HPC BACKS HEALTHCARE
Medical Solution Center will bring supercomputing to medical technology industry.

EARLIER WARNINGS
Researchers uncover innovative ways to assess risks for two of the Earth’s most destructive disasters: earthquakes and tsunamis.

QUANTUM LEAP FORWARD
In a partnership with D-Wave Systems, JSC welcomes Europe’s largest quantum computer to date.
Welcome!

Welcome to the latest issue of InSiDE, the bi-annual Gauss Centre for Supercomputing magazine showcasing innovative supercomputing developments in Germany. Our spirits and those of our staffs have been buoyed by a partial return to some in-person events, even with additional safety measures in place. We remain hopeful that the pandemic has finally slowed some, but are still actively working with partners in academia and government to develop therapeutics and track outbreaks using our HPC resources.

While our resources have always primarily been used to accelerate discovery and solve problems surrounding humanity’s most pressing and challenging problems, the latest issue of InSiDE showcases some of the science and partnerships focused on urgent computing responses to societal health and safety needs. More specifically, some of the research highlights showcase how research teams are leveraging our resources to address water issues. Researchers at the Karlsruhe Institute of Technology have been using the High-Performance Computing Center Stuttgart’s (HLRS’s) HPC resources to study how pollutants sink to the surfaces of rivers, are buried by sediment, and then can reappear after being set in motion by fluid flows (Page 18). A long-time collaboration at the Ludwig-Maximilians Universität München and Technical University of Munich used resources at the Leibniz Supercomputing Centre (LRZ) to identify three traits that can unleash devastating tsunamis after an earthquake occurs (Page 14). Researchers at the Jülich Supercomputing Centre (JSC) jumped into action after a volcano eruption in Tonga to assist atmospheric scientists in understanding the eruption’s implications (Page 33).

In the last year, our centers’ staffs have not only been focused on ensuring that today’s leading HPC technologies are available for researchers, but also have been actively co-designing, installing, and evaluating next-generation computing technologies. Our centres have long been the natural computational test beds of German and European researchers, and our staffs have eagerly embraced better understanding and scaling artificial intelligence and quantum computing capabilities at our centres. As part of its JUNIQ user facility, JSC welcomed the D-Wave Advantage™ quantum computer, the first in Europe with 5,000 Qubits (Page 6). LRZ started 8 new projects in the last year connected to its Quantum Integration Centre (Page 9). HLRS, in partnership with the University of Stuttgart, is participating in the IKILeUS project to not only strengthen education on artificial intelligence, but also develop and evaluate AI-based teaching methods (Page 28).

Our centers staffs are at home at the cutting edge of computing technologies, and we will continue to ensure that our centers can provide researchers around Europe the best possible tools to keep our citizens safe and healthy.

Prof. Dieter Kranzlmüller
Prof. Thomas Lippert
Prof. Michael Resch
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Quantum computers can help solve complex optimization problems. The D-Wave Advantage™ System, JUPSI, at Forschungszentrum Jülich can be used to optimize flight schedules, among countless other data-intensive applications.

**JSC Inaugurates Europe’s First Quantum Computer with More Than 5,000 Qubits**

The first D-Wave Advantage™ system built outside of North America comes out of an 8-year collaboration between D-Wave Systems and the Jülich Supercomputing Centre.

On Monday, January 17, the Jülich Supercomputing Centre (JSC) inaugurated a D-Wave Advantage™ Quantum Annealer. JSC and D-Wave Systems also launched the company’s first cloud-based quantum service outside of North America. Taken together, these developments represent a major milestone in the European Union’s burgeoning interest in quantum computing, a complementary computing technology to traditional high-performance computing (HPC) that shows promise in more efficiently addressing challenges currently too time-consuming or difficult for traditional computers. The inauguration was attended by Federal Minister of Education and Research Bettina Stark-Watzinger, Minister-President of North Rhine-Westphalia Hendrik Wüst, and European Commissioner Mariya Gabriel.

The machine serves as the cornerstone of the Jülich Unified Infrastructure for Quantum computing (JUNIQ), Forschungzentrum Jülich’s newest user facility. JUNIQ was started in 2019 to facilitate quantum computing access for European researchers and will serve as the quantum computing component of JSC’s modular supercomputing concept, which provides access to a variety of tightly connected high-end computing architectures.

“We operate the system directly here at Jülich. This gives us the opportunity to integrate it closely with our supercomputing infrastructure,” said Prof. Kristel Michielsen, Head of Forschungzentrum Jülich’s Quantum Information Processing Group.

While the D-Wave Advantage™ system – the largest commercially available quantum computing system to date – serves as the flagship machine for JUNIQ, JSC staff have focused on ensuring that JUNIQ would give users the opportunity to evaluate different quantum computer designs and concepts. JSC is participating in a project newly funded by the German Federal Ministry for Education and Research (BMBF) called QSolid, where JSC will build its own quantum computer prototype using superconducting qubits as the processors. Michielsen is also leading a EuroHPC Joint Undertaking project called HPCQS in which JSC staff will evaluate quantum computer architectures and then integrate a system into its JUWELS modular supercomputer, test it in use cases, and provide training material. To learn more about the HPCQS project, visit page 25.

“arly as possible, and with a variety of systems, because they all have different characteristics and don’t always behave as theory would expect them to,” Michielsen said. “One really needs the practical experience to learn how to use these systems. The other main task for JUNIQ is to look for the benefit of quantum computing, and for that, it is important to do cross-platform benchmarking. For that kind of work, you have to have an environment like JUNIQ, because scientists cannot practically be expected to go through all the administrative hurdles that would come with gaining access to these machines independently of one another.”

According to Prof. Thomas Lippert, Director of JSC, integrating quantum computing resources of this scale into an HPC facility is a novel concept, but a logical one.
"We’re also looking at ways to integrate the new system into our supercomputing infrastructure. To the best of our knowledge, this would be the first instance of a quantum computer working directly with a supercomputer,” he said.

“This is made possible because the quantum annealer has over 5,000 qubits and is therefore big enough to help with application-related problems that are typically calculated on supercomputers.”

For D-Wave Systems, one of the world’s largest companies focused purely on quantum computers, the partnership developed through JUNIQ represented the natural evolution the company sees for its products and the growth of quantum computing generally.

“Given the extent to which companies and research institutions are identifying important problems that require investments in quantum computing, the marketing potential for quantum computing will grow at a faster rate than ever before,” said Alan Baratz, CEO at D-Wave Systems. “This particularly applies to Europe, where we are seeing increasing interest from companies, universities, and even government institutions. We look forward to combining Jülich’s expertise in the field of deep computing with D-Wave’s ability to scale and commercialize transformative technologies. I am proud that this is the first commercial quantum computing system in-region in Europe, deepening the impact of quantum computing in Europe, and am excited about the innovations and applications that will emerge from the system.”

Eric Gedenk

Quotes from the event originally appeared in a press release released by Forschungszentrum Jülich. You can read the original here: https://go.fzj.de/2022-01-17-juniq-pm

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"A change in mindset is needed to move away from hardware-oriented ways of thinking."

Prof. Dr. Martin Haimerl

The vibrant medical technology community develops and tests electronic instruments, surgical tools, implants, and pharmaceuticals.

and tests electronic instruments, surgical tools, implants, and pharmaceuticals. The Solution Center model was also adapted in 2018 with the founding of the Media Solution Center Baden-Württemberg, which is facilitating new forms of artistic production by connecting cultural and media organizations from across Europe with supercomputing resources and expertise at HLRS.

The new Medical Solution Center will build a network that includes stakeholders from Baden-Württemberg’s medical technology community and experts in the development of IT-based and data-driven approaches for medical applications. Through meetings and other outreach activities, participants will determine what kinds of HPC-based solutions could most benefit the community and what resources and skills would be necessary to make them a reality. By cultivating contacts and completing pilot projects demonstrating relevant applications of simulation, data analytics, and artificial intelligence, the Medical Solution Center aims to grow steadily and to become a self-sustaining membership organization by the end of the grant period.

Prof. Dr. Martin Haimerl, Scientific Director of the Innovation and Research Center Tüttlingen, has worked closely with the local medical technology community and foresees great potential in the Medical Solution Center. “In the medical technology sector, use of simulation and high-performance computing is uncommon and will need to be built up in a systematic way,” he explained. “A change in mindset is needed to move away from hardware-oriented ways of thinking towards an openness to and familiarity with the use of supercomputing, including machine learning and data-driven approaches. The collaborative network that the Medical Solution Center plans to build could take medical technology across the state to a new level.”

Christopher Williams

The Medical Solution Center will also profit from the expertise of SICOS BW, a nonprofit organization cofounded by the University of Stuttgart and the Karlsruhe Institute of Technology that facilitates access to high-performance computing for small and medium-sized companies. “We are looking forward to sharing our experience in developing solution centers. The medical field is challenging and promising at the same time, and we see great potential for the companies to make beneficial use of HPC and data analytics!” said Dr. Andreas Wierse, managing director of SICOS BW GmbH.

