two polymer blocks spontaneously separate into different spatial regions or domains at the nanoscale, and these domains arrange in distinct ways that create patterns with cylindrical pores or other shapes.

As materials science has advanced, researchers are increasingly turning to such diblock copolymers to develop thin films and membranes to help separate complex chemical mixtures. These pores or channels can act as "gatekeepers," as their dimensions can be tailored in such a way to only allow certain molecules to pass through.

Once science had a rough understanding of the process of fabricating polymer membranes, scientists and engineers started to implement it in certain industrial separation methods. Unfortunately, membrane fabrication (i.e., the process of forming a membrane) depends on a multitude of thermodynamic and kinetic parameters and is still not well understood at a fundamental level.

In recent years, researchers at the University of Göttingen have collaborated with the experimental group of Prof. Dr. Volker Abetz (Helmholtz-Zentrum Hereon and University of Hamburg) to advance our understanding of these processes at a fundamental level in the hopes of better understanding how process-directed self-assembly in the course of solvent evaporation from a polymer film or the exchange of solvent and nonsolvent can help tailor this nonequilibrium phase separation process.

"Our work in this area is motivated by the fact that solvent evaporation is a basic and ubiquitous real-world process," said Prof. Dr. Marcus Müller, Professor of Theoretical Physics at the University of Göttingen. "Polymer solutions are frequently employed in the preparation of polymer films and membranes, yet this process is not well understood and simulation studies are in their infancy." Müller and his collaborators have been using high-performance computing (HPC) resources at the Jülich Supercomputing Centre (JSC) to study the phase separation and self-assembly at the molecular level.

Pull yourself together

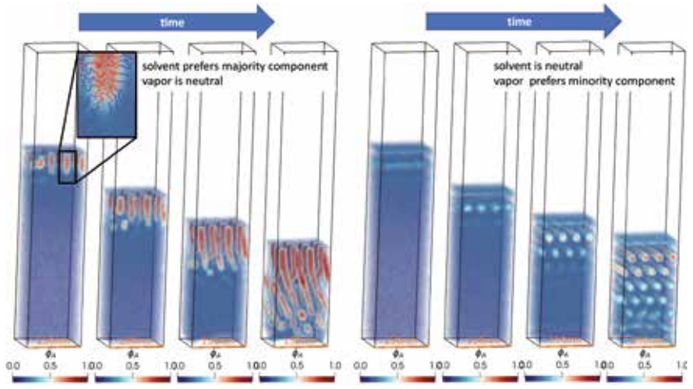
The fabrication of polymer membranes has made large advancements in recent decades, but is still an emergent field of study. While these self-assembled structures are very effective at filtering out desired molecules in a chemical mixture, they are also very fragile and prone to fouling—clogging of a polymer membrane's pores that prevents it from filtering out the desired molecules.

Müller and a group of international collaborators are investigating a suite of potential methods to improve copolymer self-assembly and polymer membranes used in filtration or separation processes. Perhaps the most exciting and promising among them lies in the realm of process-directed self-assembly.

"As a theoretical physicist, I am really fascinated by process-directed self-assembly, where the processing pathway—in our case, the evaporation or solvent exchange—is utilized to fabricate a functional nanostructure," Müller said. "This kind of processing is a well-known strategy in engineering. Japanese swordsmiths all the way back in feudal Japan knew that micrometre-sized grains in metals dictate their mechanical application properties, for instance, but processing on the molecular time and length scales is much less explored and understood."

Experiments have been the driving force in finding new ways to use polymers in this research field, but rely heavily on prior knowledge followed by trial and error. To accelerate development of new fabrication processes, researchers like Müller and his collaborators pair experiment with simulation.

Experiments serve as the basis for simulations, as researchers want to recreate the experimental conditions in their computational models as closely as possible. Unlike



Self-assembly of an AB diblock copolymer in the course of solvent evaporation from a thin film, as observed by particle simulations with the GPU-accelerated program SOMA. Time increases from left to right, and the inset illustrates the arrangement of the chain molecules into A-rich (red) and B-rich (blue) domains. Left: The solvent prefers the majority component of the diblock copolymer and the evaporation process results in cylindrical domains, vertically orientated to the polymer-vapour interface of the film. This pore orientation is desirable for filtration membranes. Right: Switching the solvent and vapour affinities, however, results in lying cylinders.

experiments, though, simulations allow researchers to not only model the process of structure formation in time and space, but also to access conditions that are difficult to create in experiments in order to highlight the role of specific interactions or process parameters. This strategy provides insights and suggests how modifications impact the structure of a polymer membrane and its ability to effectively filter a mixture.

However, in order to accurately model a given system, simulations must be large enough to capture real-world conditions while detailed enough to accurately represent molecules' interactions with one another. Further, researchers need simulations to follow the large spectrum of time scales involved in the membrane formation and usage. That means that researchers like Müller require access to HPC resources, such as JSC's modular supercomputing system JUWELS.

Using a combination of theory and experiment, Müller and his collaborators have already gained new insights into how the relationship between polymer structure, thermodynamics, and process conditions influences membrane fabrication, but stressed that this field is still emergent and more experimental and computational work remains.

Next-generation technologies advance next-generation industrial processes

Müller indicated that advancements in both experimental techniques as well as computational power have already played a big role in furthering researchers' understanding of polymer membranes. "These are exciting times, because by virtue of new techniques and resources like the JUWELS Booster module at JSC, the time and length scales of simulation and experiment are starting to truly converge," he said. "One can anticipate many opportunities of fruitful collaboration in the context of nonequilibrium structure formation of polymer materials."

Cutting-edge computational resources such as the JUWELS Booster—currently the fastest machine in Europe and among the top 10 most energy-efficient machines in the world—can only truly demonstrate their computational muscle if scientists and engineers can make effective use of them, though, and Müller indicated that JSC's emphasis on training has helped improve his team's performance significantly. Specifically, he pointed to JSC's GPU Hackathons as being beneficial for not only improving performance, but also generally sharing best practices across JSC's user base.

"Hackathons allow my group members and experts from JSC like Dr. Andreas Herten as well as NVIDIA experts like Markus Hrywniak to team up. This collaboration started for us with an event in 2016, and continued through the JUWELS Booster early-access program and Hackathon at the end of last year," he said. "This personal contact to HPC experts at JSC and NVIDIA is essential. It allows us to acquire top-notch technical knowledge and is also a great team-building activity that brings together new and experienced group members – my group members dedicate a lot of work to these exciting events, but it also provides a lot of excitement and motivation and is also a lot of fun."

Moving forward, the team plans to leverage its increased knowledge of using the JUWELS Booster to include even more processes in their simulations in the hopes of not just validating experimental hypotheses, but suggesting new potential materials. Müller indicated that by using JUWELS' modular computing concept to draw from its ultra-fast GPUs and robust CPUs, the team could combine different modelling approaches to further accelerate the iteration between computational scientists and experimentalists. *eg*

THE PPI4HPC PROJECT LEADS TO A SUCCESSFUL FIRST JOINT EUROPEAN PROCUREMENT OF HPC SYSTEMS

Intra-European procurement effort focuses on collective bargaining power to strengthen the next generation of Europe's flagship HPC resources.