Many applications of simulation and data analytics

As in other engineering fields, simulation could offer medical device companies tools that make the development and testing of new products faster and less expensive. Simulation could be used, for example, to assess the suitability of materials or components for medical instruments and implants. It could help optimize the design of electronic and software components in medical instruments, evaluate the effectiveness of production, improve quality control processes, for example, or support data-driven processes for the development of new products or business models. Such methods could revolutionize the way medical procedures are implemented and controlled.

One additional important use of HPC could be in helping medical technology companies to address Medical Device Regulation (MDR) requirements. Before a new medical device or therapy can be used in patients, companies must demonstrate that it is safe and effective, a process that is typically complicated and expensive. Although simulation and other data-based approaches alone are unlikely to eliminate the need for actual clinical trials, they can help to provide earlier insights and stronger evidence about a medical product’s quality and benefit for patients.

HLRS Director Prof. Dr. Michael Resch welcomed the beginning of the Medical Solution Center project, saying, “Since its founding, a key component of HLRS’s activities includes supporting the small and medium-sized enterprises that play such an important role in Baden-Württemberg’s economy. We have worked towards bringing medical applications to HPC for long time and are very excited for this chance to become more engaged with this community, especially because the outcomes of this collaboration could demonstrate new ways in which high-performance computing can help to improve human health.”

Christopher Williams
Bringing Quantum Computing to Scientists’ Work

Science and research are counting on the integration of diverse technologies and on hybrid computing for the future.

The course for the future has been set: “In quantum computing, we are involved in eight projects to research the new processors, develop software stacks and programming environments, and ultimately integrate quantum computing into supercomputing,” says Prof. Dr. Dieter Kranzlmüller, Director of the Leibniz Supercomputing Centre (LRZ). “The practical handling of this technology will be exciting and offers many challenges for research and development.”

In the future, growing volumes of data will continue to be analyzed in real time, if possible, and high-performance computing (HPC) will need new concepts to increase computing power and accelerate computing for greater energy efficiency. “Quantum computing could become a next development step for high-performance computing,” envisions Dr. Martin Schulz, Professor of Computer Science at the Technical University of Munich (TUM) and member of the Board of Directors at the LRZ. “The integration of quantum into supercomputers, as well as the interplay of HPC, artificial intelligence, and quantum could provide the necessary performance boost.”

Quantum as a service for research

Quantum computing is currently electrifying politics and research. As scientists and entrepreneurs come up with better methods for data analysis, politicians in Europe and Germany are hoping to catch up again in information technology and reach “digital sovereignty.” Billions of Euro are currently flowing into research aimed at bringing this technology to market maturity and faster commercial use in the next few years.

As institutes of the Bavarian Academy of Sciences and Humanities (BADW), LRZ, and the Walther-Meißner-Institut (WMI) have co-founded the Munich Quantum Valley (MQV) with Munich’s universities, research institutions, and technology providers. In addition, the computing center has started working in eight research projects throughout the last year and is now bundling its tasks in the Quantum Integration Centre (QIC). “As with all technologies, LRZ is also concerned with providing reliable IT services for science and research in quantum computing. Supercomputers are severely challenged when processing the largest volumes of data, so we will integrate quantum processors and quantum components into our high-performance systems, explore how they work and develop more services,” says Kranzlmüller.

Even though they have already left the experimental stage, quantum computers still operate largely under laboratory conditions. To stabilize and control quantum bits – the smallest computational units, also called qubits – it is necessary to avoid disturbances. Such as temperature fluctuations, vibrations, or light pollution. Computing centers, and supercomputing centers in particular, bring the technology to users as quantum-as-a-service. Only when this quantum machine can be used to develop the first codes and interfaces via which binary chips work together with universal quantum computers – the basis for all further developments.

“Scientists need programming models,” Kranzlmüller adds. “They need software stacks, access mechanisms via web or cloud portals. And above all, they need support to optimize their scientific and industrial problems on super and quantum computers.”

Prof. Dieter Kranzlmüller (left), Director of LRZ, with Dr. Jan Goetz (right), CEO of IQM at the signing of Q-EXA contract.

Through supercomputers into broader use

Operating systems and tools are consequently the focus of LRZ’s projects. Within the Munich Quantum Valley, LRZ staff members are planning a Munich Software Stack for quantum computers – the basis for all further developments. But first, efforts are focused on embedding a quantum processor into the LRZ supercomputer. For the project “Quantum Computer Extension through Exascale HPC,” or Q-Exa for short, LRZ has purchased a large quantum system from the German-Finnish company IQM in November 2021 with funding from the German Federal Ministry of Education and Research. The processor will have 20 qubits, based on superconducting metals and cooled to negative 273 degrees by a cryostat. “Q-Exa is a key project for our activities in the QIC and within the Munich Quantum Valley,” Kranzlmüller says. “By working together in this highly competitive consortium, we can set European standards that are also globally competitive.”

Even though the processor is still being developed, the quantum specialists at LRZ are already planning how the computer will be connected to HPC resources. The Quantum Learning Machine (QLM) – by French technology company Atos – offers useful help. Not only can researchers use it to develop quantum algorithms and process simulation data, this quantum simulator can also be used to develop the first codes and interfaces via which binary chips work together with universal quantum computers – the basis for all further developments.

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Susanne Vieser
Years-Long Collaboration Helps Geophysicists Better Understand Severe Earthquake-Tsunami Risks

Researchers at Ludwig-Maximilians-Universität München and their partners at the Technical University of Munich have developed innovative ways to assess risk for two of the Earth’s most destructive disasters.

For nearly a decade, researchers at the Ludwig-Maximilians-Universität (LMU) München and the Technical University of Munich (TUM) have fostered a healthy collaboration between geophysicists and computer scientists to try and solve one of humanity's most terrifying problems. Despite advancements over the recent decades, researchers are still largely unable to forecast when and where earthquakes might strike.

Under the right circumstances, a violent couple of minutes of shaking can portend an even greater threat to follow – certain kinds of earthquakes under the ocean floor can rapidly displace massive amounts of water, creating colossal tsunamis that can, in some cases, arrive only minutes after the earthquake itself is finished causing havoc.

Extremely violent earthquakes do not always cause tsunamis, though. And relatively mild earthquakes still have the potential to trigger dangerous tsunami conditions. LMU geophysicists are determined to help protect vulnerable coastal populations by better understanding the fundamental dynamics that lead to these events, but recognize that data from ocean, land, and atmospheric sensors are insufficient for painting the whole picture. As a result, the team in 2014 turned to using modelling and simulation to better understand these events. Specifically, it started using high-performance computing (HPC) resources at the Leibniz Supercomputing Centre (LRZ), one of the 3 centers that comprise the Gauss Centre for Supercomputing (GCS).

"The growth of HPC hardware made this work possible in the first place," said Prof. Dr. Alice-Agnes Gabriel, Professor at LMU and researcher on the project. "We need to understand the fundamentals of how megathrust fault systems work, because it will help us assess subduction zone hazards. It is unclear which geological faults can actually produce magnitude 8 and above earthquakes, and also which have the greatest risk for producing a tsunami."

Through years of computational work at LRZ, the team has developed high-resolution simulations of prior violent earthquake-tsunami events. Integrating many different kinds of observational data, LMU researchers have now identified three major characteristics that play a significant role in determining an earthquake's potential to stoke a tsunami – stress along the fault line, rock rigidity and the strength of sediment layers. The LMU team recently published its results in Nature Geoscience.

Lessons from the past

The team's prior work has modelled past earthquake-tsunami events in order to test whether simulations are capable of recreating conditions that actually occurred. The team has spent a lot of effort modelling the 2004 Sumatra-Andaman earthquake – one of the most violent natural disasters ever recorded, consisting of a magnitude 9 earthquake and tsunami waves that reached over 30 meters high. The disaster killed almost a quarter of a million people, and caused billions in economic damages.

Simulating such a fast-moving, complex event requires massive computational muscle. Researchers must divide the area of study into a fine-grained computational grid where they solve equations to determine the physical behaviour of...
“The computer science achievements are essential for us to do advance computational geophysics and earthquake science...”

Dr. Alice-Agnes Gabriel

The computer science achievements are essential for us to do advance computational geophysics and earthquake science...”

Dr. Alice-Agnes Gabriel

water or ground (or both) in each space, then move their calculation forward in time very slowly so they can observe how and when changes occur.

Despite being at the cutting edge of computational modelling efforts, the team used the vast majority of SuperMUC Phase 2 in 2017, at the time LRZ’s flagship supercomputer, and was only able to model a single earthquake simulation at high resolution. During this period, the group’s collaboration with computer scientists at TUM led to developing a “local time-stepping” method, which essentially allows the researchers to focus time-intensive calculations on the regions that are rapidly changing, while skipping over areas where things are not changing throughout the simulation. By incorporating this local time-stepping method, the team was able to run its Sumatra-Andaman quake simulation in 14 hours rather than the 8 days it took beforehand.

The team continued to refine its code to run more efficiently, improving input/output methods and inter-node communications. LRZ installed in 2018 its next-generation SuperMUC-NG system, significantly more powerful than the prior generation. The result? The team was able to not only unify the earthquake simulation itself with tectonic plate movements and the physical laws of how rocks break and slide, but also realistically simulate the tsunami wave growth and propagation as well. Gabriel pointed out that none of these simulations would be possible without access to HPC resources like those at LRZ.

“IT is really hardware aware optimization we are utilizing,” she said. “The computer science achievements are essential for us to do advanced computational geophysics and earthquake science, which is increasingly data-rich but remains model-poor. With further optimization and hardware advancements, we can perform as many of these scenarios as needed to allow sensitivity analysis to figure out which initial conditions are most meaningful to understand large earthquakes.”

After having its simulation data, the researchers set to work understanding what characteristics seemed to play the largest role in determining both an earthquake’s strength and its propensity for causing a large tsunami, the team has helped bring HPC into scientists’ and government officials’ playbook for tracking, mitigating, and preparing for earthquake and tsunami disasters moving forward.

Urgent computing in the HPC era

Gabriel indicated that the team’s computational advancements fall squarely in line with an emerging sense within the HPC community that these world-class resources need to be available in a “rapid response” fashion during disaster or emergencies. Due to its long-running collaboration with LRZ, the team was able to quickly model the 2018 Palu earthquake and tsunami near Sulawesi, Indonesia – an event that caused more than 4,000 fatalities – and provide insights into what happened.

“We need to understand the fundamentals of how submerged fault systems work, as it will help us assess their earthquake risks as well as cascading secondary hazards. Specifically, the deadly consequences of the Palu earthquake came as a complete surprise to scientists,” Gabriel said. “We have to have physics-based HPC models for rapid-response computing, so we can quickly respond after hazardous events. When we modelled the Palu earthquake, we had the first data-fused models ready to try and explain what happened in a couple of weeks. If scientists know which geological structures may cause geohazards, we could trust some of these models informing hazard assessment and operational hazard mitigation.”

In addition to being able to run many permutations of the same scenario with slightly different inputs, the team is also focused on leveraging new artificial intelligence and machine learning methods to help comb through the massive amounts of data generated during the team’s simulations in order help clean up less-relevant and possibly distracting data that comes from the team’s simulations.

The team is also participating in the ChEESE project, a European-Union-funded initiative aimed at preparing mature HPC codes for exascale systems, or next-generation systems capable of one billion billion calculations per second, or more than twice as fast as today’s most powerful supercomputer, the Fugaku system in Japan.

Eric Gedenk


Simulated seismic waves from a multi-physics simulation of the 2004 Indian Ocean earthquake.
Simulations of Sediment Movement Could Help Protect Waterways

Researchers at the Karlsruhe Institute of Technology (KIT) are using high-performance computing to model how waterways’ sediment beds change and what those changes mean for pollutants moving downstream.

While conservation efforts and environmental regulations have played an important role in limiting damage to our lakes and rivers, human pollution and natural disasters are still capable of wreaking havoc. Recognizing this risk, the Baden-Württemberg Stiftung in 2017 funded an expansive, multidisciplinary project aimed at better understanding how water quality is affected when pollution enters a river or stream.

The effort brings together environmental scientists, biologists, civil engineers, and chemical engineers, among others, combining high-performance computing (HPC) simulation with experimental techniques. Among the team members is a group of researchers from the Karlsruhe Institute of Technology (KIT) who are using HPC resources at the High-Performance Computing Center Stuttgart (HLRS) to do complex multiphase turbulent flow simulations of how solid pollutants settle on a river bed. This work is helping to better understand how these pollutants become buried or actively move and spread.

“If you think about a canal or a river, you always have sediment, which might act in your benefit or not,” said KIT Professor Dr. Markus Uhlmann, principal investigator on the project. “Sediment could be good in the sense that it helps support the foundation of a bridge pier, or it can contain pollutants that can be carried downstream. To predict and control the spread of pollution it is important to know if particles are going to move and your bed is going to be eroded.”

Using HLRS’s Hawk supercomputer, the team conducted the first ab initio simulation — calculations that start from first principles — of the sediment pattern on a riverbed while also simulating settling contaminant particles from above, publishing its results in the Journal of Fluid Mechanics. The work also resulted in team member Markus Scherer being awarded HLRS’s Golden Spike Award at the center’s October 2021 Results and Review workshop.

Rolling on the river

When modelling how pollutants disperse in rivers and other waterways, scientists rely on supercomputers like Hawk to better understand the chaotic, turbulent motions in fluid flows. In such studies, researchers do computationally expensive direct numerical simulations (DNS) that divide the fluid in question into a fine, three-dimensional grid — also called a computational mesh — and then solve equations in each grid box that represent changes in fluid motion over time.

Simulating turbulent fluid motion by itself is a significant challenge, but in order to understand how pollutant particles spread in a waterway, researchers must do DNS calculations of so-called multiphase flows. These simulations also account for the ability of particles to influence and modify fluid flows. Although this approach results in a more realistic model, it also significantly increases the computational demands.

Solid particles also add another complication to the research: the team must model how particles disperse as they float toward the bottom of a river bed. This is not a trivial issue, as particles do not permanently stay where they land on the stream bottom. Because of water currents, the bottom of a river or stream is always in motion. When a pollutant first enters a waterway, this can actually be advantageous; the particles fall to the bottom of the river and can be buried by moving sediment. Unfortunately, over a longer period, the opposite is true: pollutants that were buried and forgotten can be re-released during flooding events as sediment is pushed downstream, allowing it to spread once again.

Predicting the cycle in which pollutants are buried and resurface is further complicated by the uneven nature of sediment motion. Grains of sand, pulverized stones, and other microscopic debris that form the sediment bed will often form “ridges,” creating an uneven distribution that further influences water flow and, in turn, how sediment moves downstream.

“The main thing we are interested in is the effect of different patterns in the sediment,” said Michael Krayes, a KIT researcher and collaborator on the project. “We started with simulations of these dune-like features, what we call ripples—they propagate with the current flow and propagate while moving from side to side, which is generally good for burying things, but the meandering ridges that form are much less effective at doing so. When charting pollutants’ movements, it makes a big difference what kind of pattern you have.”

“When it comes to these sediment ridges, they are closely related to very complex turbulent structures,” said Markus Scherer, KIT researcher and another collaborator on the project. “When modelling these interactions, you have to ask if you’ve captured everything, or do what we do — resolve all scales and see what is most relevant for studying the changes and movement of sediment ridges. This can be used, of course, for computational models that can run on more modest computing resources and be performed quicker in the event of an environmental emergency.”

Many rivers to cross

With access to HLRS resources, the team has made significant progress in better understanding pollutant transport in waterways, although they know more work needs to be done. Uhlmann indicated that the team does not necessarily need to run a larger or higher-resolution version of its model, although in the future it would benefit from the ability to run “parameter sweeps.” Here, the team could make single modifications in the simulations and watch how they impact the entire system.
Aided by HPC, Researchers Aim to Carve Out New Treatment Methods to Selectively Interfere with mRNA

Scientists and public health officials want to better understand how to modify genetic building blocks to target the diseases that manipulate and hijack them. Using a combination of simulation and experiment, a multidisciplinary team is getting closer to that goal.

A s humanity fights against emergent illnesses and a host of difficult-to-cure, long-familiar diseases, scientists have started to focus research efforts on fundamentally new methods of combating diseases. Specifically, scientists are looking at ways to use specific chunks of deoxyribonucleic acid (DNA), the class of molecule that houses the genetic information central to all living things’ development, to selectively break down mutated or overly abundant pieces of ribonucleic acid (RNA). With more research, scientists hope these so-called DNAzymes could provide successful therapies for a host of illnesses.

During the COVID-19 pandemic, pharmaceutical companies threw their efforts behind developing new vaccines that would use slices of a virus’s genetic code to engage our immune system rather than weakened versions of the virus itself. These next-generation vaccines exemplify a pivot happening in multiple areas of healthcare research — using genetic building blocks to fight back against difficult diseases or generally improve health outcomes.

“Ultimately, our work in this area is similar to other biomedical work — the goal is, in part, to find new ways to optimize biological systems so that they perform better,” said Prof. Holger Gohlke, researcher at Heinrich Heine University in Düsseldorf and Forschungszentrum Jülich. Gohlke serves as principal investigator on a project that uses high-performance computing (HPC) resources at the Jülich Supercomputing Centre (JSC) in his team’s efforts to interfere with one of our body’s primary messaging services — RNA — in fighting against diseases that hijack, manipulate, or impersonate RNA.

Many viruses, for instance, are based on a sequence of RNA. Normally, RNA molecules fulfill a plethora of functions within cells, including taking on information for protein synthesis from DNA.