In May 2018, a tender was published to procure high-performance computing and storage systems at four leading European supercomputing centres. It was the first joint procurement in this field that was initiated and financially supported by the European Commission (EC). It served as a precursor for later European HPC procurements. The joint procurement formally ended in May 2020 after all contracts had been successfully awarded. The project itself ended in September 2021 after the last supercomputer was accepted.

The project, the Public Procurement of Innovations for High-Performance Computing (PPI4HPC) implemented a so-called public procurement of innovative solutions, which is an instrument introduced by the EC to stimulate innovation. The idea is to make the public sector act as a launch customer of new, innovative products. In a joint procurement, several public organisations form a buyers' group, which allows them to leverage their collective bargaining power to push for products that meet their needs. In the case of PPI4HPC, BSC (Spain), CINECA (Italy), Forschungszentrum Jülich (Germany), and GENCI with support of CEA (France) formed such a group.

After a joint market consultation and a joint selection of the candidates, the procurement process was split into four different lots. Within each of the lots, a contract for a large-scale system was awarded. All PPI4HPC supercomputers are among the top 60 of the most recent Top500 list. At the Jülich Supercomputing Centre (JSC), the PPI4HPC procurement resulted in the installation of the JURECA-DC system.

Given the focus on promoting innovation, the buyers' group folded an innovation criterion into the bidding process, putting further emphasis on the program's focus. This forced suppliers to explicitly identify opportunities to develop and integrate new and relevant features to the system. In the case of JURECA-DC, the bid resulted in not only using the most recent computing devices, but also introducing advanced power management and energy monitoring capabilities. Furthermore, the successful supplier integrated fast storage devices based on non-volatile memory managed by a new software stack into the system.

This joint procurement required all partners to enter new territory and a willingness to jointly work on technical specifications and legal documents. Getting motivated, available, and highly competent teams in place involving experts from all sites was a key for success. For legal aspects, the group relied on consultancy from an international law firm that was capable of understanding potential conflicts between French law, which was used for this joint procurement, and local laws.

The joint work on the technical specifications allowed for a significant enhancement of the quality of the documents. The project participants were able to learn from one another, ultimately helping improve different aspects of such procurements, including risk management strategies, acceptance procedures, and methodologies for assessing offers based on total cost of ownership (TCO).

The PPI4HPC project demonstrates that a joint procurement is feasible and that procurements can be run in a better way while promoting the deployment of new and innovative technologies. The project had been a true collaborative effort and the authors conclude this short report with acknowledging all people involved in this partnership for their good work as well as the shared expertise and knowledge. *(dp, mb, va)*

PPI4HPC

Funding:
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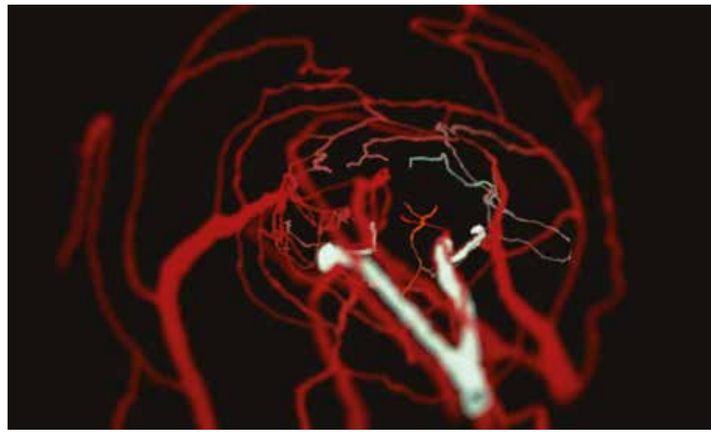
Runtime:
01.04.2017 – 30.09.2021

Partners:
BSC (Spain)
CEA (France)
CINECA (Italy)
GENCI (France)
Forschungszentrum Jülich (Germany)

SOFTWARE FOR MEDICINE AND PHARMACOLOGY

In its second funding phase, the European Centre of Excellence CompBioMed combines codes and software to develop tools for the simulation and visualisation of organs and drug development.

HemeLB is a freely available high-performance computing (HPC) program developed in the CompBioMed Centre of Excellence that models three-dimensional fluid flows at scale. The data obtained can be visualised with the oneAPI rendering toolkit from Intel. Using a combination of these tools, the visualisation specialists at the Leibniz Supercomputing Centre (LRZ) created a video that shows what happens in the arteries and veins of the forearm during one heartbeat.



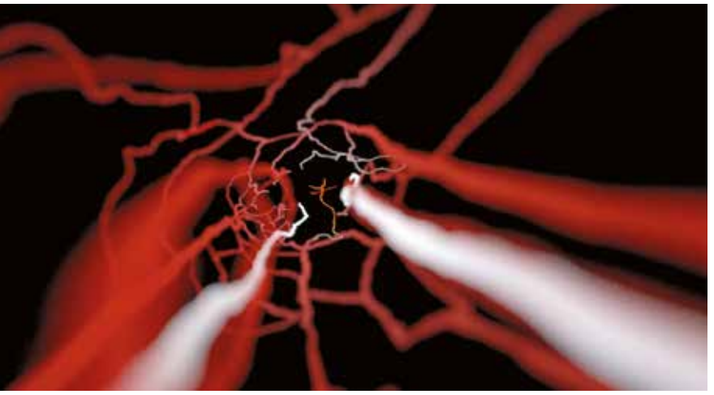
In addition to these next-generation visualization capabilities enabling greater insight into the inner workings of the human body, pharmacology also benefits from supercomputing: the interaction of smart pattern recognition with HPC software accelerates the search for active ingredients for drugs. Together with CompBioMed researchers, HPC experts at the LRZ set up innovative screening processes, tested them at the SuperMUC-NG in Garching and on the Summit supercomputer in the USA and found millions of substances that interact with spike proteins of the SARS-Cov2-virus in a significantly shorter time than using experimental trial and error.

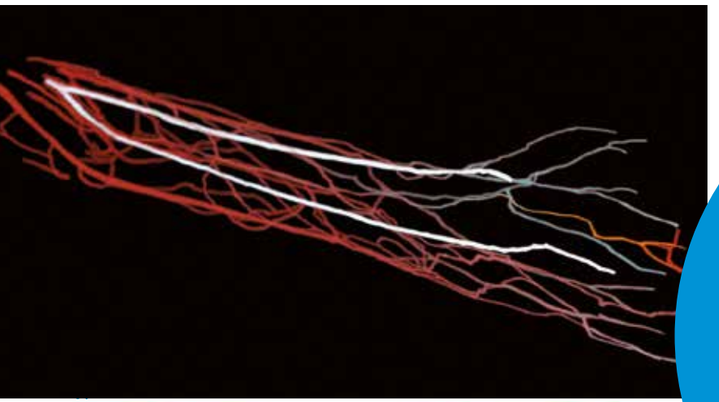
Both works are milestones for the digitization of medicine, molecular biology, and pharmacology as well as for the construction of a digital twin of humans: CompBioMed has been working on the latter since 2016. Around 20 research institutes and supercomputing centres, including LRZ, are developing and researching software, algorithms, and applications. In the second phase of the project, further tools are now being created by combining tools and codes to help improve research as well as therapies.