Masking its RNA, a virus like SARS-CoV-2 or those causing the common cold can enter the cell and hijack its normal functions, co-opting them to create more viral RNA strands. While its origins are still mysterious, cancers seem to also develop when contributions by RNA viruses are possible, cancers also develop when corrupted or overly abundant proteins are synthesized based on damaged or corrupted genetic material.

Gohlke and his collaborators are using a combination of experimental techniques and HPC simulations to understand how to cause a DNAzyme-catalyzed reaction that could selectively cleave the “unhealthy” RNA within human cells. While the method is still in its early stages, the team has focused its studies on this particular class of molecules as it expects it to play a central role.

Carving out a path toward precision therapeutics

DNAzymes are small, specific chunks of a DNA sequence that can be used in a catalytic reaction within a cell — essentially, DNAzymes can trigger certain molecular behaviours within a cell without radically altering them—
selves in the process. While they have not been observed in nature, scientists first identified them via experiment in the 1990s and have been researching how certain DNA-zyme sequences might provide new methods for fighting off difficult-to-cure, or even incurable, diseases.

For this process to work, though, researchers have to get a fundamental understanding of the mechanism through which DNAzymes cleave RNA and what role other cellular components, chief among them metal ions, play before they can design effective therapies. While experimental research helps scientists better understand how DNAzymes interact with other molecules, the size and speed at which these interactions take place leave researchers with only a limited view of these interactions.

In order to observe how molecules’ atomic components interact with one another, researchers have turned to HPC for computationally demanding molecular dynamics (MD) simulations. MD simulations allow scientists to model individual atoms and their movements over time to see these interactions play out in sub-nanometer, sub-nanosecond detail. Seeing a large-enough system over a meaningful amount of time would take months or years on a normal computer, and considering that the researchers have many permutations of atomic arrangements to model, they need access to HPC.

“We needed to represent DNAzymes’ interactions, focusing on their interactions with metal ions specifically. When dealing with DNA, you also need a good representation of solvent effects. On top of that, we also needed to represent the interactions between and within the DNA and RNA correctly,” Gohlke said. “At the same time, we needed to be able to deal with a sufficient amount of systems, because from the experimental work, there were four different structures that the DNAzyme we are studying could have, and we needed to test all of these against four different concentrations of metal ions.”

Gohlke, who has a joint appointment at Forschungszentrum Jülich, the parent organization of JSC, was able to gain access to the JUWELS Booster module — currently Europe’s fastest computer — to run the team’s MD simulations. Using an iterative approach between simulation and experiment, the team was able to specifically replace an atom in the system to yield higher cleavage activity. This result shows that the team’s simulation work accurately represented experiments, ultimately helping expand the team’s knowledge of how to further experiment for developing novel DNAzymes as possible treatment options. The team published its results in Nature.

**HPC as a trailblazing technology for next-generation healthcare**

Gohlke was an early adopter of using GPUs to accelerate his biomedical research, beginning to use the accelerators around 2010 when they began being adopted by HPC centers as a way of improving HPC systems’ peak performance. As a result, the team was able to very efficiently use the GPU-accelerated JUWELS Booster. “I think we are easy customers,” Gohlke said. “The Amber code that we use for our simulations was co-developed with NVIDIA, and that makes it very efficient for running on GPUs and the setup and installation is straightforward. We do get strong support from the JSC Biology Simlab, and they are always there for us helping to install new Amber versions on the machine.”

With the team’s newly gained foundational knowledge of DNAzymes and how they interact with molecules, Gohlke feels confident that the team, and indeed researchers focused on exploring these new therapies generally, will be able to move closer to using DNAzymes to help patients in the years to come. “I think it is important to stress that, if successful, this would provide a new means for a very targeted type of therapy for cancer,” he said. “You would be able to remove proteins that carry a wrong mutation or appear too abundantly. These things still have to be demonstrated experimentally, but that is the vision.”

Eric Gedenk

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Average structure of the DNAzyme (red) wrapped around the RNA (black) from molecular dynamics (MD) simulations overlaid with the structural ensemble generated from the MD trajectory. The MD-derived picture suggests that the DNAzyme shows increased conformational plasticity in the catalylic-loop region compared to the binding arm and, particularly, the cleavage-site region.

Figure adapted from work that appeared in Nature (Borggräfe et al. DOI: https://doi.org/10.1038/s41586-021-04225-4).
JSC Plays an Active Role in Several EU-Funded Pilot Projects Connected to Emerging Technologies

Last year, the European High-Performance Computing Joint Undertaking (EuroHPC JU) issued a call for proposals with two topics: “Advanced pilots towards the European exascale supercomputers” and “Pilot on quantum simulator.” Only three proposals in this call have been chosen to be funded as pilot projects: EUPILOT (The European PILOT: Pilot using Independent Local and Open Technologies), EUPEX (European Pilot for Exascale), and HPCQS (High Performance Computer and Quantum Simulator hybrid).

The projects are funded in equal parts by EuroHPC JU and the participating member states, which in case of Germany is by the German Federal Ministry of Education and Research (BMBF). The Jülich Supercomputing Centre (JSC) is proud to be a partner of all three projects and also takes on a leading role as coordinator of the HPCQS project. While EUPILOT and EUPEX will integrate the two processor technologies built in the European Processor Initiative (EPI) project (an accelerator and general-purpose processor, respectively), HPCQS is devoted to the integration of a quantum computer into an HPC system. The experiences in these three pilots will be very valuable for the next-generation HPC and artificial intelligence (AI) infrastructures in Europe. EUPILOT and HPCQS were launched on 1 December 2021, while EUPEX was launched on January 1, 2022.

The project EUPILOT focuses on creating demonstrators using open-standard-based RISC-V accelerators. The project is the first example of a pilot HPC ecosystem designed and manufactured entirely in Europe and is aimed at power-efficient exascale supercomputers. Within EUPILOT, the RISC-V based accelerators created as part of the EPI project will be further developed and integrated into a full computational ecosystem. The project’s primary goal is to integrate both open-source software and open and proprietary hardware into a pilot system, and demonstrate its viability for real-world applications.

The EPEX consortium aims to design, build, and validate the first EU platform for HPC, with European assets covering the spectrum of required technologies end to end: from architecture, processors, system software, and development tools to applications. The EUPEX prototype will be designed to be open, scalable, and flexible, and will include a modular OpenSequana-compliant platform and a corresponding HPC software ecosystem for its modular supercomputing architecture.

Scientifically, EUPEX is a vehicle to prepare HPC, AI, and Big Data processing communities for upcoming European exascale systems and technologies. Being the first of its kind, EUPEX has set itself the ambitious challenge of gathering, distilling, and integrating European technologies that its scientific and industrial partners will use to build a production-grade prototype.
EUPLEX runs for three years with a total budget of about €40 million. In the project 17 European academic and industry partners are collaborating. JSC will bring as one of the partners its many years of experience in the design, installation, and operation of large HPC systems into the project. Furthermore, JSC will contribute its well-known open-source software in the form of tools for performance measurement and analysis (Scalasca, Score-P, CUBE) and for system monitoring (LLview). Finally, JSC will port and adapt AI applications that cover machine and deep learning. The software developed by JSC within this project will be made openly available to help support the platform within the HPC community and beyond in the long term.

On the other end of the spectrum, the new HPCQS project aims to develop, deploy, and coordinate a European federated infrastructure that tightly integrates two quantum simulators that each control more than 100 qubits (quantum bits) in the Tier-0 HPC systems Joliot Curie of GENCI, operated at CEA/TCGCC, and the JUWELS modular supercomputer at JSC.

The seamless integration of quantum hardware with classical computing resources is an essential step towards utilizing the power of quantum computers to handle the first practical applications. As JSC, HPCQS is a logical continuation of the efforts driven by JUNIQ (the Jülich Unified Infrastructure for Quantum computing) to establish tight hybrid quantum HPC simulations.

HPCQS receives a total budget of €12 million and runs for four years. HPCQS is carrying out a public procurement of innovative solutions (PPI) to implement the two 100+ qubit quantum simulators and will launch an ambitious research program. Prof. Kristel Michielsen from JSC, one of the five participating European HPC centers, is coordinating the project. Apart from these five HPC centers, other European partners from academia and industry and three linked third parties are participating in the project. HPCQS will develop the programming platform for the quantum simulator. It is based on two European software developments: the Atos Quantum Learning Machine (QLM)TM and ParTec’s ParaStation ModuloTM. Together, these technologies allow the deep, low-latency integration of quantum simulators into classical modular HPC systems. In addition, HPCQS will work on the deployment of a full hybrid software stack. It will include cloud access, resource management of hybrid workloads, tools and libraries, as well as benchmarking and certification/ performance analysis. Engaging users in the co-design process will lead to prototype applications in machine learning and scientific simulations.