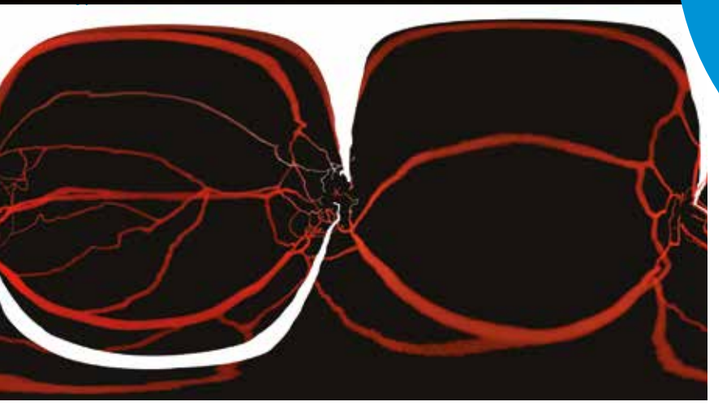
In research on COVID-19, CompBioMed's simulation software clarified the multiplication behaviour of the SARS-Cov2-virus. Above all, however, the Centre of Excellence found substances that bind to the virus more quickly: a groundbreaking result that may help to shorten the usual development times for marketable drugs to combat the virus. To speed things up, CompBioMed coupled machine learning with molecular dynamics simulations in a multi-step process. SuperMUC-NG ran thousands of calculations using the ESMACS and TIES codes to predict how strongly substances interact with four spike proteins of the corona virus. To do this, the LRZ optimised existing software and codes and developed management tools so that they utilise as many of SuperMUC-NG's more than 311,040 compute nodes as possible. With the simulation data, researchers trained artificial neural networks to accelerate screening of active substances. And with each additional combined analysis and calculation step, more precise results were available more quickly.

In a short time, SuperMUC-NG and Summit screened billions of compounds that potentially interact with the target proteins of SARS-Cov2. In parallel, workflows for implementing HPC software—including Gromacs, NAMD, AMBER and OpenMM—and the tools for training smart neural networks were built. RADICAL cybertools were also used to create middleware that connects software, databases and smart systems. Researchers and HPC centre staff feel confident in this hybrid approach of machine learning and simulation to help accelerate drug design for fighting pandemics and other emergent disease.

The further development of the open Lattice Boltzmann code, HemeLB, which was developed by CompBioMed to simulate blood flow, has now been optimised and adapted at the LRZ to achieve 80 percent scaling efficiency on SuperMUC-NG, and brings similarly high practical benefits. The data calculated with it from the human forearm was also visualised with the open-source programme OSPRay from the Intel oneAPI rendering toolkit. The specialists also developed tools and processes for the interaction of







HemeLB with graphics software and for the processing of measured values and other data. With this toolkit, blood flow can now also be visualised in other parts of the body. Surgeons are thus provided with a useful tool for preparing operations, and the views from inside the human body are likely to enter medical teaching and clarify the role of vessels. *sv*

Visualisations of a forearm data set from HemeLB using Intel® OSPRay Studio on LRZ's SuperMUC-NG.
© LRZ: Elisabeth Mayer (Visualisation, VR), Salvatore Cielo UCL/CompBioMed/HemeLB: Jon McCullough, Peter Coveney

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Department of Energy
National Cancer Institute

AS PART OF THE CATALYST PROJECT, FESTO-HLRS PARTNERSHIP WILL USE ARTIFICIAL INTELLIGENCE TO DEVELOP SAFER AUTOMATION

Industrial controls manufacturer Festo is looking to high-performance computing to help design safer, more efficient human-robot collaborations in manufacturing processes. Company researchers are collaborating with HLRS staff to "teach" robots how to learn from their environments.

Using a combination of experiment in the Festo R&D lab (pictured) and reinforcement learning, Festo and HLRS researchers are collaborating to train robots to safely interact with humans in automated manufacturing processes. © Festo

Festo, an Esslingen, Germany-based automation and industrial controls manufacturer, has helped businesses large and small improve their efficiency by delivering various forms of automation technology to businesses looking to streamline difficult tasks. As manufacturing processes become increasingly complex, though, Festo has turned to the power of high-performance computing (HPC) to help better tailor solutions to customers' individual needs.

"Festo has years of experience with automation, and until recently, these processes were more or less built once in a facility, then perform the task it needs to do," said Dr. Shahram Eivazi, researcher at Festo and a collaborator on the project. "But with artificial intelligence (AI) and other new tech, people are starting to ask for more custom-made solutions in their factories. Automation processes we have developed might need to be changed and tweaked for a company's specific needs, and that means that these systems have to be adaptive so they can change in a reasonable amount of time, while also being safe and interactive with humans that are involved in the manufacturing process."

The Festo team recently started a collaboration with the High-Performance Computing Center Stuttgart (HLRS) through the CATALYST project in order to train robots to perform complex tasks safely. Using the center's world-class HPC resources and partnering with HLRS staff, the Festo team is developing an AI workflow for training robots based on biological learning principles. CATALYST supports activities aimed at evaluating AI solutions and the eventual convergence of AI and HPC to enable full support of AI workflows on HPC.

Build on your best behavior

When training a machine to "learn" a new behavior, researchers primarily use three different methods. The first two, supervised and unsupervised learning, involve using large amounts of data to train an algorithm to pick out patterns effectively—either specific patterns that a programmer wants them to focus on (supervised learning) or noticing correlations of any kind in a given data set (unsupervised learning).

When training a computer to distinguish between cars and trucks, for example, supervised learning would involve feeding an algorithm many images of both and giving feedback about which are cars and which are trucks. For an unsupervised learning application, though, researchers might show the algorithm many pictures of cars and trucks, but let the algorithm define its own parameters for grouping the images. While it might notice structural differences between cars and trucks and filter the images that way, it might also choose vehicle color as the most important parameter and distinguish all the red vehicles from the blue vehicles.

While these are the most common AI methods, robots being designed to automate complex tasks need to be trained in a more detailed manner. The Festo team uses reinforcement learning to train its algorithm, an approach that draws heavily from methods used in early childhood development. Simply put, researchers train the algorithm by giving it feedback on its decisions. It boils down to sequence of trial-and-error. An algorithm wants to achieve a specific goal, such as getting a robot to tighten a screw, and each time it turns the screw driver in the correct direction, it gets positive feedback, a so-called award (the screw goes deeper into the material), otherwise, there will be negative feedback (the screw falls on the ground, because it is too loose).

Using a mixture of input data from the Festo R&D lab as well as video and sensor data from real-world manufacturing environments, the researchers train the algorithm to replicate behaviors while receiving feedback

"Once collected, you can take these different data sets and turn it into simulation," Eivazi said. "We wind up with a large dataset that can show the algorithm what is considered good or bad behavior. Using this method, we can achieve roughly 80 percent of the performance we want without actually ever touching a real environment. Then the last 20 percent of the work is tuning it to a specific environment for a specific need."

By tailoring these solutions to specific scenarios, Festo can help clients develop more complex automation workflows that involve humans interacting with robots safely. "We want to make these kinds of interactions safer, so we don't have to put barriers between robots and workers, because ultimately, we want our systems to support humans," Eivazi said.

Data-driven training methods need world-class HPC infrastructure

The principles behind using reinforcement learning to train an algorithm sound relatively simple, but the devil is in the details—in order to train its algorithm, the Festo team requires about 70 to 100 terabytes of data (100 terabytes is equivalent to saving roughly 50,000 hours of high-definition video to a computer). Using their own in-house computing resources, the team was unable to efficiently analyze such a massive dataset. By partnering with HLRS, however, Festo researchers can take advantage of the center's Cray CS-Storm system.

The team knew that it would need GPU accelerators to effectively train its algorithm, and while it had previous experience with accelerators, large-scale simulations require a different approach.

"We had experience with GPUs, but always in small clusters—3 GPUs and 100 CPU cores," Eivazi said. "As researchers in industry, we have limited access to large-scale computational resources and we already passed the point of training what we can on in-house resources, and coming to work with HLRS lets us answer the question, 'What if we have access to thousands of CPUs instead?'"

To take advantage of that performance, though, the researchers need to build out their software with a larger system in mind.

In order to scale its application appropriately, the team has started closely collaborating with Dennis Hoppe, Head of the HLRS Service Management and Business Processes Division, and his team member, Oleksandr Shcherbakov. The HLRS staffers are working with Festo to port their application to run effectively on HLRS's resources, and will soon start running their application on HLRS systems.

Having access to raw computational power does not mean all that much if researchers are unable to efficiently move and store these large datasets, though, and with a robust storage infrastructure, HLRS can effectively manage Festo's data in a secure environment that integrates with multiple computational and data analysis tools.

As the collaboration grows, Festo indicated three main challenges the team will have to overcome. First, the team needs to effectively train its algorithm to get "smarter" as it goes. "Training an algorithm with reinforcement learning doesn't mean it thinks like a human," he said. "If I train a machine to pick up something, and move it somewhere else, it learns it. Unfortunately, if you then decide to ask it to cut something or screw in a bolt after the first task, you are basically starting from the beginning again." He indicated that throughout the project, Festo wanted to investigate ways to reuse datasets for additional training opportunities.

Second, collecting meaningful datasets is a challenge. While simulations can go as fast as processing power allows, conducting experiments in the Festo R&D lab means keeping robots moving at real-world speeds, which, for safety reasons, cannot be too fast for humans to react to or interact with.

Finally, the team has to optimize how to move data containing insights gained on HLRS resources and quickly apply it to real-world manufacturing scenarios. As part of the Deutsches Forschungsnetz, with access to its ultra-high-speed X-WiN network, and through the Gauss Centre for Supercomputing's (GCS's) InHPC-DE initiative, HLRS has built out high-speed data transfer infrastructure to German universities, research facilities, and its fellow GCS centers. The center will rely on its experience in building out its data transfer capabilities in order to further improve the data management abilities for countless industrial partners.

"The CATALYST project gives us the opportunity to work closely together with researchers from both academia and industry on real-world solutions that combine AI and HPC," Hoppe said. "The collaboration with Festo goes beyond applying classical machine learning by focusing on reinforcement learning, which is currently a very active research area. It comes with different hardware and software requirements, making the Festo collaboration an excellent example for evaluating HPC's capabilities in supporting reinforcement learning." *eg*

CATALYST Project

Funding:
Ministry of Science, Research and the Arts Baden-Württemberg

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Runtime:
October 2016 to December 2021

Partners:
HLRS
HPE

E-CULTURE CONVENTION EXPLORES INTERSECTION OF ART AND DIGITAL TECHNOLOGIES

Bringing artists and HPC experts together could promote new kinds of creativity and support economic development in the culture industry.

Technologies such as simulation, artificial intelligence, data analytics, and data visualization have steadily been transforming the arts and culture industries. From theater to music to sculpture to the visual arts, computational methods now inspire and enable artists to produce new kinds of artworks. The results often make science and technology more accessible, present data in ways that are more understandable and facilitate critical perspectives, or dazzle audiences by creating experiences that would be impossible to achieve using other methods.

On September 15-17, 2021, HLRS and the Media Solution Center Baden-Württemberg (MSC) hosted a convention focused on this emerging "eCulture." The gathering, titled "The Economic and Cultural Impacts of the Digital Age," was designed to facilitate an exchange of ideas related to recent trends in art, culture, and the economy and provoke reflection on what new opportunities they offer for research at the intersection of digital technologies and the arts.

The Media Solution Center was co-founded by HLRS in 2018 to address a growing need in the media arts industry for large-scale computing resources and expertise in high-performance computing. Since then, the MSC has steadily built a network of artists and cultural organizations interested in exploring this new territory, facilitating collaboration with scientists and engineers who can provide the technical expertise to help realize their visions. To date, this includes 40 organizations located in 10 countries that are united by a vision in which cooperation between artists and scientists can enrich both worlds. The number of MSC members continues to grow.

The eCulture convention for the first time brought together many protagonists within the MSC network, and provided convention attendees the chance to discover state-of-the-art applications of computing technologies in the arts and culture industry. Presentations at the event fell into three general categories. In the first, speakers demonstrated examples of recent innovative projects in which artists and cultural institutions have experimented with and applied new applications of digital technologies. In the second, cultural managers and researchers of the culture industry discussed how cultural innovation can promote wider economic success, as well as model programs for uniting the arts and sciences that are sustainable and impactful. A third category of talks also explored philosophical and ethical questions concerning the growing influence of new technologies that have attracted interest within the media arts and society at large, particularly artificial intelligence.

"The diverse talks and the discussions that took place at the eCulture convention made it clear that creativity will be an essential part of future economic prosperity," said Media Solution Center General Manager Matthias Hauser, organizer of the event. "It is also clear that multidisciplinary networking and collaboration will be necessary to realize this potential in Europe. MSC, by connecting the art and media communities with computing resources and expertise at HLRS, is well positioned to help build these bridges."

Among the participants in the eCulture convention were (l-r): Bernd Eberhardt (Hochschule der Medien), Bastian Koller (HLRS), Matthias Stroezel (SSC Services), Daria Tataj (Tataj Innovation), Matthias Hauser (General Manager, Media Solution Center), Uwe Wössner (HLRS), Bernd Fesel (European Creative Business Network), Clara Gonçalves (CUNY Firefly Innovations), Ellen Seehusen (Consultant). © HLRS

At the convention, Javier Iglesias Garcia (Fundación Èpica) and Pep Gatell (La Fura dels Baus), related how Barcelona-based performance troupe La Fura dels Baus evolved over the last 40 years by using new technologies in its spectacular productions.

© Fundación Èpica.