Kristel Michielsen, Bernd Mohr, and Andreas Herten

| PROJECT | The European PILOT |
| FUNDING | European Union’s Horizon 2020 and BMBF |
| FUNDING AMOUNT | €30 million |
| RUNTIME | Dec 2021 to May 2025 |
| PARTNERS | 19 European partners |
| WEBSITE | https://eupilot.eu/ |

| PROJECT | HPCQS |
| FUNDING | European Union’s Horizon 2020 and BMBF |
| FUNDING AMOUNT | €12 million |
| RUNTIME | Dec 2021 to Nov 2025 |
| PARTNERS | 18 European partners |
| WEBSITE | https://www.hpcqs.eu/ |

| PROJECT | EUPEX |
| FUNDING | European Union’s Horizon 2020 and BMBF |
| FUNDING AMOUNT | €40 million |
| RUNTIME | Jan 2022 to Dec 2025 |
| PARTNERS | 17 European partners |
| WEBSITE | https://eupex.eu/ |

The LEXIS Project Furthers Big Data Analysis and Exchange in Europe

Research data can often inspire more questions than it initially answers. Extended analysis and exchange of research data from various supercomputers is becoming more important in Europe.

Ideally, European researchers should be able to run simulations where systems are readily available and fit their requirements. “Researchers just want to analyze and model their data on different supercomputers as simply and efficiently as possible, independently of location,” says Stephan Hachinger, PhD physicist and Head of the Research Data Management team at the Leibniz Supercomputing Centre (LRZ).

“While moving data from one place to another is part of everyday life for many researchers, it is a highly complex task in high-performance computing (HPC). Tera-bytes to petabytes worth of data are often processed at LRZ, which, despite fast networks, cannot be easily moved back and forth between strongly secured, heterogeneous systems,” says Hachinger. User-friendly workflows for processing, analyzing, and exchanging data between locations are therefore required.

Simplifying complex HPC and cloud workflows

Big Data analysis, distributed workflows, and data exchange between European HPC centers have been at the focus of the EU project “Large-Scale Execution for Industry and Society (LEXIS).” Coordinated by the Czech national supercomputing center IT4Innovations (IT4I), 18 institutes, companies, and data centers, including the LRZ, have developed workflows and HPC and cloud technologies aimed at streamlining this exchange.

The result is the LEXIS platform, which builds on existing cloud systems, networks, and supercomputers in Europe and organizes the data flow. Users from academia and industry can find tools at https://portal.lexis.tech that efficiently start and simplify analysis and simulation processes. The portal also offers tools for managing data based on EUDAT services. Companies and researchers can process large datasets in the Czech Republic even when they are stored in Germany or Italy, and vice versa, and collaborations can work together on data projects across Europe.

“Within LEXIS, data is easily findable and it is immediately apparent how and for what purpose it can be further used,” explains Hachinger. Although the LEXIS project ended in December 2021, the portal and platform will continue to exist: Developed and optimized with partner organizations from the fields of meteorology, geophysics, polar and marine research, and aircraft technology, the first companies and research groups are now testing the platform via the portal.

New services for the LRZ?

LRZ staff feel strongly about the positive impact of LEXIS. “We spent a long time looking for solutions for workflow control, for example in the processing of weather and climate data,” Hachinger said. “EUDAT’s combination of workflows and data management is exciting because it enables European computing from different locations.”

LEXIS will be used and further developed in the coming years. Hachinger and his LRZ team collaborators also hope for further teamwork with LEXIS partners, especially with IT4I and the Irish supercomputing center ICHEC. Looking further ahead, LRZ could also benefit from the technology and thus expand its services.

Susanne Fiszer

| PROJECT | LEXIS Project |
| FUNDING | European Horizon 2020 |
| FUNDING AMOUNT | Total cost: €13 997 428,71 EU contribution: €12 218 545,50 |
| RUNTIME | Jan 2019 to Dec 2021 |
| PARTNERS | 18 |
| WEBSITE | https://lexis-project.eu/web/ |
As new applications of artificial intelligence (AI) emerge, there is a growing demand across many industries for university graduates with the understanding needed to develop and use such technologies effectively. A new project funded by the German Federal Ministry for Education and Research (BMBF) aims to address these needs at the University of Stuttgart.

The project, called IKILeUS (Integrated AI in Teaching at the University of Stuttgart) is bringing together multidisciplinary AI expertise from several institutes across the university in ways that will better prepare students to create and work with AI tools. The High-Performance Computing Center Stuttgart (HLRS) is serving as the coordinating institute for this project and will strengthen several subprojects by contributing both its expertise in artificial intelligence and access to computing resources that are optimized for AI applications.

IKILeUS is pursuing a holistic approach that involves bringing both AI “for” teaching and AI “in” teaching to the entire student body across all stages of study. On the one hand, this means ensuring that all students graduate with an understanding of the fundamentals of artificial intelligence, including practical experience with AI, in an interdisciplinary and sustainable way. On the other, IKILeUS will develop and introduce AI-based technologies that can improve instruction.

New educational programs will better prepare students

Under the auspices of IKILeUS, partners from across the University will develop new educational content to prepare students to identify potential applications of AI in their field of study, while giving them the necessary skills to develop and implement them. This will include curriculum enhancements and event series in which students learn about specific applications of AI for scientific research and in industry.

In addition, HLRS will develop related continuing education content for individuals who have graduated from university and work in industry. This new, AI-focused content will become an established course in the center’s Supercomputing Academy.

These various activities will also include instruction on ethical issues concerning the trustworthiness and responsible use of artificial intelligence. Members of the HLRS Department of Philosophy of Computational Sciences, led by Dr. Andreas Kamiński, will develop these resources to encourage students to reflect on their interaction with and use of AI technologies, both during their studies and in their careers that follow.

AI for improved instruction

In addition to curriculum development, IKILeUS will support the development of AI technologies that could improve instruction at the University. This could include AI-supported learning assistants that help students improve concentration when studying, and tools for improving accessibility to teaching resources for students with vision or hearing impairments. The project will also investigate how AI could simplify some teaching tasks, such as through the automatic evaluation of student work.

“It is important that the University prepare students for their lives after graduation,” said HLRS Director Prof. Dr. Michael Resch. “Today, this means ensuring that they both understand the theoretical foundations of artificial intelligence and that they graduate with practical experience in using AI tools and methods. We are excited about the potential of IKILeUS to make significant improvements in this effort.” Christopher Williams
CIRCE Kickoff Meeting Highlights Needs for Urgent Computing

Scientific staff at HLRS met with representatives of public agencies to discuss how high-performance computing could help in preparing for and responding to sudden crises.

I n recent years the COVID-19 pandemic, devastating floods, the rapid spread of misinformation, and sudden surges in migration have all tested public administration’s abilities to manage crisis situations. In the high-performance computing (HPC) community, such events have also raised the question of how tools using simulation, high-performance data analytics, and artificial intelligence might better assist governments in protecting citizens and crucial infrastructure when confronted with such challenges.

At the High-Performance Computing Center Stuttgart (HLRS), the need to think about this problem quickly became apparent in 2020 during the early months of the COVID-19 pandemic. To support the German government in preventing its health care system from being overwhelmed, hardware and software experts at HLRS worked closely with investigators in the Federal Institute for Population Research (Bundesinstitut für Bevölkerungs-forschung, BiB) to quickly implement a model on HLRS’s supercomputer that predicts demand for intensive care units across Germany up to four weeks in advance. This tool, which continues to run at HLRS and delivers daily information to the federal government once every week, has helped national policy makers to manage public health related to the pandemic.

Building on this collaboration, HLRS, under the auspices of the Gauss Centre for Supercomputing, launched a new project called CIRCE (Computational Immediate Response Center for Emergencies) in late 2021 that has begun to investigate how HPC could help in future crisis situations. The three-year effort, which is co-financed by the German Federal Ministry for Science and Education (BMBF) and the State of Baden-Württemberg Ministry for Science, Research and Art (MWK), will identify potential emergencies in which high-performance computing and related technologies could better support decision-making in government. To improve preparedness, CIRCE also aims to determine what technical and organizational changes are needed to ensure that HLRS supercomputing resources are immediately available to public administration when crises arise.

In February 2022 CIRCE held its first meeting to begin exploring these challenges. While HLRS can provide technical infrastructure and scientific expertise in high-performance computing, the discussion made clear that building relationships between HLRS and government agency representatives will be essential for improving emergency preparedness. This approach will help to identify what specific risks exist, and where high-performance computing power is needed to manage them. Moreover, these exploratory discussions will need to determine what data government agencies could provide as a basis for simulation or data analysis. This includes considering both what data they currently collect and how existing data protection regulations affect how data can be shared, analyzed, and used for simulations.