The convention also marked the announcement of several new initiatives being organized by the Media Solution Center. This included a Research and Creation Center for Computational Based Art, Culture, and Economy, which will support young creators by introducing them to high-tech tools and connecting them with companies that can help them realize their ideas. Other upcoming MSC-led programs include a new CreativeLab, an Advanced School for the Computational Culture, and an Observatory of eCulture aimed at gathering, analyzing, and publicizing news and information from around the field. Rollout of these programs is planned over the coming years. *cw*

H³: HELMHOLTZ HERBST HACKATHON HELPS STUDENTS REENGAGE WITH COMPUTATIONAL SCIENCE CHALLENGES

Young Helmholtz researchers solve scientific data challenges and start filling the pandemic communication vacuum.

As part of the H³ hackathon, young researchers from various Helmholtz research facilities were able to come together to solve scientific data challenges. **© Ramona Kloß**

For all participants, the Helmholtz Herbst Hackathon was a relief. After months of pandemic self-isolation, young scientists were finally able to be absorbed in the unique atmosphere of a collaborative, engaging scientific workshop. The Helmholtz Herbst Hackathon, a cooperation project within the Helmholtz Association of German Research Centres, ran at a hotel near Cologne, Germany Sept 8–12.

"We wanted to create an event that truly stands out after the depressing pandemic time," said Daniela Henkel of Digital Earth, GEOMAR. "We wanted to get young scientists engaged in Machine Learning and let them get in touch again." The hackathon consisted of 46 young researchers from different research areas and different Helmholtz research programs who worked together to solve scientific data challenges.

The data challenges, a broad collection of datasets and research questions from various domains, were collected by a team from Forschungszentrum Jülich (FZJ) and released as the "Jülich Challenges Platform." "We firmly believe that creating data challenges is a great way to foster science," said Hanno Scharr, researcher from the Institute for Advanced Simulation (IAS-8) at FZJ. The challenges originate in various scientific fields, such as plant research, neuroscience, and physical analytics, and most approaches are centered around leveraging machine learning methods. For solving the challenges, participants could use the computational power of JUWELS Booster, the flagship of the Jülich Supercomputing Centre (JSC), which is ranked no. 8 in the current Top500 list. For many researchers, it was their first contact with a supercomputer. "The Jülich team gave a great introduction before the event. We have now made our first steps in using the JUWELS Booster for our own research," said Max Pargmann, a PhD student from the German Aerospace Center (DLR).

Stefan Kesselheim (JSC), scientific organizer of the program from FZJ, was also enthusiastic. "The results are extraordinary. All teams could beat the previous leaders in the respective leaderboard," he said. "The root counting challenge can now be considered solved." In this challenge, participants are asked to find methods to estimate the length of complex plant root systems from image data. When the two teams working on the challenge joined forces, they were able to complete the task with even higher accuracy. Sören Möller, researcher from the Institute of Energy and Climate Research (IEK-1) in Jülich, was also very happy with the outcome. "The task of my challenge is the automated analysis of ion beam spectra. The approach of the team was very innovative, and a true step forward for our research field," he said.

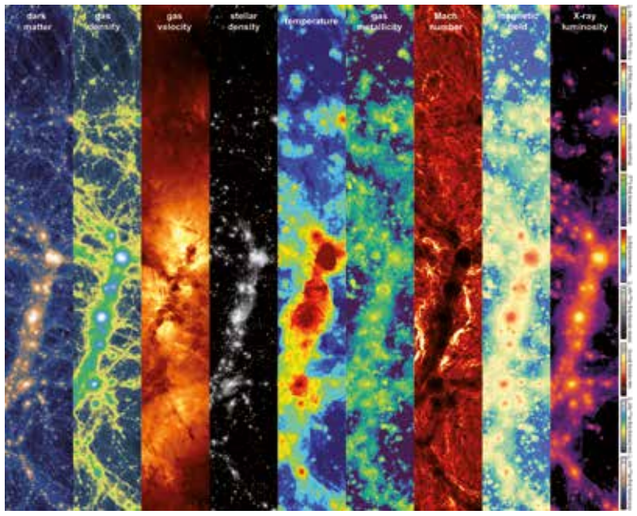
Sophie Ehrmanntraut of the Helmholtz Information and Data Science Academy (HIDA) is sure of the impact of hackathons like these. "Hackathons like this can play a very important role in the education of young researchers. They benefit on so many levels, personally and scientifically, and taking part will help them develop career goals," she said." After very positive feedback, the organizing team is already planning a similar hackathon for next year. *sk*

WELL DONE, SUPERMUC-NG

During the bi-annual Status and Results Workshop, LRZ invited the international HPC community to learn about the projects running on its flagship system.

The Status and Results Workshop of the Leibniz Supercomputing Centre (LRZ), which took place as virtual-only event from June 8–10, 2021, attracted a lot of attention, bringing roughly 160 participants from around the world. During the workshop, scientists discussed their results gained from large-scale computations done on LRZ's flagship supercomputer, SuperMUC-NG. And the results were impressive: since the machine went into full production in 2019, the 311,040 compute cores of the supercomputer in Garching have worked almost 30 billion core hours and completed around 195,000 jobs across 840 research projects. 17 of the 26 lectures are available as "LRZ Lectures on Demand" via the LRZ YouTube channel.

Prof. Volker Springel of the Max Planck Institute for Astrophysics, vividly described how his team used sophisticated modeling techniques to track a trillion particles and the distribution of matter in the universe in a cube with an edge length of several billion light years. The simulations of the multiple award-winning Millennium Illustris TNG runs created about a petabyte of data as they reconstructed the evolution of billions of galaxies and black holes since the Big Bang, and incidentally explain physical processes that also take place on Earth. His was just one of many presentations highlighting SuperMUC-NG's role as a machine for advancing science.



Prof. Dr. Volker Springel (Max Planck Institute for Astrophysics) described how his team used sophisticated modeling techniques to track a trillion particles to simulate the distribution of matter in the universe. © The TNG Collaboration

Simulate and visualize

The wide variety of presentations during the HPC workshop shows that demand for HPC is growing in other fields of science as well, such as in the natural, engineering, biological, and environmental sciences, for instance, as well as in pharmaceuticals and medicine. Researchers used SuperMUC-NG to simulate the impact of earthquakes, calculate the effects of emissions from road and air traffic on climate change, and model blood flow through veins: For this last project, led by the research consortium CompBioMed, LRZ experts completed a visualization on SuperMUC-NG that shows in high resolution how blood is pumped through the veins in the forearm during a heartbeat, enabling medical professionals to learn and understand better and faster. The book, *HPC in Science and Engineering*, which came out shortly before the event, gives insights in even more research projects on SuperMUC-NG.

However, the Status and Results Workshop did not only offer the opportunity to present research results; it also showcased what LRZ generally has to offer for researchers and students.

Naturally, the programme included an outlook into the future of supercomputing at LRZ as time passes faster between each new generation of HPC systems. After just over two years in operation, SuperMUC-NG will be extended with Phase 2. The system will integrate 240 nodes, which will also enable artificial intelligence and deep learning methods. An Infiniband network will ensure the fastest-possible data transfer. This, however, is just one way in which the LRZ is responding to constantly varying needs of classic and new HPC user communities.

In a separate track of the 3-day workshop programme, LRZ experts gave an encompassing overview on topics like the LRZ Compute Cloud, the centre's efforts in Research Data Management (RDM), artificial intelligence, and quantum computing to round-up the all-virtual experience.