Women’s Power for Science

According to a recent UNESCO Science Report, more women are choosing to study mathematics, computer and natural sciences, or engineering. Women now comprise 40 percent of all computer science graduates, and 40 percent of engineering graduates, and for good reason: “I really enjoy building my own programs, looking for solutions to experiments, reading from data how a supercomputer handles software or algorithms,” says computer scientist Dr. Carmen Navarrete of the Computational X support team at the Leibniz Supercomputing Centre (LRZ) when speaking to how she became interested in HPC. Her colleague Elisabeth Mayer, a specialist in virtual reality and visualization, agreed: “My work is diverse and challenging; we support researchers and work on the front lines alongside cutting-edge hardware and software. I like that.”

Still, according to Eitan Frachtenberg and Rhody Kaner, researchers at Reed College in Portland, women remain underrepresented in HPC space. For their study, prepared for the SC21 conference, they analyzed the programs of nine HPC and high-tech conferences in 2017, and found that 2,136 authors of scientific papers, only 10% were women; the program of four events did not involve any female scientists at all. The UNESCO Science Report confirms that female scientists are underrepresented at conferences and in publications, passed over for promotions, paid less, and receive lower funding for projects. “There can be a pretty competitive atmosphere at times in the science and the technology sector,” said Viktoria Paun, PhD student and a researcher at LRZ. “But women typically are very welcome and should be confident to take part and not feel intimidated to present their work and ideas. I would personally take this path again anytime – being active in science broadens my horizon and teaches me new things every day.”

Empowering female scientist and ensuring visibility

This spirit has to be supported from an institutional perspective, according to Sabine Ooster, head of human resources at LRZ. “Women enrich IT, technology, and supercomputing and make economy and society fit for the future. With women on the team, the approaches and ideas become more diverse.”

The LRZ adopts various strategies to increase its female workforce, and making its staff more diverse generally. For instance, the LRZ HR team avoids expressions in job advertisements that discourage women from applying. Participating in Girls’ Day has been on the agenda of LRZ for more than 10 years to encourage girls getting involved with technology from an early age. The LRZ team hopes to improve networking opportunities again in person to exchange ideas and experiences.

But most importantly, LRZ also strives to offer its female employees more visibility – most recently with a series of portraits and video interviews with female scientists launched between Women in Science Day in February and International Women’s Day in March. This strategy has proven to be successful, as the study by Frachtenberg and Kaner shows: in order to promote women, lead authors of scientific papers on supercomputing are cited more often and female HPC specialists are deliberately invited to give lectures. Susanne Vieser
GPU Programming Scales to New Heights at the JUWELS Booster Tuning and Scaling Workshop 2022

Multi-day event allows new and old JSC users to scale applications for better use of the JUWELS Booster’s GPU-heavy architecture.

With roughly 70 petalops of theoretical peak performance, the JUWELS Booster at the Julich Supercomputing Centre (JSC) is quite a performance powerhouse. However, using the bulk of its 400,000 GPU cores efficiently requires diligent scientific software engineering effort. To support the journey of achieving performance heights, the first JUWELS Booster Tuning and Scaling Workshop was held virtually at JSC March 7-11.

The workshop was conducted as a combination of lectures on advanced topics, interactive code improvements, and opportunities to test the scalability. In the lectures, tools and libraries were presented to assess and improve code performance on one node and many nodes by experts from JSC and NVIDIA. Tools like Nsight Systems and Score-P were introduced and libraries like NCCL explained. Experts went into great detail in describing features and benefits.

Immediately afterwards, participants could apply their freshly-gained knowledge to their own applications in the interactive sessions. Guided by their respective tutors from JSC and NVIDIA, they worked towards the common individual goal of improving single-GPU performance and, especially, multi-GPU scalability. Nine application teams from the diverse JUWELS Booster user base participated, with teams from the weather and climate domain, hydrological modelling, neuroscience, plasma physics, molecular dynamics, and materials science simulations.

Some teams studied in detail their single-GPU performance, using the tools to identify their respective application’s bottlenecks to optimize memory transfers, cache hit rate, asynchronous operations, and other aspects. Eventually, every group focused also on the multi-node behaviour of their application and studied them on multiple nodes, going up to 200 nodes (800 GPUs) or even further. Some dedicated runs were instrumented to study and improve the communication pattern in detail and optimize for least idle time.

In presentations, teams reported on the current status and their plans for the near hours, allowing for exchanges of ideas and identification of needs for support. Finally, on the last day, the teams reported about their successes, experiences, and future plans. Every team was able to improve various aspects of their application using the introduced tools for assessments – and advanced the application’s scalability in the process. Every group enjoyed the workshop and also noted the long-term effect that the week will have on their respective applications.

Because of the productive atmosphere and positive outcome, JSC will host the event again in 2023.

Andreas Herten

Preparatory Study for the Helmholtz Platform for Research Software Engineering Started

Scientific software is becoming increasingly important in our quest for new knowledge. Research Software Engineering (RSE) is forming as a new subject of investigation, in Europe, Germany, and the Helmholtz Association specifically.

In this context, the HiRSE concept (“Helmholtz Platform for Research Software Engineering”) sees the establishment of central activities in RSE and the targeted sustainable funding of strategically important codes by so-called community software infrastructure (CSI) groups as mutually supportive aspects of a single entity.

In a first “preparatory study,” HiRSE_PS will evaluate the core elements of the HiRSE concept and their interactions in practice over the funding period of two years. The study is led by FZJ and KIT, who are joined by HZB and Hereon. JSC plays a key role in the consulting and networking activities and will help code developers to make use of modern continuous integration, testing, and delivery techniques, especially in the context of high-performance computing.

Nic Excellence Project 2021 on Polymer Physics

The John von Neumann Institute for Computing (NIC) Peer Review Board regularly awards the title “NIC Excellence Project” to outstanding simulation projects. At its October meeting, the board decided to honor Prof. Kurt Kremer (Max Planck Institute for Polymer Research) for his project, “Bridging Drastically Coarse-Grained and Microscopic Descriptions in Hierarchical Modeling of Soft Matter. Application: Non-Linear Viscelasticity of Polymer Melts”.

This project investigates molecular-level mechanisms underlying polymer rheology at strong deformations, which presents tremendous challenges for basic science and industrial processing, Prof. Kremer and his group study these mechanisms by simulating experiments with molecular dynamics simulations. The computational experiments must start from samples of...
molten polymers that are much larger than the entanglement length—the average number of monomers between two consecutive topological constraints on chain motion. For that a novel strategy based on hierarchical fine-graining of polymer melts has been developed. This backmapping method proceeds from blob-based chains down to the microscopic description and is applicable to generic polymer models (bead-spring) as well as actual materials, e.g. polyisoprene.

OpenGPT-X: JUWELS Booster Trains Large European Language Models

Through the OpenGPT-X project, JSC is taking part in one of the most exciting European endeavors in the field of machine learning: the creation of a large-scale language model that speaks not only English, but all major European languages. The project consortium of 13 organizations from academia, industry, and media has been granted funding of 435 million by the German Federal Ministry for Economic Affairs and Climate Action (BMWK) over three years. It seeks to bring large language models all the way from creation to application, using open-source technologies and publishing results as such. OpenGPT-X is a Gaia-X project, aiming to supply its developed services within the federated Gaia-X infrastructure.

Large language models have exciting potential. They are capable of processing and generating text with a quality that only two years ago would have been unthinks: The OpenGPT-X partners would like to use these models for different real-world scenarios. The German broadcaster WDR, for example, intends to make its library of audio more accessible. The Russian broadcaster WDR, for example, intends to make its library of audio.

Bundesverdienstkreuz for LRZ Advisory Council Member

Prof. Dr. Martin Wirsing was awarded the Bundesverdienstkreuz am Band by Bundespräsident Frank-Walter Steinmeier. The prestigious award was given to Wirsing, an LRZ advisory board member, by Markus Blume, Bavarian Minister for Science and the Arts, at the beginning of March. Wirsing has been an elected LRZ advisory board member since 1999, was vice-president of Ludwig Maximilians-Universität München (LMU) and held the chair of programming and software engineering. The mathematician and computer scientist is the author and editor of 20 books on software, IT systems and programming languages, has published approximately 220 scientific studies, and led several European research projects. Wirsing studied mathematics at the LMU and in Paris, worked at the Technical University of Munich (TUM) for the computer science pioneer and LRZ co-founder Prof. Dr. Friedrich Bauer, and was appointed to the chair of computer science at the University of Passau in 1989. He moved to Munich to LMU in 1992.

25 Years of the Archive and Backup System at LRZ

At night, the work of the robots begins with a whir in the data archive room of LRZ. With their gripper arms, they pull tapes out of the compartments of the libraries, use them to store 40 million backup copies that around 5,000 computer systems in the Munich Scientific Network (MWN) send to Garching every day, and put them back again. For 25 years, the LRZ centralized data storage has performed this kind of essential and often unnoticed work, and Werner Bauer accompanied the change, seeing the archive and backup system (ABS) grow. “Data is becoming more and more important in our society; it must not be lost,” he said. “That was true 25 years ago and is even more true today. Today, the security measures are correspondingly multiplied, at the end of which, as the ‘last line of defence’ we need to rely on us, is our archive and backup system.” In a recent interview, he back up his knowledge with details and figures. Read more at: https://www.lrz.de/presse/ere-spnisse/2020-10-05-LRZ-Archivbackupsys-tem-en/

LRZ cooperates with TUMjuniour

LRZ is going to schools. The scientific computing center participates in the TUMjuniour program, which is intended to raise interest in mathematical and scientific topics and computer science among school children. TUMjuniour is supported by the Bavarian Ministry of Education and is aimed at students in grades 5 to 10. Three excursions to different places of learning are planned for each class per school year. The vision behind the program is based on the premise that when students see and experience technology first-hand, their motivation to study it increases dramatically. The cooperation started in autumn 2021. Approximately 450 students came to visit LRZ in the first round. The program will continue and be expanded in 2022.

https://www.lrz.de/presse/ere-spnisse/2021-11-01-LRZ-juniourSchool/
“As I see it, at the moment, there is a lot of momentum in quantum computing, so I am quite sure that more and more of these devices will become available with different types of technologies.”
Prof. Dr. Kristel Michielsen

Staff Spotlight: Standing at the Forefront of the Next Major Quantum Computing Revolution

JSC Quantum Information Processing Group Leader Takes a Holistic View of the Field.

Since beginning her graduate studies at the University of Groningen in the Netherlands in the 1990s, Prof. Dr. Kristel Michielsen has participated in several periods of scientific research that could only be described as “quantum revolutions,” or moments where the principles of quantum mechanics were better understood and applied in new ways that carried large implications for physics research and beyond.

“When I did my post-doctoral work in Groningen, we were focused on simulating all kinds of problems by solving the time-dependent Schrödinger equations, and around that time we had the first ‘revolution in quantum computing,’” she said. “We built a quantum computing emulator on our laptops, and we for the first time could really simulate a realistic model of a quantum computer. We learned a lot from these early experiences.”

She may not have realized it at the time, but over the next 25 years, Michielsen would find that these early experiences were laying the groundwork for a career at the forefront of what is now the burgeoning field of quantum computing.

While classical computers give instructions through long chains of 1s and 0s, called binary code, quantum computers can use the principles of quantum superposition – in essence, when a subatomic particle is representing both a positive and negative charge at the same time – so that so-called “qubits” can represent both a 1 and a 0 at the same time. While still in its infancy, the technology promises researchers a fundamentally new way to calculate complex, data-intensive problems.

In 2004, the Director of the Jülich Supercomputing Centre (JSC), Prof. Dr. Thomas Lippert, formed a group that would take the nascent research on quantum computing and begin to explore it in the context of a high-performance computing (HPC) center.

After finishing her post-doctoral work at the University of Groningen, Michielsen joined JSC in 2009 to become group leader of the quantum information processing (QIP) group. It was there that Michielsen and Lippert began to collaborate and think strategically about not only how to leverage quantum mechanics in the context of computing, but also how to think of HPC as a broader ecosystem and develop a concept where distinctive, complementary computing architectures could co-exist with one another.

Since then, JSC has experimented with quantum computing emulators and prototypes, but in 2019, the center experienced a quantum revolution of its own – JSC and its parent organization, Forschungszentrum Jülich, launched the Jülich Unified Infrastructure for Quantum computing (JUNIQ) user facility as a way to further develop and evaluate quantum computing designs, concepts, and applications in collaboration with research partners from around the globe. In January 2022, JSC celebrated JUNIQ’s biggest acquisition to-date: in partnership with D-Wave Systems, the centre inaugurated the D-Wave Advantage™ Quantum Annealer, the first quantum computer in Europe with more than 5,000 qubits. (More information about JUNIQ can be found on page 6).

While the Advantage™ system is a major milestone for JUNIQ’s growth, Michielsen sees JUNIQ as a place to experiment with the variety of new technologies being rapidly developed in quantum computing space. “As I see it, at the moment, there is a lot of momentum in quantum computing, so I am quite sure that more and more of these devices will become available with different types of technologies,” she said.

As the field has grown, so too have Michielsen’s responsibilities. In addition to being the QIP group leader at JSC, Michielsen also has an appointment at RWTH Aachen University, is the head of JUNIQ, and leads a project funded by the EuroHPC Joint Undertaking called HPCQS (High Performance Computer and Quantum Simulator hybrid), which tasks JSC with evaluating quantum computing technologies and integrating a system into the center’s HPC ecosystem. Michielsen is a true scientist at heart, and despite lamenting that her administrative and managerial tasks can take away from her time doing...
“We need to provide quantum computing resources to outside users so they can see what the technology is about and see for themselves what is possible and what isn’t.”

Prof. Dr. Kristel Michielsen

Jülich as a Europe’s leading quantum computing-HPC nation of video conferencing software, chat programs, and other collaborative tools.

Education and Training

GCS and its member centres provide first-class training opportunities for the national and European HPC communities. More than 50 highly qualified scientists work as trainers for over 100 courses (or 200 course days), which positions GCS as one of the leading training institutions in all of Europe.

Over the past two years, we have seen a significant shift in the way training events are conducted. Before the Corona pandemic took hold in early 2020, virtually all courses and workshops took place on site at one of the supercomputer centers, typically spanning multiple full days in a row. As face-to-face meetings were suspended, all our training offers were switched to online events, employing a combination of video conferencing software, chat programs, and other collaborative tools.

For a full list of training courses offered, please visit:

<table>
<thead>
<tr>
<th>GCS</th>
<th>HLRS</th>
<th>JSC</th>
<th>LRZ</th>
</tr>
</thead>
</table>

Now that on-site events are gradually becoming possible again, we see that many of our course participants have grown accustomed to being able to attend high-quality training events without the need for travel, and international participation is on the rise. Going forward, we thus expect to see a permanently changed training landscape, with a mixture of on-site courses, online workshops, and hybrid events being the norm. As a side effect, training collaboration between the different GCS centers has further increased, with more events being co-organized by multiple locations, and instructors from different centers supporting each other’s training efforts.

research, she feels connected to her group’s work and plays an active role in shaping its research fociuses. “The issues my team members are dealing with are problems that have a lot of my interest,” she said. “They often have to do with how these devices operate in real conditions. Seeing what the deviations are and finding explanations for them is still something which I’m involved in and very much like to be involved in.”

JSC’s flagship computer, JUWELS, is currently Europe’s fastest supercomputer, and is based on the modular supercomputing architecture — that is, a computer that is comprised of a variety of modules including CPU clusters or boosters featuring GPUs and/or other accelerators and a storage system. Additional modules can include, among others, future technology modules, such as a quantum computer or a neuromorphic system, and an interactive computation and visualization system. The modules are interconnected at system level, forming a system of autonomous modules. JSC has applied to the hosting entity for Europe’s first exascale computer – the next major performance horizon in classical computing – and Michielsen sees one of JSC’s main tasks in the years to come as tightly integrating quantum computing resources and classical computing resources to serve the widest variety of users’ needs.

For Michielsen, training current and prospective users about quantum computing’s advantages and limitations is a big part of the job. While quantum computers show promise in solving certain classes of problems better than classical computers, they have not matured to the same extent as classical machines, and Michielsen tries to ensure that expectations for their present-day abilities are always in context.

“There is hype surrounding these systems,” she said. “A lot is promised, of course, and if someone asks me to give examples of potential future applications, then I can mention them, but I usually refrain from saying when, because we are also looking at this subject openly and critically, and approach this from a scientific point of view. We need to provide quantum computing resources to outside users so they can see what the technology is about and see for themselves what is possible and what isn’t. I still often get questions from potential users about doing massive calculations that we can’t currently solve with these machines, and from the start I have to disappoint them and tell them that it isn’t how this works. We have to bring very large expectations down to something that is more realistic, but is obviously still interesting to be studying and may even have some practical application already.”

In the years to come, the QIP group will continue to collaborate with partners in GCS and Europe as a whole to innovate in the realm of quantum computing. Between acquiring new technologies and ramping up a robust training program for users dedicated to quantum computing, Michielsen feels confident that JSC’s path leads to academic and industrial users realizing the promises of this paradigm-shifting technology. “We really plan to develop Jülich as a Europe’s leading quantum computing HPC hybrid infrastructure,” she said. Erich Gedenk
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.

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.