"While we highly value the personal exchange with our users, we were very happy to see how well the digital version of our status and results workshop was received and how much interest it received also on an international scale," Dr. Gerald Mathias, Head of the Computational X Support Team, explained. "This is definitely something to consider when we design the next edition of this bi-annual meeting," he added. *sv*

HLRS AND AMD RUN FOR CHILDREN'S HOSPICE

HLRS and computer manufacturer AMD teamed up this summer to raise money for the Stuttgart Hospice for Children and Youth as participants in the Hand in Hand Spendenlauf. The "Core Performance Unit" finished in second place in the team rankings, running the equivalent of 1,948 laps. Seventy-eight team members from HLRS and AMD participated, with three placing within the top ten of the individual runners' ranking. In recognition of the team's efforts, AMD contributed 2,000 Euro to the Kinder- und Jugendhospiz der Hospiz Stuttgart, which provides support to seriously ill children and their families.

MPI AND THE NEXT PERFORMANCE LEVEL FOR HPC

Message passing interface (MPI) was the focus of the EuroMPI conference, which took place on September 7, 2021 and was hosted by LRZ as fully virtual conference by LRZ. Users and researchers discussed newly proposed concepts of the programming scheme and extensions to the MPI standard, libraries and languages based on MPI, as well as necessary interfaces to other standards in parallel programming. It also dealt with applications and their adaptations to new, more powerful computer architectures and networks with a session called "MPI goes Exascale." This year, Prof. Dr. Martin Schulz, Director of the LRZ, was responsible for the EuroMPI program. (https://www.eurompi21.lrz.de/)

HAWK GPU EXTENSION GOES INTO OPERATION

Installation of an important extension of HLRS's flagship supercomputer, Hawk, was recently completed and the system is now available for use. The upgrade consists of 24 HPE Apollo 6500 Gen10 Plus systems with 192 NVIDIA A100 GPUs based on the NVIDIA Ampere architecture. It offers 120 petaflops of AI performance and will provide a dramatic increase in HLRS's capabilities for supporting applications of machine learning, deep learning, high-performance data analytics, and artificial intelligence. The new AI platform has three times the number of NVIDIA processors found in HLRS's Cray CS-Storm system, its other go-to system for AI applications, making it possible to run larger-scale deep learning projects and expanding the total amount of computing power for AI that HLRS provides. With the integration of GPUs into Hawk's existing CPU architecture, computer scientists at HLRS also look forward to working with system users to develop new hybrid computing workflows that integrate traditional simulation methods with AI approaches.

PROJECT FMHUB: SUSTAINABLE FMM LIBRARY FOR THE SCIENTIFIC COMMUNITY

The rapid increase of hierarchically parallel hardware as well as the advent of accelerators has made it harder for those responsible for maintaining scientific simulation software to retain flexibility and high performance for each part of the code. In recent years, many communities therefore parted from large, intricately connected applications and moved towards an application model of highly specialized, modular and reusable components. The Fast Multipole Method (FMM) for long-range interactions is such a component that can serve researchers in multiple scientific communities.

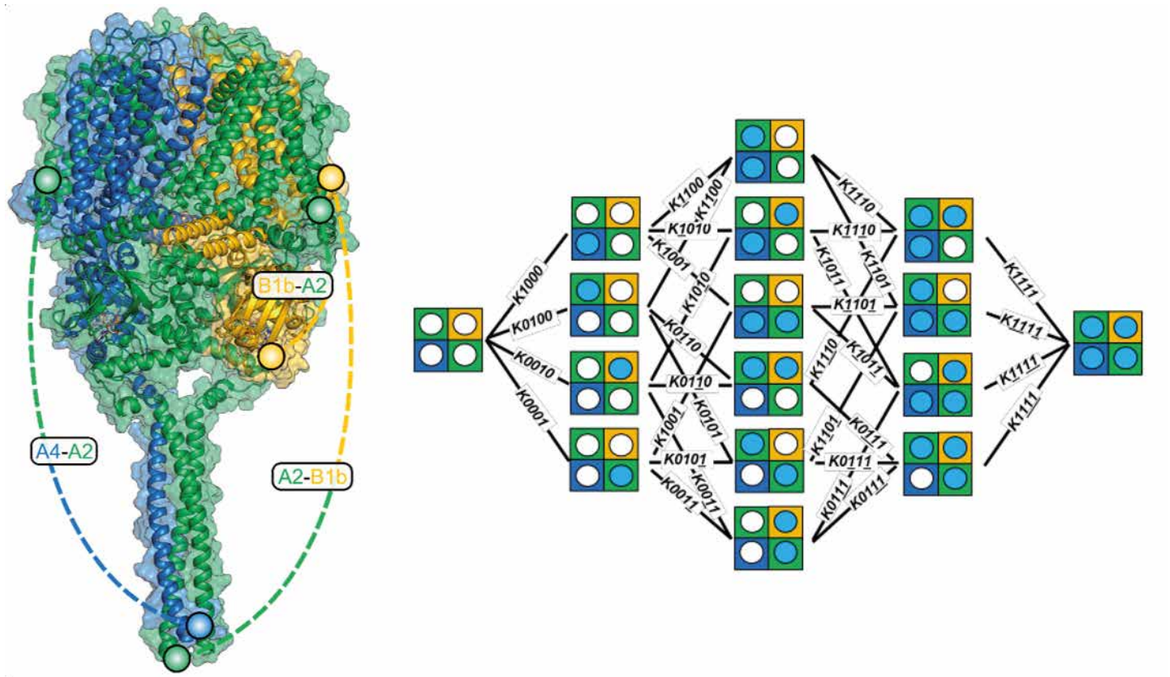
To establish a community hub for linear-scaling Coulomb solvers, project FMhub was devised. This DFG-funded joint-venture between JSC and Chemnitz University of Technology launched in September. With the goal of software sustainability in mind, the C++ library FMSolvr will be fully decoupled from its current application and made freely available together with community-building tools such as bugtracker and CI/CD to allow other HPC users an easy adoption to their code.

HPC IS AT AN INFLECTION POINT

Martin Schulz, Dieter Kranzlmüller, Directors of LRZ, among others, contributed a position paper to the 11th Symposium on Highly Efficient Accelerated and Reconfigurable Technologies (HEART) titled, "On the Inevitability of Integrated HPC Systems and How they will Change HPC System Operations." They advocate for a reduction of internal communication among nodes in HPC systems by a more integrated approach of different compute elements needed for machine learning, quantum computing, and other emergent technologies such as ARM kernels, GPUs, and tensor units sitting near to common compute architectures as well as teaching programmers how to use these systems efficiently (https://dl.acm.org/doi/10.1145/3468044.3468046)

IMPROVING ENERGY EFFICIENCY IN DATA CENTRES

HLRS has launched two new research projects focused on making HPC and data centres more sustainable. In the first, called DEGREE, HLRS and investigators at the University of Stuttgart's Institute for Building Energetics, Thermotechnology and Energy Storage (IGTE), will test an approach that dynamically regulates the operation of the cooling system for HLRS's flagship supercomputer, Hawk, maximizing the use of energy-efficient free cooling over more energy intensive active cooling while ensuring that the cooling circuit temperature climbs no higher than is necessary for free cooling. Using a numerical model of Hawk and validating it with real operating data, the goal is to understand the impact of dynamic control of the cooling loop temperature on energy consumption, IT component performance and reliability, operating costs, and CO_2 emissions. The second project, called ENRICH, will develop a digitalization atlas to forecast the future growth of the IT sector across Baden-Württemberg and identify opportunities for increasing energy efficiency. HLRS researchers will also look closely at issues related to the lifecycle of digital technologies, including procurement processes, responsible supply chain management, and disposal of electric waste at the conclusion of a product's life cycle. Both projects include partners from the IT industry, who will assist in developing recommendations to improve environmental performance in commercial data centres.



DISENTANGLED IN FOUR DIMENSIONS – SWITCHING BEHAVIOUR OF MEMBRANE RECEPTORS

A research team comprising researchers from Jena University Hospital, Schmalkalden University of Applied Sciences, Heinrich Heine University Düsseldorf (HHU), and Forschungszentrum Jülich were able to decode the switching process of a membrane receptor that occurs in olfactory neurons. Their scientific findings were recently published in the journal Proceedings of the National Academy of Sciences of the United States of America (*PNAS*, DOI: 10.1073/pnas.2100469118). In the article, the team presents a thermodynamic profile for the interactions of the ion channel's four subunits using an analysis method that can in principle be transferred to other membrane receptors.

A MULTIDIMENSIONAL VIEW OF THE CORONAVIRUS SARS-COV-2

What exactly happens when the coronavirus SARS-CoV-2 infects a cell? In an article published in Nature, a team led by Prof. Dr. Andreas Pichlmair from the Technical University of Munich (TUM) and the Max Planck Institute of Biochemistry paints a comprehensive picture of the viral infection process. For the first time, the interaction between the coronavirus SARS-CoV-2 and a cell is documented at five distinct proteomics levels. This knowledge will help to gain a better understanding of the virus and find potential starting points for therapies. Experimental data from mass spectrometry and extensive simulations on the Linux cluster at LRZ discovered 1,484 interactions between viral and human cell proteins. The result is a freely available database accessible at: (https://covinet.innatelab.virologie.med.tum.de/home). The paper was published in *Nature* (https://doi.org/10.1038/s41586-021-03493-4).

GERMAN AND RUSSIAN SCIENTISTS JOIN FORCES TO IMPROVE HPC PERFORMANCE TUNING

HPC is a key technology of the 21st century and performance measurements are of crucial importance to ensure the efficient usage of the computing power those systems provide. Unfortunately, many HPC systems expose their jobs to substantial amounts of interference (aka noise), leading to significant run-to-run variation. This makes performance measurements generally irreproducible. Thus, performance analysts usually have to repeat performance measurements several times and then apply statistical analysis to capture trends. This has a negative impact in terms of cost and time. This has become a major focus for Prof. Felix Wolf of TU Darmstadt, Dr. Bernd Mohr of JSC, and Drs. Dmitry Nikitenko and Konstantin Stefanov of Moscow State University, who are now addressing this problem in a joint project, named ExtraNoise. It is funded by Deutsche Forschungsgemeinschaft (DFG, German Research Foundation) and the Russian Foundation for Basic Research (RFBR). Moreover, Prof. Torsten Hoefler of ETH Zurich is contributing his expertise as an associated partner. In addition to making performance analysis more noise-resilient, the partners also aim to achieve a better understanding of how applications respond to noise in general and which design choices increase or lower their active and passive interference potential. The project, which will run for three years, is coordinated by TU Darmstadt.

HLRS COMPLETES DATA SECURITY ASSESSMENT

The University of Stuttgart has been registered on behalf of the High-Performance Computing Center Stuttgart (HLRS) as a participant in the Trusted Information Security Assessment Exchange (TISAX). By following this international standard for data security HLRS will ensure the protection of the data belonging to users of its computing systems. Governed by the ENX Association on behalf of the German Association of the Automotive Industry (VDA), TISAX prescribes a standardized set of strict requirements for the management of data centres that are intended to protect data confidentiality, data integrity, and data availability. Among the many facets of information security covered by TISAX, certification ensures that HLRS follows best practices in protecting physical access to its computing room, defining security responsibilities for technology providers and vendor staff, and implementing formal processes for managing security risks and information breaches. In addition, it details HLRS employees' responsibilities for data security, outlines relevant considerations in the procurement of new systems, and provides for formal review processes to guarantee that the centre is meeting all relevant legal requirements. Following registration with TISAX, HLRS's data security practices were assessed by an independent, accredited audit provider. Results are available on the ENX Portal.

FEDERAL ENVIRONMENT MINISTER SVENJA SCHULZE VISITS JSC

Svenja Schulze, the Federal Minister for the Environment, Nature Conservation and Nuclear Safety (BMU), visited Forschungszentrum Jülich as part of her summer tour. At the JSC, she learned about energy-efficient supercomputing and the use of AI for climate and environmental protection. The minister was welcomed by Jülich's new members of the Board of Directors, Dr. Astrid Lambrecht and Prof. Frauke Melchior. Afterwards, Dr. Scarlet Stadtler from JSC and her colleagues provided insights into the KI:STE project (AI Strategy for Earth System Data), which is funded by the BMU. The aim of the project is to use deep learning methods for the in-depth analysis of environmental data, for example to assess risks from natural hazards that are becoming increasingly frequent as a result of climate change. Prof. Thomas Lippert, Director of JSC, concluded by speaking about the ongoing activities on energy-efficient supercomputing at JSC, especially with regard to the development of future exascale systems.

WHEN THE FAST FOURIER TRANSFORMATION GETS TOO SLOW

The invention of the Fast Fourier Transformation (FFT) by Cooley and Tukey in 1965 accelerated many areas of computation, among them the Carr-Parinello Molecular Dynamics (CPMD). But with ever more processors, the communication between compute nodes has become the primary bottleneck. Tobias Klöffel, Bernd Meyer, and Gerald Mathias from the Friedrich-Alexander-Universität Erlangen-Nürnberg and LRZ, respectively, were able to multiply the performance of *ab initio* molecular dynamics on massively parallel multicore supercomputers like SuperMUC-NG at LRZ by integrating state-of-the-art compute, communication, and autotuning strategies. The new algorithms have been implemented in CPMD (www.cpmd.org) and the paper was published in *Computer Physics Communication* (https://doi.org/10.1016/j.cpc.2020.107745).

JOINT VIRTUAL LAB AIDAS IMPLEMENTED BY CEA AND FZJ

Forschungszentrum Jülich (FZJ) and the French Alternative Energies and Atomic Energy Commission (CEA) Paris are joining forces and will enhance their cooperation in the field of artificial intelligence, data analytics, and scalable simulation (AIDAS). To this end, François Jacq, General Administrator for CEA, and Prof. Wolfgang Marquardt, Chairman of the Board of Directors at FZJ, signed an Implementing Agreement on the Joint Virtual Lab AIDAS that runs until the end of 2024. AIDAS aims at advancing simulation in Europe by bringing together the partners' expertise in numerics with respect to AI, quantum computing, and HPC. So far, around 70 scientists are represented in AIDAS. The lab is led by Christophe Calvin and France Boillod-Cerneux from CEA and Prof. Thomas Lippert and Prof. Kristel Michielsen from the JSC. AIDAS is also intended to become a blueprint for further cooperation within the EU and to strengthen the potential and synergies of intra-European strategic partnerships.

ARM AND FORSCHUNGSZENTRUM JÜLICH SIGN MULTI-YEAR COLLABORATION AGREEMENT

Hardware provider Arm and the Forschungszentrum Jülich signed a multi-year cooperation agreement. Its goal is to strengthen their joint effort in identifying the requirements of HPC applications and advancing their porting and optimization on Arm-based architectures. The collaboration of Arm with the JSC focuses on the analysis and optimization of strategic HPC applications on Arm-based HPC systems, including Arm accelerated platforms (for example, Arm+GPU). The joint team carries on performance analysis and code engineering, taking advantage of specific features of Arm-based hardware to further advance application performance. The code requirements identified in this effort will help in the design of future HPC technologies and systems.

GOLDEN SPIKE AWARDS PRESENTED AT HLRS'S 24TH ANNUAL RESULTS AND REVIEW WORKSHOP

On October 7–8, scientific users of HLRS's HPC systems gathered virtually to present their latest results and discuss their experiences and lessons learned in optimizing the performance and scalability of their codes. The online event featured scientific talks and a virtual poster session. At the conclusion of the workshop, Prof. Dr. Dietmar Kröner and members of the HLRS steering committee presented the annual Golden Spike Awards to three investigators whose presentations demonstrated excellence in the application of high-performance computing. The awardees included Markus Scherer of the Karlsruhe Institute of Technology for his presentation, "Secondary flow and longitudinal sediment patterns in turbulent channel flow over a bed of mobile particles in domains of small to intermediate size"; Jakob Dürrwächter of the University of Stuttgart for his presentation, "Uncertainty quantification in high order computational fluid dynamics"; and Daniel Mohler of the GSI Helmholtzzentrum für Schwerionenforschung GmbH for his presentation, "Hadronic contributions to the anomalous magnetic moment of the muon from lattice QCD."

STAFF SPOTLIGHT: YEARS AT HLRS SET THE STAGE FOR TRANSITION TO UNIVERSITY OF TENNESSEE INNOVATIVE COMPUTING LABORATORY

Dr. Joseph Schuchart, HLRS

Ever since he was 10 years old, Dr. Joseph Schuchart has been fascinated by computers. Specifically, he has been drawn to understanding how computers work at a fundamental level, and began learning programming languages and fiddling with the family PC through command lines in his early teens.

Such purebred passion does not always translate to a clear career path, though, and entering college at the Technical University of Ilmenau (TU Ilmenau), Schuchart convinced himself that he should study electrical engineering. However, Schuchart quickly came to realize that this passion could and should play a central role in shaping his professional future.

"After one year, I decided to change my major to computer science at the Technische Universität Dresden—I find the field fascinating because you can build such complex systems basically out of nothing. Computer science allowed me to really focus on learning how to get these systems working efficiently," Schuchart said.

After changing his academic focus, Schuchart began working as a student assistant for TU Dresden Professor Dr. Wolfgang Nagel, head of the Center for Information Services and High-Perfomance Computing (ZIH) at the university. During this period, Schuchart's general interest in computer science further sharpened into a focus on improving efficiency for computational science applications. When he finished his master's degree, his interest in tools for improving efficiency and performance led to a desire to do so on the largest computing resources available. He earned an opportunity in 2012 to work at Oak Ridge National Laboratory (ORNL) in the United States. At the time, ORNL was transitioning between having one of the prior fastest supercomputing resources in the world, the Jaguar Supercomputer, to building its next world-leading system, one that would also herald the beginning of using GPU accelerators in large-scale HPC systems.

While his time at ORNL was enriching, Schuchart ultimately decided to return to Dresden and began working in projects concerning energy efficiency. In 2016, he learned about an open position with the Dash project at the High-Performance Computer Center Stuttgart (HLRS), and jumped at the opportunity. "I really came for the project, which was focused on task-based programming, because that fit perfectly with what I wanted to do—finding ways to create and handle a lot of concurrency and parallelism in applications. In my opinion, that is really at the heart of doing HPC," he said.

Not only did his transition to HLRS get him more closely aligned with his professional passions, it also offered him the opportunity to get more deeply involved in the specific communities where he could deepen his knowledge of the field. With the encouragement of Dr. Rolf Rabenseifner, Head of HLRS's Training and Application Services group, Schuchart got more involved in the MPI forum, a group dedicated to developing the Message Passing Interface, a software standard used worldwide to parallelize codes running across many different compute nodes—a key component to making efficient use of large HPC systems.

Ultimately, Schuchart got his PhD at the University of Stuttgart under the tutelage of HLRS Director Prof. Dr. Michael Resch and Dr. José Gracia, Head of HLRS's Scalable Programming Models and Tools group. He focused specifically on distributed task-based runtime systems, which seek to find efficient methods to coordinate millions of individual tasks and calculations across a large amount of computer nodes. This work wound up pairing extremely well with a research group in familiar surroundings: the University of Tennessee's Innovative Computing Laboratory (ICL), which has close connections to and is roughly 40 km away from Schuchart's prior position at ORNL. In 2020, Schuchart accepted a post-doctoral research position at ICL, hoping to bring his experiences at HLRS into a team that has been focused on similar goals from a different perspective. "I'm merging into the existing world that has already been here," he said. "There is learning potential on both sides, which is nice, and I'm definitely learning a lot, and I hope to contribute something to the efforts already going on here."

Schuchart indicated that his experiences at HLRS and TU Dresden prepared him to join the team at ICL at a time of transition and evolution for the field of HPC, and that his dynamic experiences provide a solid foundation for working in a quickly changing field. Based on his own experiences, Schuchart advised those just beginning to study computer science to be flexible, curious, and willing to explore different avenues and niches within the field.

"For anyone just coming into the field, you have to have a broad view on computer science," he said. "You have to look into AI and machine learning, you should look into quantum computing because of its potential. But most importantly, you have to have a solid, theoretical background in numerics and programming models—the theoretical side of computer science, so thinking about the design of languages to be more efficient in how we're using the systems that we have." *eg*

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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

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 cooperation with neighbouring universities.

JSC's Modular Supercomputer "JUWELS", Booster on the left, Cluster on the right hand side. **© Forschungszentrum Jülich**

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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 Research 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

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.

www.gauss-centre.eu

Cover image: During the bi-annual LRZ Status and Results workshop, Prof. Dr. Volker Springel (Max Planck Institute for Astrophysics) described how his team used sophisticated modeling techniques to track a trillion particles to simulate the distribution of matter in the universe. For more information, visit page 31. © The TNG Collaboration

GCS
Gauss Centre for Supercomputing

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MINISTRY OF SCIENCE, RESEARCH AND ARTS

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