Compute servers currently operated by JSC

<table>
<thead>
<tr>
<th>System</th>
<th>Size</th>
<th>Peak Performance (Tflop/s)</th>
<th>Purpose</th>
<th>User Community</th>
</tr>
</thead>
<tbody>
<tr>
<td>MODULAR SUPERCOMPUTER JUWELS</td>
<td>Cluster (Atos): 10 cells, 2,567 nodes 122,768 cores Intel Skylake 224 NVIDIA V100 GPUs 275 TByte memory</td>
<td>12,266</td>
<td>Capability Computing</td>
<td>European (through PRACE) and German Universities and Research Institutes</td>
</tr>
<tr>
<td></td>
<td>Booster (Atos): 39 racks, 936 nodes 44,928 cores AMD EPYC Rome 3,744 NVIDIA A100 GPUs 629 TByte memory</td>
<td>75,020</td>
<td></td>
<td></td>
</tr>
<tr>
<td>MODULAR SUPERCOMPUTER JURECA</td>
<td>Data-Centric Cluster (Atos): 768 nodes, 98,304 cores AMD EPYC Rome 768 NVIDIA A100 GPUs 443 TByte memory</td>
<td>18,515</td>
<td>Capacity and Capability-Computing</td>
<td>European (only on the Data-Centric Cluster) and German Universities, Research Institutes, and Industry</td>
</tr>
<tr>
<td></td>
<td>Booster (Intel/Dell): 1,640 nodes, 111,320 cores Intel Xeon Phi (KNL) 157 TByte memory</td>
<td>4,996</td>
<td></td>
<td></td>
</tr>
<tr>
<td>FUJITSU CLUSTER QPACE 3</td>
<td>672 nodes, 43,008 cores Intel Xeon Phi (KNL) 48 TByte memory</td>
<td>1,789</td>
<td>Capability Computing</td>
<td>SPB TR55, Lattice QCD Applications</td>
</tr>
<tr>
<td>ATOS CLUSTER “JUSUF”</td>
<td>205 nodes, 26,240 cores AMD EPYC Rome 61 NVIDIA V100 GPUs 52 TByte memory</td>
<td>1,372</td>
<td>Capacity and Cloud Computing</td>
<td>European and German Universities and Research Institutes through PRACE and Human Brain Project</td>
</tr>
<tr>
<td>MODULAR SUPERCOMPUTER DEEP-EST PROTOTYPE</td>
<td>Cluster: 50 nodes, 1,200 cores Intel Xeon Gold 6146 9.6 TByte memory + 25.8 TByte NVM</td>
<td>45</td>
<td>Capacity Computing</td>
<td>Partners of the “DEEP” and “SEA” EU-project series and interested users through Early Access Programme</td>
</tr>
<tr>
<td></td>
<td>Booster: 75 nodes, 600 cores Intel Xeon Silver 4215 75 NVIDIA V100 GPUs 6 TByte memory</td>
<td>549</td>
<td>Capacity and Capability Computing (high-scalable code parts)</td>
<td></td>
</tr>
<tr>
<td>MODULAR SUPERCOMPUTER “D-WAVE”</td>
<td>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</td>
<td>170</td>
<td>Capacity and Capability Computing (data analytics codes)</td>
<td></td>
</tr>
<tr>
<td>D-WAVE QUANTUM ANNEALER JUPSI</td>
<td>More than 5,000 qubits</td>
<td>No classical performance measure applicable</td>
<td>Quantum Computing</td>
<td>German Universities and Research Institutes (50%), Industry Applications and D-Wave customers (50%)</td>
</tr>
</tbody>
</table>
Leibniz Supercomputing Centre

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 center 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 levels. Top-notch specialists for HPC code portability and scalability support the broad user base at LRZ and ensure that the systems are running their operations in the most energy efficient way possible.

Future computing at LRZ

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 that touches on HPC, machine learning, artificial intelligence, and big data complements LRZ’s offerings.

IT backbone for Bavarian science

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

CONTACT

Leibniz Supercomputing Centre (LRZ)
Prof. Dr. Dieter Kranzlmüller
Boltzmannstraße 1, 85748 Garching near Munich, Germany
Phone +49- 89 - 358-31-80 00
kranzlmueller@lrz.de
www.lrz.de

Compute servers currently operated by LRZ

<table>
<thead>
<tr>
<th>System</th>
<th>Size</th>
<th>Peak Performance (TFlop/s)</th>
<th>Purpose</th>
<th>User Community</th>
</tr>
</thead>
<tbody>
<tr>
<td>SUPERMUC-NG INTEL/LENOVO THINKSYSTEM</td>
<td>6,336 nodes, 304,128 cores, Skylake</td>
<td>26,300</td>
<td>Capability Computing</td>
<td>European (through PRACE) and German Universities and Research Institutes</td>
</tr>
<tr>
<td>SUPERMUC-NG INTEL/LENOVO THINKSYSTEM</td>
<td>144 nodes, 8,192 cores Skylake</td>
<td>600</td>
<td>Capability Computing</td>
<td>Bavarian Universities (Tier-2)</td>
</tr>
<tr>
<td>SUPERMUC-NG COMPUTE CLOUD</td>
<td>64 nodes, 3,072 cores, Intel Xeon (“Skylake”), 64 Nvidia V100</td>
<td>458 (CPUs + GPUs) 7,680 AI Performance</td>
<td>Cloud Computing</td>
<td>Bavarian Universities (Tier-2)</td>
</tr>
<tr>
<td>COOLMUC-2 LENOVO NEXTSCALE</td>
<td>384 nodes, 10,752 cores Haswell</td>
<td>447</td>
<td>Capability Computing</td>
<td>Bavarian Universities (Tier-2)</td>
</tr>
<tr>
<td>COOLMUC-3 MEGWARE SLIDE SX</td>
<td>148 nodes, 9,472 cores, Knights Landing, 17.2 TByte, Omnipath</td>
<td>459</td>
<td>Capability Computing</td>
<td>Bavarian Universities (Tier-2)</td>
</tr>
<tr>
<td>DGX Systems (A100, V100 &amp; P100 Architecture)</td>
<td>7 Nodes, per Node: 40-64 CPUs, 32-64 GB GPU HBM Memory, 512-2048 GB DDR4 Memory;</td>
<td>1066 26,000 AI Performance</td>
<td>Machine Learning, AI applications</td>
<td>Bavarian Universities</td>
</tr>
<tr>
<td>Nvidia GPUs Nodes (V100 &amp; P100 Architecture)</td>
<td>5 Nodes, per Node: 40-64 CPUs, 32-64 GB GPU HBM Memory, 256-368 GB DDR4 Memory; 12 Nvidia Tesla GPUs in total</td>
<td>261 1,045 AI Performance</td>
<td></td>
<td>Bavarian Universities</td>
</tr>
<tr>
<td>“MankAI” (AMD MI50 Architecture)</td>
<td>6 Nodes, per Node: 64 CPUs, 8 AMD MI50 GPUs, 128 GB GPU HBM Memory, 512 GB DDR4 Memory;</td>
<td>317 1,272 AI Performance</td>
<td>Selected research on COVID-19 and/or with high society impact</td>
<td>Bavarian Universities</td>
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<td>Atos QLM</td>
<td>Quantum simulation</td>
<td>Bavarian Universities</td>
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<td>QMWare</td>
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<tr>
<td>SUPERMUC-NG INTEL/LENOVO THINKSYSTEM</td>
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<td>Machine Learning, AI applications</td>
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</tr>
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</table>
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.

Compute servers currently operated by HLRS

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</tr>
</thead>
<tbody>
<tr>
<td>HPE APOLLO 9000</td>
<td>5,632 nodes 720,896 cores 1.44 PB memory</td>
<td>26,000 TF</td>
<td>Capability Computing</td>
<td>European (through PRACE) and German Universities, Research Institutes, and Industry</td>
</tr>
<tr>
<td>HAWK GPU EXTENSION</td>
<td>24 nodes 191 NVIDIA A100 GPUs</td>
<td>120,000 TF AI performance</td>
<td>Machine Learning, Artificial Intelligence applications</td>
<td>German and European (PRACE) research organizations and industry</td>
</tr>
<tr>
<td>NEC CLUSTER</td>
<td>653 nodes 17,192 cores 117 TB memory</td>
<td>974 TF</td>
<td>Capacity Computing</td>
<td>German universities, research institutions, and industry</td>
</tr>
<tr>
<td>NECX: AURORA TSBASA</td>
<td>64 nodes 512 cores 3072 GB memory</td>
<td>137.6 TF</td>
<td>Vector Computing</td>
<td>German universities, research institutions and industry</td>
</tr>
<tr>
<td>CRAY CS: STORM</td>
<td>8 nodes 64 GPUs 2,048 GB memory</td>
<td>499.2 TF</td>
<td>Machine Learning, Deep Learning</td>
<td>German universities, research institutions and industry</td>
</tr>
<tr>
<td>AMD COVID-19 SYSTEM</td>
<td>10 nodes 80 AMD MI50 GPUs</td>
<td>530 TF</td>
<td>COVID-19 Research</td>
<td>German and European researchers focused on COVID-19 research</td>
</tr>
</tbody>
</table>

Contact

High-Performance Computing Center Stuttgart (HLRS), University of Stuttgart

Prof. Dr.-Ing. Dr. h.c. Dr. h.c. Hon.-Prof. Michael M. Resch
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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 centers. 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.

GCS
Gauss Centre for Supercomputing

www.gauss-centre.eu

Funding for GCS HPC resources is provided by: