HLRS

High-Performance Computing Center | Stuttgart

2018 ANNUAL REPORT

ENERGY HEALTH CLIMATE MOBILITY PHILOSOPHY

2018

HLRS ANNUAL REPORT

The High-Performance Computing Center Stuttgart (HLRS) was established in 1996 as the first German national high-performance computing (HPC) center. As a research institution affiliated with the University of Stuttgart and a founding member of the Gauss Centre for Supercomputing, HLRS provides HPC services to academic users and industry. We operate leading-edge HPC systems, provide training in HPC programming and simulation, and conduct research to address key problems facing the future of supercomputing. Among our areas of expertise are parallel programming, numerical methods for HPC, visualization, grid and cloud computing concepts, data analytics, and artificial intelligence. Our system users conduct research across a wide range of scientific disciplines, with an emphasis on computational engineering and applied science.

Director's Welcome

Grußwort

Welcome to the HLRS 2018 Annual Report. We are pleased to present this look back at our activities over the past 12 months, which were marked by many successes.

At the top of our list of achievements was certainly our procurement of a new high-performance computer. After an intense, yearlong competition among leading hardware vendors, HLRS signed a contract with Hewlett Packard Enterprise (HPE) in November to build Hawk, our forthcoming next-generation supercomputer. As part of this collaboration, HLRS and HPE will also work together on improving services, optimizing codes, and developing new types of high-performance computing (HPC) applications for machine learning and artificial intelligence. In the coming years we look forward to being able to offer our users a much more powerful supercomputing resource and will be well positioned to lead as HPC technologies continue to advance.

HLRS also successfully participated in the launch of several new EU-funded projects, including new European Centres of Excellence (CoE's) in high-performance computing that will form the backbone of the European HPC strategy. As a member of multiple new CoE's created in 2018 — EXCELLERAT, HIDALGO, CHEESE, and POP2 — HLRS is involved in four of the nine European centers. As project leader of the new European Centre of Excellence for Engineering Applications (EXCELLERAT), HLRS will strengthen its position as Europe's leading center for simulation in engineering, a critical tool for high-tech innovation. Our support for the computational engineering and applied science communities is the focus of this annual report's spotlight article.

Also important in 2018 was the positive evaluation of several key research projects that HLRS leads or

Wir freuen uns, mit Ihnen auf die zahlreichen Erfolge der letzten zwölf Monate am HLRS zurückzublicken.

An oberster Stelle der wichtigsten Ereignisse steht sicherlich die Beschaffung unseres neuen Höchstleistungsrechners. Nach einer intensiven, einjährigen Ausschreibungsphase, an der führende Hardware-Anbieter teilnahmen, unterschrieb das HLRS im November 2018 einen Vertrag mit Hewlett Packard Enterprise (HPE), um „Hawk" — unseren Höchstleistungsrechner der nächsten Generation — in Betrieb zu nehmen. Als Teil dieser Zusammenarbeit werden das HLRS und HPE gemeinsam Services ausbauen, Codes optimieren und neue Anwendungen für Maschinelles Lernen und Künstliche Intelligenz vorantreiben. Wir freuen uns darauf, unseren Nutzern in den kommenden Jahren deutlich leistungsfähigere Ressourcen für das Hoch- und Höchstleistungsrechnen (HPC) anbieten zu können und damit unsere führende Position für die Weiterentwicklung zukünftiger HPC-Technologien auszubauen.

Das HLRS konnte seine Arbeit in zahlreichen neuen, EU-geförderten Projekten beginnen — darunter vier neue europäische Exzellenzzentren (CoEs) für HPC-Anwendungen, die das Rückgrat der europäischen HPC-Strategie bilden sollen. Als Mitglied von EXCELLERAT, HIDALGO, CHEESE und POP2 ist das HLRS in vier der neun in 2018 gestarteten europäischen Exzellenzzentren vertreten. Als koordinierender Partner des neuen European Center of Excellence for Engineering Applications (EXCELLERAT), wird das HLRS seine Position als führendes europäisches Zentrum für Simulation in den Ingenieurwissenschaften stärken. Unsere Unterstützung für die computergestützte Ingenieur- und angewandten Wissenschaften ist ein Schwerpunkt dieses Jahresberichts.

participates in as a major partner. In September the Deutsche Forschungsgemeinschaft (DFG, or German Research Foundation) once again recognized the University of Stuttgart's Cluster of Excellence in Simulation Technology (SimTech) as a German national center of excellence for its proposal to expand our focus on data-integrated simulation science. As the prominent facility for high-performance computing at the University, HLRS looks forward to the coming seven years, in which we will work closely with our colleagues here to push the limits of using big data in simulation.

HLRS recognizes that the future of high-performance computing lies not just in new technologies, but also in addressing humanity's greatest challenges. Considering important relationships among supercomputing, society, and politics we created a new Sociopolitical Advisory Board, which held its first meeting this year. The gathering identified many topics that will feed back into our research and enable HLRS to remain focused on society's needs and requirements. Throughout the year we were also glad to welcome prominent politicians from Germany and Europe to HLRS to discuss the future of high-performance computing and how its potential could be maximized to benefit society.

HLRS's focus on HPC training grew in strength this year with the completion of the first course offered by the Supercomputing-Akademie. Its "blended learning" curriculum is designed to address the needs of HPC users in industry, and complements HLRS's existing state-of-the-art training program. Trainers and trainees were overwhelmingly positive about the Supercomputing-Akademie's first test-run, and we look forward to watching this innovative program grow in the coming years.

Another highlight of 2018 was the inauguration of the Media Solution Center Baden-Württemberg (MSC), through which HLRS will work closely with partners from industry and academia to find solutions to challenges facing the fields of media and the arts. The MSC is the latest product of our industrial strategy, which began with the Automotive Simulation Center Stuttgart (asc(s). This year the asc(s celebrated its 10th anniversary, showing just how sustainable our strategy can be. We thank asc(s director Alexander Walser for using the occasion to talk with us for this annual report about the economic and scientific benefits of networking the German automotive industry.

In terms of key performance indicators HLRS can proudly look back on a very successful year. Our third-party funding saw an increase over previous years, our income from industrial HPC users was again at a high level, and the number of people benefiting from our training and education activities remained strong.

Users of our HPC systems also had a very productive year. This annual report showcases some examples of our users' research, including a new sound prediction model that could help reduce machinery noise, applications of HPC and machine learning to make power plants more efficient, and a computational approach that is helping to point the way toward new semiconductor technologies. Such applications show how simulation is making important contributions in areas that are critical for our wellbeing.

With this annual report we express our heartfelt thanks to our supporters and funders, who have made our successes in 2018 possible. At the same time, we look forward to tackling new challenges in 2019.

With best regards,

Prof. Dr.-Ing. Dr. h.c. Dr. h.c. Prof. E.h. Michael M. Resch
Director, HLRS

Ein weiteres Ereignis in 2018 war die positive Bewertung einiger wichtiger Forschungsprojekte, die das HLRS leitet oder daran als bedeutender Partner teilnimmt. Die Deutsche Forschungsgemeinschaft hat zum Beispiel im September das Exzellenzcluster SimTech der Universität Stuttgart wieder als deutsches Exzellenzzentrum anerkannt, das seinen Fokus auf daten-integrierte Simulationswissenschaft legen wird. Als herausragende Einrichtung für das Höchstleistungsrechnen an der Universität Stuttgart, freut sich das HLRS auf die nächsten sieben Jahre, in denen wir in enger Zusammenarbeit mit unseren Kollegen die Grenzen der Simulation unter Benutzung von Big Data erweitern werden.

Für uns liegt die Zukunft des Höchstleistungsrechnens nicht nur in der Entwicklung von neuen Technologien, sondern auch darin, die größten Herausforderungen der Menschheit zu adressieren. Unter Berücksichtigung wichtiger Zusammenhänge zwischen dem Höchstleistungsrechnen, der Politik und der Gesellschaft haben wir einen neuen Gesellschaftspolitischen Beirat geschaffen, der 2018 zum ersten Mal zusammengetroffen ist. Die Sitzung hat mehrere Themen identifiziert, die unsere Forschung voranbringen können und es dem HLRS ermöglichen werden, sich stärker als bisher auf die Bedürfnisse und Anforderungen der Gesellschaft zu konzentrieren. Dieses Jahr haben wir uns auch darüber gefreut, viele prominente Politikerinnen und Politiker aus Deutschland und Europa am HLRS willkommen zu heißen, um die Zukunft des Höchstleistungsrechnens und dessen Nutzen für die Gesellschaft zu diskutieren.

Der Schwerpunkt des HLRS auf die HPC-Weiterbildung verstärkte sich in diesem Jahr durch den Abschluss des ersten Moduls der Supercomputing-Akademie. Ihr Kursplan im „Blended Learning"-Format entspricht den Bedürfnissen der HPC-Nutzer aus der Industrie und ergänzt das wegweisende Schulungsprogramm des HLRS. Nach den vielen positiven Reaktionen der Ausbildenden und Teilnehmenden auf den ersten Testlauf der Supercomputing-Akademie freuen wir uns darauf, dieses innovative Programm in den nächsten Jahren wachsen zu sehen.

Ein weiteres Highlight von 2018 war die Gründung des Media Solution Centers Baden-Württemberg (MSC), in dem das HLRS eng mit unseren Partnern aus Industrie und Forschung arbeiten wird, um technischen Herausforderungen aus den Bereichen Medien und Kunst zu begegnen. Das MSC ist der neueste Bestandteil unserer industriellen Strategie, die mit dem Automotive Simulation Center Stuttgart (asc(s) begann. In diesem Jahr feierte das asc(s sein zehnjähriges Bestehen und demonstrierte somit, wie nachhaltig diese Strategie sein kann. Wir danken asc(s Geschäftsführer Alexander Walser dafür, dass er für diesen Jahresbericht mit uns über die Vorteile des Networking innerhalb der Automobilindustrie sprach.

In Bezug auf unsere Leistungskennzahlen kann das HLRS stolz auf ein erfolgreiches Jahr zurückblicken. Unsere Drittmitteleinnahmen stiegen über die letzten Jahre hinweg, unser Einkommen aus industrieller HPC-Nutzung war wieder auf einem hohen Niveau und die Anzahl der Personen, die von unserem Weiterbildungsprogramm und unseren Vorlesungen profitieren, blieb hoch.

Auch die Benutzer unseres HPC-Systems hatten ein sehr produktives Jahr. Dieser Jahresbericht verdeutlicht anhand einiger Beispiele aus der Forschung unserer Nutzer, wie wichtig Simulation für unser Wohlergehen ist. Dazu gehören ein Geräusch-Vorhersage-Modell, das helfen könnte, den Lärm von Maschinengeräuschen zu reduzieren; eine Machine Learning-Anwendung, die Kraftwerke effizienter machen könnte; sowie einen Berechnungsansatz, der den Weg zu einer neuen Halbleitertechnologie ebnet.

Mit diesem Jahresbericht bringen wir auch unseren Dank an unsere Unterstützer und Förderer zum Ausdruck, die uns diese Erfolge in 2018 ermöglicht haben. Gleichzeitig freuen wir uns darauf, die neuen Herausforderungen 2019 in Angriff zu nehmen.


IMPRINT

© Mathis Bode, Institute for Combustion Technology, RWTH Aachen

SPOTLIGHT

Engineering the Future

HLRS has decades of experience supporting computational engineering for academic and industrial research. With recent expansions in its infrastructure and services, it is now laying a foundation that will enable engineers and applied scientists to take full advantage of the next generation of faster supercomputers.

Located in the capital of the state of Baden-Württemberg, the High-Performance Computing Center Stuttgart (HLRS) sits at the epicenter of one of Germany's most dynamic regions for high-tech engineering. The region is not only home to prominent international concerns such as Daimler, Bosch, and Porsche, but also to a large and thriving ecosystem of small and medium-sized companies with a long tradition of manufacturing high-quality mechanical, electronic, and chemical products. Together, these communities have been a major engine of Germany's economic prosperity.

This regional strength in engineering has also played an important role in shaping HLRS's evolution. Based on the campus of the University of Stuttgart — itself a center for research and higher education with an emphasis on engineering and the applied sciences — HLRS has for decades maintained a state-of-the-art infrastructure for computational simulation, visualization, and data analytics. Such tools have become essential for creating models of natural phenomena that are so complex or that occur at such small scales that they are difficult to study in any other way. In engineering, the design of many precision products for which Germany is renowned has become unimaginable without such computational models.

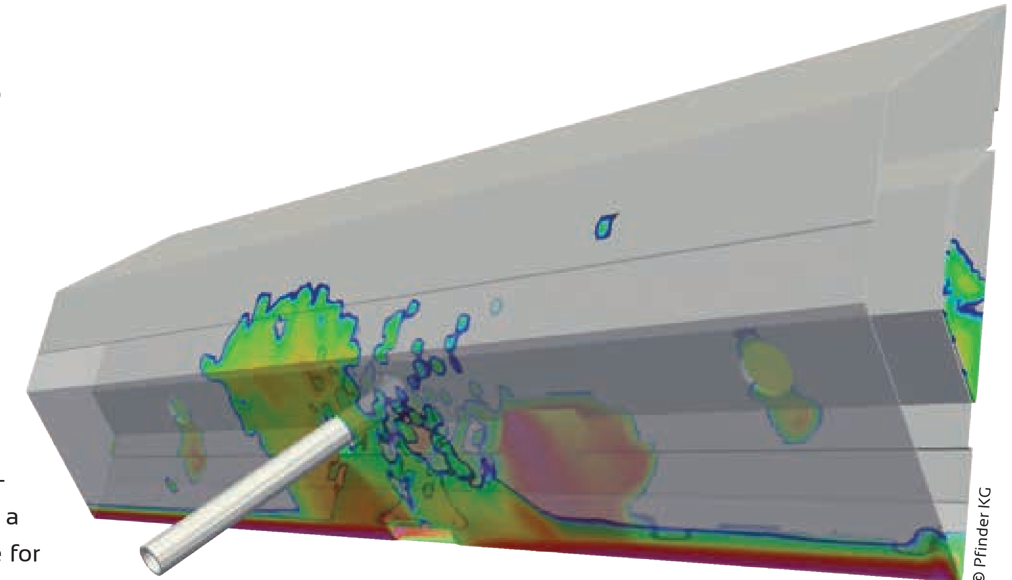
HLRS has long provided essential supercomputing resources for scientists in disciplines such as computational fluid dynamics, physics, chemistry, and materials science, among other fields. This includes not only academic researchers, but also scientists in industrial research and development — for example, in the automotive, energy, and aerospace industries. In fact, approximately 10% of HLRS computing hours are dedicated to industrial users, a figure that stands out as particularly noteworthy in Germany's academic supercomputing landscape.

Bridging the academic and industrial worlds in this way has enabled HLRS to develop expertise in applying high-performance computing (HPC) to many kinds of real-world computational engineering problems. This knowledge has, in turn, guided its strategy for growth. HLRS's goal of providing resources that optimally serve the needs of computational engineers has been a key driver of investments in its new computing infrastructure, professional training offerings, and in-house computer science research. As HLRS lays the groundwork for ever-larger supercomputers in the future, the center is also focused on providing the tools and services the engineering community will need to take full advantage of these resources as they become available.

HPC improves automotive manufacturing

For Stefan Hildenbrand at chemicals manufacturer Pfinder KG, HLRS has become an important partner, enabling the company to develop new services for clients in the automotive industry.

Pfinder supplies wax-based anticorrosive coatings that are typically applied by assembly line robots during car manufacture. As team leader for digital engineering, Hildenbrand performs computational simulations to



© Pfinder KG

Sample simulation of the application of wax to a sill. The colors indicate the thickness of coverage.

help optimize this process. Specifically, he uses OpenFOAM, a widely used software package for computational fluid dynamics, to predict how the coatings will behave when injected by a nozzle, the paths the droplets will follow through the air, and how they will form films on surfaces. These models are used to optimize the amount of fluid that needs to be sprayed for a specific application, to identify the best nozzle layout, and to ensure they are fully protective and durable.

Pfinder has a small parallel computing system in-house, but when complex questions arise or when results need to be delivered quickly, Hildenbrand turns to HLRS. "When we are deep in a project for a client that requires a large-scale simulation," Hildenbrand explained, "we can't wait four weeks to run the computation on our own system. HLRS makes it possible for us to quickly run a job on many hundreds of cores as opposed to on the 16 we have here. Instead of waiting for up to 4 weeks, this can deliver a result in as little as 3 to 4 days."

Being able to call on HLRS also has other advantages over installing its own larger HPC system. Because Pfinder's computational workload fluctuates widely, it would not make economic sense to install a large system of its own, only to have it sit idle for multiple months of the year. Moreover, Hildenbrand can be confident that HLRS uses reliable, state-of-the-art hardware that continually grows in power as HPC systems evolve. Keeping up with changes in HPC technologies would be impossible for a small company.

Having access to this kind of computing power became particularly important for Hildenbrand in 2018, when for the first time his team simulated the application of Pfinder coatings not just for one component, but for an entire automobile simultaneously. This jump in scale required a leap in computing power that was far beyond the reach of its own system. He anticipates continuing to utilize the HLRS supercomputer in the future, as this ability to model entire systems could offer a new market opportunity for his firm to provide complete coating application solutions.

Hawk to offer new capabilities for industrial production

Users of HLRS's HPC systems will soon have even more power at their fingertips. In November 2018, HLRS and Hewlett Packard Enterprise announced a joint collaboration to build a next-generation supercomputer that will be 3.5 times faster than Hazel Hen, HLRS's current flagship system. The upcoming supercomputer, called Hawk, will be the fastest in the world for industrial production, powering computational engineering and research across science and industrial fields to advance applications in energy, climate, mobility, and health. The 5,000-node Hawk system will have a theoretical peak performance of 24 petaFLOPs.

An important feature of Hawk is that its technical specifications were chosen with the specific needs of computational engineers in mind. Hawk's architecture is based on chip manufacturer AMD's next-generation EPYC processor, code-named Rome. HLRS picked the Rome processors because they utilize a memory subsystem that makes them particularly well suited for simulation applications in fields such as computational fluid dynamics, molecular dynamics, and other research areas in which many of HLRS's users are engaged. In addition, the AMD EPYC processors complement the use of competing processors at the other two centers in the Gauss Centre for Supercomputing — the alliance of Germany's three national supercomputing centers. The choice supports GCS's goal of offering its users a diverse set of computing architectures.

"We are excited that Hawk constitutes a sizable increase in the performance of our flagship supercomputing system," said Prof. Dr. Michael M. Resch, Director of HLRS. "But the real winners will be our user community of computational engineers in academic research and industry who will benefit from the ability to run much more complex simulations."

Getting to the next level

There is no doubt that larger supercomputers enable larger simulations and increase the number of core hours available for the research community. At the same time, however, it has become clear that building hardware alone is not enough to meet the growing needs of computational engineering. Writing software for large-scale parallel computing systems like Hazel Hen or Hawk is much more complex than running the same algorithm on a desktop computer or a small computing cluster. Indeed, developing and implementing effective and efficient codes for HPC systems requires specialized knowledge, and will be especially important as supercomputers approach the exascale, the next major plateau in computing power over that of current petascale systems. Optimizing codes for such extremely parallelized systems will be necessary to accelerate individual computational scientists' research and to make the operation of supercomputers more efficient — this will, in turn, help save energy and make HPC resources available to the largest number of potential users.

For many years, HLRS has recognized that the future of high-performance computing lies in developing and increasing access to state-of-the-art codes capable of scaling to ever-larger systems. For these reasons, the center has undertaken several projects aimed at preparing computational engineers for the future.

Bringing industrial engineering up to scale

In 2018, for example, HLRS became the lead coordinating center of a new Horizon 2020-funded research program called EXCELLERAT (European Centre of Excellence for Engineering Applications). A collaborative network including 13 partners from across Europe, EXCELLERAT will provide the HPC and engineering communities access to scalable applications and facilitate their availability through technology transfer. (See page 28 to learn more about EXCELLERAT.)

Recognizing the need for such resources and expertise, companies including Porsche, Ansys, and Festo have expressed support for EXCELLERAT. Aircraft manufacturer Airbus has also been an early participant in the project, as EXCELLERAT will enable academic knowledge to be connected with industrial needs.

In addition to EXCELLERAT, HLRS participates in projects focused on identifying and addressing opportunities for supercomputing in specific industries. For more than 10 years it has been a key partner in the Automotive Solution Center Stuttgart (see page 30), an alliance of companies that use simulation in automotive development and design. In 2018, it also joined the Hochschule der Medien und the Center for Art and Media in Karlsruhe (ZKM) in founding the Media Solution Center, an alliance of organizations interested in exploring opportunities for high-performance computing in the media arts. (see page 27). In coming years, HLRS intends to implement this solution center model to focus on increasing access to high-performance computing for health research and other areas.

Supercomputing-Akademie trains HPC experts in industry

Providing HPC training has long been a key activity for HLRS. In 2018, however, the center opened a new continuing education program designed with the needs of computational engineers in industry in mind.

To make these training activities as accessible as possible, the new program, called the Supercomputing-Akademie, uses a "blended learning" format. This means that only a small part of the training actually takes place in a classroom. Approximately 80% of a participant's time spent learning can be done online, making it easy for someone with a full-time job to join in the course alongside his or her normal responsibilities.

In July, the Supercomputing-Akademie — which is supported by the Baden-Württemberg Ministry for Social Affairs and Integration through the European Social Fund, and by the Baden-Württemberg Ministry of Science, Research, and Art — completed its first 15-week course on parallel programming. In 2019, it will begin offering a second course, focusing on simulation. In the coming years, the curriculum will grow to include additional modules on visualization; performance optimization; cluster, cloud, and high-performance computing; ecology and economics of supercomputing; and data management — topics that are of great interest to system administrators, programmers, and HPC software users in industry.

The Supercomputing-Akademie is just one component of an ongoing dialogue between HLRS and computational engineers in industry. Working with the nonprofit organization SICOS-BW, the center has for the last two years also organized the Industrial HPC User Roundtable (iHURT), a full-day event designed to promote information exchange in industrial R&D. This dialogue also enables HLRS to understand the most important challenges that HPC users in industry face, and will continue to guide its development of new infrastructure and services in the coming years.

Putting all the pieces together

In the coming decade, simulation, visualization, data analytics, and machine learning will remain critical for research and development, and will play important roles in addressing some of our greatest challenges. By identifying and focusing on the needs of engineers and applied scientists, HLRS aims to provide the widest possible access to such tools.

Representatives of the University of Stuttgart and Hewlett Packard Enterprise celebrated the contract signing for the new Hawk supercomputer.

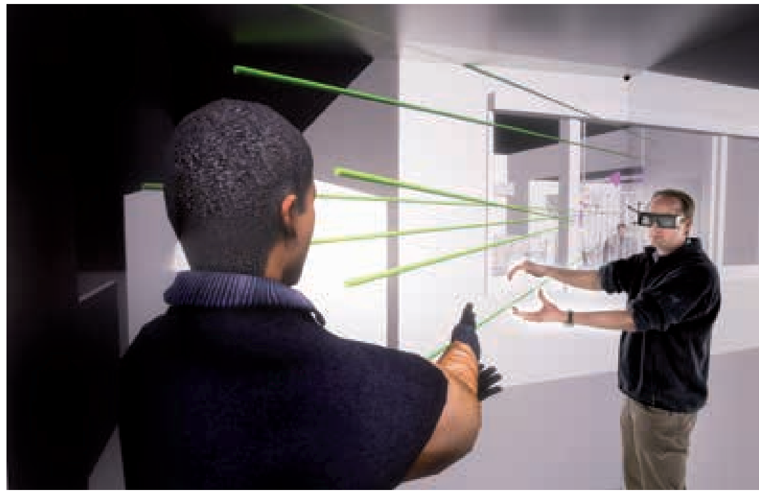
Installing the next-generation Hawk supercomputer in 2019 will be one important step toward this goal. Additionally, HLRS's ambitious training program and its outreach and training programs focused on industry are important parts of this effort. Through such activities, HLRS is positioned to be a key partner for innovation in Baden-Württemberg, in Germany, in Europe, and beyond. *(CW)*

NEWS HIGHLIGHTS

Günther Oettinger HLRS Director Michael Resch

Commissioner Oettinger Visits HLRS

As a longtime supporter of HLRS in his previous role as minister president of the state of Baden-Württemberg, European Commissioner for Budget and Human Resources Günther Oettinger is acquainted with the needs and challenges facing high-performance computing. On May 17 Oettinger and HLRS Director Michael Resch discussed the importance of a European strategy for high-performance computing capable of providing European scientists access to state-of-the-art technology. One topic of discussion was how European HPC will be supported through the EuroHPC Joint Undertaking (EuroHPC), which plans to fund two pre-exaflop systems and two exaflop systems in the coming years. Both Oettinger and Resch expressed a need to make high-performance computing available and productive for both scientific applications and industrial research. *(LB)*



HLRS Supports Crime Investigation with 3D Visualization

An October 8, 2018, episode of the ARD television program *Kriminalreport* focused on how 3D modelling and simulation can help solve complex crimes. The episode detailed methods the State Office of Criminal Investigations, Baden-Württemberg (LKA) uses in analyzing 3D images of crime scenes, as well as HLRS's recent advances in developing such approaches. HLRS Visualization Department leader Uwe Wössner explained that investigators can use visualization environments to accurately study bullet trajectories or conduct autopsies, among other aspects of crime scene investigation. Such methods can provide critical forensic evidence that would be hard to gather using other methods. In recent years, HLRS has been collaborating with the LKA to develop new methods for 3D-digital reconstruction of crime scenes to study them even more effectively. *(EG)*

HPC User Forum Considers State of European Supercomputing

Organized by HPC industry consultants Hyperion Research, the 2018 HPC User Forum took place at HLRS on October 1-2. It offered an intimate venue for promoting interactions among HPC users and technology suppliers, and provided insights into how supercomputers and their uses are evolving. In addition to updates from HLRS and its partners in the Gauss Centre for Supercomputing, the meeting featured presentations by Leonardo Flores (European Commission) on the EuroHPC Joint Undertaking; by Hyperion's Earl Joseph and Steve Conway on trends in the HPC industry; by leading HPC hardware manufacturers about technical challenges they face; by industrial HPC users focusing on autonomous driving; and by SICOS-BW, the Fortissimo Project, and the EXCELLERAT project looking at unique challenges faced by HPC users in industry. *(CW)*

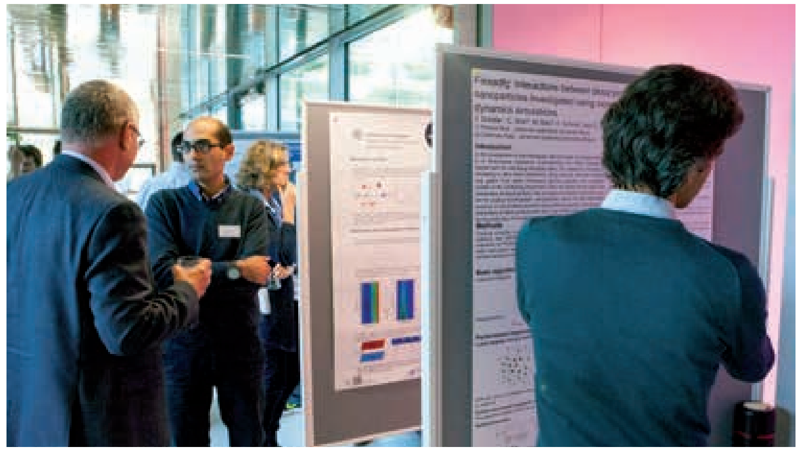
Stuttgart and Wuhan Sign Collaboration Agreement

On April 3, HLRS took its next step in strengthening its scientific cooperation in Asia. In a short ceremony in Wuhan, China, Supercomputing Center of Wuhan University Director Dengyi Zhang and HLRS Director Michael Resch signed an agreement pledging collaboration for the next three years. HLRS and the Supercomputing Center at Wuhan University plan to exchange scientists and to focus on key research topics in high-performance computing. Both sides will also share experience in installing large-scale computing systems. In addition to its cooperation with Wuhan University, HLRS maintains agreements with many other HPC centers in Asia, Europe, Russia, and the United States with the goal of promoting the exchange of HPC knowledge and expertise. *(CW)*

Dengyi Zhang Michael M. Resch

Golden Spike Awards Recognize Outstanding Research

Each year, the Results and Review Workshop offers an opportunity for HLRS supercomputer users to discuss their research and best practices in HPC. On October 4-5, the 21st annual workshop featured 41 user projects in 22 scientific talks and 19 posters. The event showcased research from computational fluid dynamics, climate research, computer science, chemistry, physics, and biology. At the workshop HLRS also presented Golden Spike Awards to representatives of three outstanding projects: Mathis Bode of RWTH Aachen ("Towards clean propulsion with synthetic fuels"), Travis Jones of the Fritz Haber Institute of the Max Planck Society ("Sulfur in ethylene epoxidation on silver"), and Christoph Wenzel of the University of Stuttgart ("DNS of compressible turbulent boundary layers with adverse pressure gradients"). *(CW)*



Girls' Day 2018

Girls' Day is an annual event that takes place across Germany to encourage girls to pursue careers in science, engineering, and information technology. As part of the 2018 festival, ten students between the ages of ten and twelve visited HLRS to learn about the world of high-performance computing. Visitors received a hands-on introduction to computing hardware, a tour of the HLRS computing room, and training in using the programming language Scratch. On their last stop, they hopped into a flight simulator in HLRS's 3D visualization room to paraglide virtually above the Black Forest. After learning to "fly," each girl obtained an HLRS pilot's license. Girls' Day offered the students enjoyable experiences that would raise their interest in technology; at the end of the day all agreed that they would take home good memories. *(AL)*

Illustris Project Featured on Postage Stamp

In December the Deutsche Post announced the release of a new postage stamp design featuring the Illustris project. The international scientific collaboration, led by Volker Springel at the Heidelberg Institute for Theoretical Studies in partnership with researchers at the Massachusetts Institute of Technology, Harvard University, and the Max Planck Institute for Astrophysics, has created the world's largest cosmological simulation of galaxy formation. Currently, the Illustris team is working with HLRS to run its next-generation simulations on Hazel Hen, a project called IllustrisTNG. In 2018 the project released five simultaneous papers documenting results of the first two IllustrisTNG simulations. The project is a two-time winner of the Golden Spike Award, an annual prize recognizing outstanding research using HLRS computing resources. *(CW)*

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Stuttgart Wins Formula SAE Michigan for Third Consecutive Year

The Formula Student Racing Team of the University of Stuttgart won the 2018 Formula SAE Michigan, the unofficial world cup of the international Formula Student network. It was the third consecutive year that a team from the University of Stuttgart won the contest. In addition to constructing a racecar and testing it on the track, team members presented it to experts from the motorsport, automotive, and aerospace industries. Teams are judged on the car's performance, design, construction, cost, and their sales presentations. HLRS has been an official supporter of the University of Stuttgart team since 2016, sponsoring computing hours for computational fluid dynamics simulations to improve the car's aerodynamics. "The support from HLRS is one of the cornerstones for developing our race cars," said team member Johannes Burgbacher. *(AL)*

Artist Visualizes Air Quality Problems in Stuttgart

For the Drehmoment Produktionskunst-Festival, organized by the KulturRegion Stuttgart, artist Michael Saup collaborated with HLRS to make the city's notorious air pollution visible. His virtual reality project, called *Staub* (*Dust*), interpreted and visualized sensor measurements of particulate emissions, integrating them with open-source street imagery and real-time data about traffic conditions. Visitors to the installation could wear a VR headset to explore this otherwise hidden environment. "It is inspirational to work with people who use similar tools but have a completely different sense of what to do with them," Saup said. "Exchanging ideas with people working in computing … can lead to new narratives about the future and what it could look like." The installation was shown in St. Maria's Church in Stuttgart for two weeks in October. *(CW)*

© Michael Saup

Third Annual German-Russian Workshop

On April 23-26, investigators from academic institutes across Russia and Germany met in Kaliningrad to forge closer ties between the two research communities and identify opportunities for potential shared research projects. The meeting was the third in a series of annual workshops organized to promote international dialogue. Following welcoming remarks by Prof. Dr.Sci. Boris Chetverushkin (Keldysh Institute of Applied Mathematics, Russian Academy of Sciences) and Prof. Dr.Sci. Andrei Klemeshev (Rector, Immanuel Kant Baltic Federal University), the packed three-day conference explored a wide range of topics related to HPC and its applications. Talks focused on scientific challenges in fields such as computational fluid dynamics, cosmology, and structural mechanics, and on cutting-edge methods in high-performance computing. *(CW)*

New Cloud-Based File System Offers Users Greater Flexibility

To enhance its user service, HLRS implemented a new Quobyte cloud-based file system. The system complements HLRS's existing Lustre file system, offering an optimal platform for users whose computation relies on millions of small data files. Because the cloud-based platform is connected to Baden-Württemberg's BelWü high-speed digital network, it also offers the possibility for users to access their data directly from their home institutions, speeding their research. In addition, the scalability and affordability of the new platform will permit users to save data on the system for the duration of their project allocations, rather than 60 days as required on Lustre. Moving suitable projects to the Quobyte system not only offers a cheaper solution but also reduces bottlenecks on the Lustre system so that it can be dedicated to projects for which it is best suited. *(CW)*

Minister of Hungary Visits to Discuss HPC in Europe, Industry

On October 19, Hungarian Minister for Innovation and Technology Prof. Dr. Laszlo Palkovics and Hungarian Foreign Trade Attaché Dr. David Bencsik visited HLRS. Following an introduction to HLRS research and industrial activities — focusing on collaboration between HLRS and the automotive engineering industry, particularly with respect to research on autonomous driving vehicles — Minister Palkovics and HLRS Director Michael Resch discussed the current high-performance computing landscape in Europe, including the EuroHPC joint undertaking and the Partnership for Advanced Computing in Europe. HLRS has existing collaborations with the University of Pécs and Hungarian Academy of Science, and both sides agreed to continue searching for new avenues for cooperation in autonomous driving and high-performance computing. *(EG)*

Michael Resch Laszlo Palkovics

Joseph Schuchart

Joseph Schuchart Wins Best Paper Award at IWOMP 2018

At the International Workshop on OpenMP in Barcelona, HLRS scientist Joseph Schuchart was recognized for his investigation of taskyield, an important piece of software for scheduling parallel computing tasks. Schuchart examined several potential implementations of taskyield, comparing their correctness and performance. Because it can be difficult to know how taskyield prioritizes tasks, he and his colleagues presented a test that can detect which variant of taskyield is used in different OpenMP compilers and runtimes. "Our motivation is to help developers and users by informing them about the weak spots of the taskyield feature and providing a tool that offers insights into the inner workings of OpenMP implementations," says Schuchart. In the future he intends to explore other types of applications and add to the research on OpenMP tasks. *(AL)*

HLRS Opens its Doors on Tag der Wissenschaft

On June 30 HLRS took part in the Tag der Wissenschaft (Science Day) at the University of Stuttgart. Welcoming more than 300 visitors, the event offered the general public an opportunity to experience high-performance computing and to learn about its use in research and technology development. Visitors toured the HLRS computer room and visited the CAVE, a 3D virtual reality facility. There, they enjoyed the thrills of piloting a driving simulator through city streets or flying a paragliding simulator high above a virtual landscape. Staff also demonstrated visualization applications for city planning, and HLRS Director Michael Resch presented a lecture titled "Simulation auf Supercomputern: Wunderwerke der Technik und des Geistes." The talk provided a lively introduction to supercomputing as well as its cultural and philosophical context. *(CW)*

Sustainability Days

This year's Nachhaltigkeitstage (Sustainability Days) at the University of Stuttgart took place in June as part of N!-Tage, a program focusing on sustainability efforts across the state of Baden-Württemberg. Bringing together sustainability initiatives at the University — including HLRS's sustainability in supercomputing program — the event promoted networking and idea exchange. Over the course of two days, it featured talks about sustainability challenges and progress the university is making, with a focus on the challenges of energy consumption and cooling in high-performance computing. "With the Nachhaltigkeitstage we want to demonstrate that sustainable action has to be an overarching goal that is based on a common conviction and will benefit all parties involved in the long run," says Sabine Eger, a member of the HLRS sustainability team. *(AL)*

Run for Digitalization

On July 27, digitalization experts ran around the University of Stuttgart's Vaihingen campus — literally. Held with special guests Thomas Strobl, Baden-Württemberg's Minister of the Interior, Digitalization and Migration, and ultramarathon runner Jürgen Mennel, the event, titled "Digitalisierung: Läuft," raised awareness of Baden-Württemberg as a location of digital expertise. During a press conference, HLRS Director Michael Resch emphasized that the state has the ideal foundation for a successful digitalization strategy, pointing out that HLRS's successful collaborations with municipalities and German industry could be further developed through collaboration among politics, industry, and the scientific community. Strobl praised Baden-Württemberg's progress in digitalization and encouraged ongoing persistence in the effort. *(LB)*

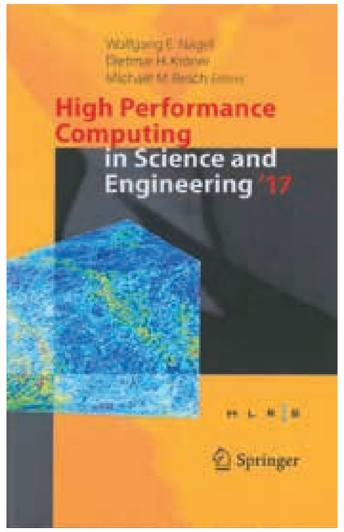

© Courtesy of KISTI

HLRS and KISTI Identify Collaboration Opportunities

Meeting in Daejeon, South Korea, HLRS Director Michael Resch and Korean Institute of Science and Technology Information (KISTI) President Dr. Choi Heeyoon identified several collaboration opportunities. One specific topic involves developing new tools for digital product design and fabrication. By combining HEMOS-Fluid (a software platform developed at KISTI for fluid analysis) with COVISE (a software environment developed at HLRS for simulation post-processing and visualization), the centers see opportunities to develop a powerful new approach for visualizing simulation data. The centers anticipate that pooling their institutes' expertise and strengthening collaboration on this topic could benefit the competitiveness of small- and medium-scale enterprises (SMEs) that use simulation in product design and development. *(CW)*

New Book: High Performance Computing in Science and Engineering '17

Including findings from researchers using HLRS high-performance computing systems in 2017, this book presents the state-of-the-art in supercomputer simulation. The reports cover all fields of computational science and engineering, ranging from computational fluid dynamics to computational physics, and from chemistry to computer science, with a special emphasis on industrially relevant applications. Presenting findings made possible by HLRS's Hazel Hen supercomputer, this volume covers the main methods in high-performance computing and applications that deliver a high level of sustained performance. Scientists and engineers will find accomplishments in achieving the best performance for production codes of particular interest. The book includes a wealth of color illustrations and tables of results.



HLRS Blooms

The spring of 2018 arrived at HLRS with more color than in the past. Led by the HLRS Sustainability in HPC Centers project, employees volunteered in late 2017 to plant beds of flower bulbs on the HLRS grounds. Their efforts paid off in April, when fields of crocuses and narzissuses burst through the earth. The activity was organized with the twin goals of strengthening biodiversity on the HLRS grounds and promoting feelings of wellbeing among the staff. In this way, it supported the general mission of the HLRS sustainability project, which aims through a wide array of activities to simultaneously address environmental, economic, and social dimensions of sustainability. *(CW)*

2nd Industrial HPC User Roundtable

Organized by HLRS and SICOS-BW, the second annual Industrial HPC User Roundtable (iHURT) focused on the diverse challenges that industrial users of HPC face, including complex programming codes, new technologies, licensing models, user support, and the organization of workflows, among others. Among the more than 30 participants were representatives from companies spanning a wide assortment of industries, including from Pfinder (supplier for the automobile industry), Putzmeister (cement pumping technology), Bosch, Porsche, Stihl, and BASF. Lectures by HPC users provided insights into a variety of industrial HPC user scenarios, covering topics including methods for simulating fire protection systems, the use of HPC in the development of new cement pumps, and the importance of HPC for the chemical industry. *(CW)*

New European Centres of Excellence Funded

Four new COEs will address important social and industrial challenges.

In 2018 the European Commission approved all proposals for "Centres of Excellence on HPC" (CoE's) containing an HLRS contribution, with HLRS participating in four out of nine funded EU CoE's in this call. HLRS will receive three-year funding totalling €7 million. The projects started operation in late 2018.

HLRS will play the largest role in EXCELLERAT (European Center of Excellence for Engineering Applications), acting as project coordinator thanks to its experience with industrial engineering partners. EXCELLERAT will support industrial HPC users by improving simulation technologies for engineering applications, making the development and testing of high-tech products safer and more efficient. The goal of EXCELLERAT is to support industry in scaling such applications to (pre)-exascale HPC systems.

POP 2 will support scientific users and software developers by helping them more efficiently parallelize and, in turn, improve the performance of their codes. Researchers who optimize their codes with HPC experts ultimately make better use of European supercomputers and improve their individual productivity.

The CheeSE project will use HPC to predict natural disasters quicker and more reliably in order to reduce response time.

HiDALGO will combine data analysis, machine learning, and HPC to address global challenges in finance, health care, migration, and energy. In this unique consortium, the computational and social sciences will join forces, with HLRS providing HPC expertise and its infrastructure for high-performance data analysis.

HLRS is also part of FocusCoE, a collaboration support action that will bring all nine CoEs together to facilitate knowledge exchange. HLRS will contribute to training activities aimed at identifying and solving shared problems among the CoEs. *(LB)*

HLRS is contributing to four new European Commission COE's.

HLRS Visualization Supports Stuttgart 21 Construction

3D virtual reality models created at HLRS helped engineers to successfully build a complex new kind of reinforced concrete column for the new Stuttgart train station.

In 2018 construction began on the most architectonically distinctive elements of the new Stuttgart central train station. The so-called "Kelchstütze" are a set of massive, chalice-shaped columns that will cradle windows to bring natural light into the subterranean station. At a height of over 12 meters and a diameter of approximately 32 meters, the elegantly curving forms of reinforced concrete promise to become a landmark in the city.

For construction engineers working on the project — called Stuttgart 21 — the columns' complex geometry created unique challenges. Although CAD drawings of the structures existed, the curving volumes and need to precisely arrange an enormous number of steel bars to reinforce the concrete proved more challenging than is the case with more conventional pillars.

To better plan the structures' fabrication, engineers at the Deutsche Bahn called upon HLRS to develop a 3D visualization. Using CAD and point cloud data, HLRS staff created an interactive digital model of one of the columns for display in the CAVE, a walk-in virtual reality environment.

Meeting at HLRS, representatives of the Deutsche Bahn and construction managers at Ed. Züblin AG could then explore and interact with the visualization to develop a strategy for erecting the column most efficiently and at the highest possible structural integrity. Once the first column was poured onsite, the HLRS team also created 3D scans of the physical structure to compare the virtual model to the actual column and determine whether it had been erected to specifications.

According to Uwe Wössner, who heads the HLRS Visualization Department, "The effort was extremely productive, as the participants had an easier time visualizing the complex geometry, identified problems in the original design, and were able to develop effective solutions." *(CW)*

A 3D visualization of one of the Stuttgart 21 "Kelchstütze," in the HLRS CAVE.

Supercomputing-Akademie Completes First Course

Using a "blended learning" approach, the new training program will provide engineers and computer scientists with essential HPC skills.

On July 17, fourteen participants completed the first three-month training module offered by the Supercomputing-Akademie. Participants included engineers and computer scientists interested in developing their skills for working in high-performance computing environments.

The course, which focused on code development for parallel computing systems, included interactive online content, animations, programming exercises, and explanatory videos. Participants also met with one another and with instructors in virtual online meetings. The course covered the architecture of parallel systems and programming models such as MPI and OpenMP, and taught participants how to use programming libraries and key parallelization concepts efficiently.

With funding from the European Union and the State of Baden-Württemberg, HLRS has been developing the Supercomputing-Akademie in collaboration with the University of Freiburg and University of Ulm, and in partnership with SICOS-BW, which promotes access to high-performance computing for small and medium-sized enterprises (SMEs). The Supercomputing-Akademie aims to provide continuing education program that is attractive for both large and small companies.

The Supercomputing-Akademie courses are conceived using a "blended learning" format, meaning that only a small part of the training takes place in a classroom. Approximately 80% of a participant's course time is spent online, reducing the need to travel to participate. Courses are held in the German language, focusing on the needs of the country's precision technology community.

The Supercomputing-Akademie's training program continues to develop with future modules to cover topics such as simulation; visualization; performance optimization; cluster, cloud and HPC; ecology and economics of supercomputing; and data management. *(CW)*

Sociopolitical Advisory Board to Help Guide HLRS Vision

A new multidisciplinary committee will provide counsel on how computer simulation can benefit society and help address its key challenges.

© Julian Rettig

Attendees at the first HLRS Sociopolitical Advisory Board meeting.

From predicting weather and discovering new medicines, to enabling the more efficient design of cars and traffic flow, simulation indirectly benefits society in many ways. However, it is also often driven by scientific or economic interests, while knowledge about it can be limited to experts in a particular field. This reality can lead to limitations in vision about how simulation could best benefit society.

"There is no question that computer simulations provide added value, but they must not be a privilege of elites," says HLRS Director Michael Resch. For this reason, he and Andreas Kaminski, head of the HLRS Department of Philosophy of Computer Simulation, convened the inaugural meeting of a new sociopolitical advisory board on April 9. "We want to ensure that a wider cross-section of society benefits from the use of simulation," Resch explained. The sociopolitical advisory board includes 13 members from different areas of society, representing socially relevant disciplines including nursing, architecture, design, art, education, and journalism.

"Simulation can make social phenomena more accessible to decision-makers and affected people," said advisory board chairman Prof. Ortwin Renn, Scientific Director at the Institute for Advanced Sustainability Studies in Potsdam. "Against the background of this progress, however, it must be ensured that ethical values are not violated and that social preferences are taken into account."

Discussions at the inaugural meeting focused on topics in which simulation can have an impact, such as urban development, social inequality, and populism, as well as questions regarding the methodology of simulations. In the future the board will gather and refine such thematic and methodologic ideas, with the goal of developing a pilot proposal for a research project. *(LB)*

SimTech Named National Center of Excellence

A University of Stuttgart research consortium focused on data-integrated simulation technologies was awarded a prestigious seven-year grant.

Since 2007 the Excellenzcluster SimTech (SimTech Center of Excellence) has nurtured a multidisciplinary community at the University of Stuttgart focused on the field of simulation. The cluster includes developers of models, methods, and other simulation technologies as well as computational scientists who use simulation for research in molecular and particle physics, mechanics, dynamic systems, and numerical mathematics.

Recognizing the University of Stuttgart's role as a national leader in simulation technology and applications, the Deutsche Forschungsgemeinschaft announced on September 27 its selection of SimTech as a national center of excellence in its latest funding cycle. This highly selective program supports key research centers that are advancing Germany's national strategy for scientific excellence.

The new grant will enable SimTech to grow in new directions. For the next seven years, it will focus on increasing capacities for data-driven simulation. Such applications are important in fields in which large amounts of data are produced using sensors, experiments, simulations, and other methods.

High-performance computing could enable simulation based on such datasets and so improving supercomputing infrastructure to enable efficient and effective high-performance data analytics is one of the key problems facing the field. For this reason, HLRS is an important partner in the SimTech cluster, with HLRS Director Michael Resch participating as a principal investigator for high-performance computing systems. "HLRS is well networked within SimTech and so we are delighted to see it once again recognized as a national center of excellence," said Prof. Resch. "Our collaborations with scientific investigators will not only support exciting new discoveries, but also enable HLRS to continue to improve its capabilities." *(CW)*

Perfusion MRI is a promising method for supporting therapy for multiple sclerosis. In one project, SimTech researchers conduct detailed small-scale simulations of how MR contrast agents spread in the brain. The method could potentially improve interpretation of images of MS-lesions.

Media Solution Center to Promote Innovation in Film and Digital Art

A new association will facilitate the integration of applications of high-performance computing and simulation into media production.

In October HLRS, together with the Center for Art and Media Karlsruhe (ZKM) and the Hochschule der Medien Stuttgart (HdM) founded a new association called the Media Solution Center Baden-Württemberg (MSC). The MSC's mission is to identify technical challenges in media production where high-performance computing and simulation could help, and to accelerate the development of technologies that address these needs.

The MSC will undertake collaborative research and development projects aimed at solving problems that media producers face. It will also facilitate sharing of the knowledge and technologies that result from these collaborations and organize events focusing on themes that are important to the media industry. One key set of application areas in which the MSC will be engaged includes animation, simulation, and visual effects (VFX). In coordination with the HdM, HLRS will also organize scientific continuing education activities that train people working in media to use high-performance computing more effectively. This includes focusing on the use and development of software for high-performance computing environments.

The MSC is open to membership of other individuals and companies working in the media industry — including animation studios, visual effects specialists, and arts organizations — as well as leaders of scientific and technical research groups in Baden-Württemberg whose work has relevance for media production. Ultimately, the MSC aims to facilitate a precompetitive exchange of knowledge and information among all organizations that choose to participate.

Prof. Dr. Bernd Eberhardt of the Hochschule der Medien was named chairman of the association. HLRS Director Prof. Dr. Michael Resch will serve as deputy chairman. *(CW)*

HLRS was recognized in 2017 with an HPC Innovation Award for its work with M.A.R.K. 13 and Studio 100 Media, who used high-performance computing to accelerate production of the animation film Die Biene Maja (Maya the Bee).

EXCELLERAT Will Bring HPC Applications to Engineering Industry

A new European Union Centre of Excellence coordinated by HLRS will support industrial HPC users in adopting more powerful hardware and software technologies.

Participants at the kick-off meeting of the EXCELLERAT Project.

HLRS launched EXCELLERAT (excellerat.eu), a new European Union Centre of Excellence (CoE) for engineering applications. With roughly €8 million in EU funding, the center includes 13 partners in 7 European countries. Its mission is to accelerate technology transfer of leading-edge HPC developments to the engineering sector.

EXCELLERAT will facilitate the further development of important codes for high-tech engineering, maximizing their scalability to increasingly large computing architectures and supporting the technology transfer that will enable their uptake within the industrial environment. These activities will support engineers through the entire HPC engineering application lifecycle, including data pre-processing, code optimization, application execution, and post-processing. In addition, EXCELLERAT will provide training that prepares engineers in industry to take advantage of the opportunities that the latest HPC technologies offer.

EXCELLERAT will work with consortium partners who have developed important codes for academic applications in engineering fields such as aerospace, automotive, combustion, and fluid dynamics. To facilitate the codes' integration into real-life industrial applications, these partners will work closely with end users outside the consortium. This will ultimately lead to fast feedback-cycles in all areas of the HPC engineering application lifecycle, from consultation on methodology and code implementation to data transfer and code optimization. End users will benefit by gaining first-hand access to the project results. This concept of a one-stop-shop for all services is unique in the area of industrial HPC. *(LB)*

Building a Sustainable HPC Infrastructure

A two-day meeting at HLRS focused on the challenges of designing environmentally responsible facilities for supercomputing.

The march toward faster, more powerful supercomputers shows few signs of slowing down. Although such growth is good for science and technology development, it also leads to increased physical needs for supercomputing centers — building spaces able to accommodate larger machines, cooling systems that efficiently manage greater heat production, and energy to keep everything running. How can the need for more resources be managed in a sustainable way?

On October 23-24, IT specialists and research infrastructure experts from the German-speaking HPC community met at HLRS to discuss holistic strategies for addressing such challenges. The event — the second annual meeting organized by HLRS on the topic of sustainability in supercomputing centers — revealed how sensors, new cooling technologies, and creative planning can make HPC more sustainable, while at the same time highlighting some important challenges and problems to be addressed.

The goal of any design for a supercomputing center is to have the newest technology installed when the center opens. But considering the fact that erecting a brick and mortar structure can take 5-7 years, the best technologies often only become available after a project is underway. As the meeting revealed, this fact requires close communication among stakeholders and a planning approach that accounts for future expansion or other potential requirements that could arise when new technologies materialize. In addition, close cooperation with funding agencies and implementing better metrics for tracking progress toward sustainability are important parts of the puzzle. *(CW)*

Networking the German Auto Industry: An Interview with Alexander Walser

Competition in the automobile industry is intense, but the Automotive Simulation Center Stuttgart has showed that cooperation can offer important advantages.

Car manufacturer Porsche has long used computer simulation resources at HLRS to develop better vehicles. In the early 2000s, however, it became clear that existing commercial software packages were not keeping pace with the constantly doubling performance of new supercomputing hardware. To accelerate the development of more efficient and effective simulation software, Porsche joined forces in 2008 with HLRS, Daimler, Opel, and other companies — with support of the Baden-Württemberg Ministry for Science, Research, and the Arts — to found the Automotive Simulation Center Stuttgart, also called asc(s.

Since then the asc(s has built a network of large and small companies from across the automobile industry, with HLRS playing a central role. Recently, we spoke with asc(s Director Alexander F. Walser about the association's activities, HLRS's contributions to them, and why simulation is growing in importance for the field.

? How do you describe the asc(s?

› The asc(s is a nonprofit association that brings car manufacturers, software developers, hardware manufacturers, engineering service providers, start-ups, and scientific organizations together to steer the future of virtual automobile development. Just as an OEM (original equipment manufacturer) can buy a screwdriver to build a car, we try to ensure that manufacturers have access to the simulation methods they need. To make this possible, the asc(s gathers the critical mass of interested parties necessary to get projects off the ground, in terms of expertise or financing.

It is also important to our mandate to integrate small and medium-sized enterprises (SMEs), as well as scientific institutions. SMEs sometimes develop very innovative software packages, but if the interfaces aren't built correctly or if the workflow doesn't fit, industry might not be able to use them. Getting OEMs and SMEs to work together reduces this risk. Building these relationships also incorporates industry's needs into software development early and makes it possible to design solutions that meet the needs of multiple OEMs at the same time.

Ten years ago the foundational idea of the asc(s was very innovative. Today, it fits contemporary needs perfectly and in the future it will be indispensable for driving innovation.

? What role does HLRS play in this network?

› High-performance computing is a key focus at the asc(s, a fact that distinguishes our organization from other interest groups in the automotive industry. It is only through our work with HLRS that we can maintain this strong focus on HPC.

Cooperation with HLRS enables us to have access to the newest hardware architecture. HLRS is always a step ahead of what's available in industry, where the update cycles are longer and the cluster sizes are smaller. Using HLRS resources, we can show relatively early that new methods will work on future cluster systems.

The projects we work on are very diverse in terms of the number of computing cores used or of the parallelization necessary to achieve research goals. By including HLRS in project planning, we also learn about potential problems and how to address them.

Another important question for OEMs and small businesses is how to design a workflow that connects the workstation under your desk with the HLRS cluster system. In the past we have built workflows in which data and results are automatically transferred between classical workstations and HLRS using only the necessary software resources. In practice this means that engineers don't just push everything onto the HLRS supercomputer, but rather they can integrate it into their workflows.

? What are the most important topics in simulation for the future of automobile design and development?

› Ten years ago no one was talking about self-driving vehicles. Electric cars were a theme that was in the air, but not something that was as prominent as it is today. Now everything must develop much, much faster.

Virtual crash tests — which are necessary for safe and efficient development — are also becoming increasingly important. Countless test scenarios need to be conducted, raising the question of how HPC and driving simulation can be better combined. In the medium-term, such tests will have to be conducted on a supercomputer.

Technological trends related to artificial intelligence are also gaining in importance. This will result not only in the use of the newest AI-technologies in driving systems, but also in asking how we can use AI to lessen the burden on engineers during the virtual development process. How can we apply AI in designing simulation models? How can we extract more knowledge from the simulation results that now exist?

Because of these new trends, the horizontal networking of automobile manufacturers that the asc)s promotes is very important, particularly as new key players enter the market that have never been integrated into the supply chain.

? What plans does the asc(s have to make the automotive industry better and to prepare for the future of simulation?


asc(s Director Alexander F. Walser

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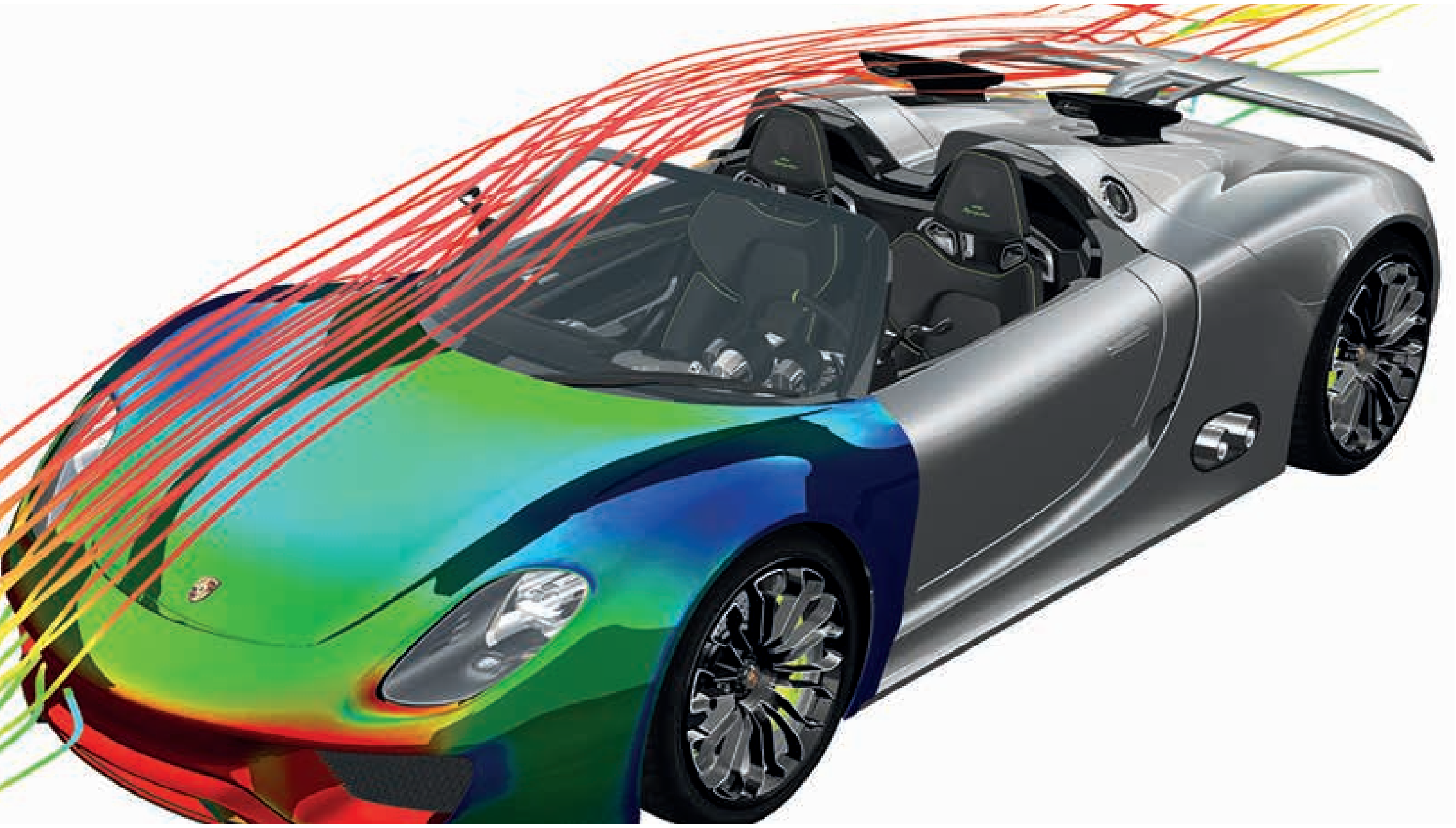


Simulation is becoming ever more important for the auto industry. This presents an important question: what qualifications will tomorrow's simulation engineer or even an engineer in another field need?
At the asc(s we have been asking ourselves how we could support our member organizations by helping to ensure that university students gain the right knowledge during their studies. This includes engaging in dialogue with universities, as well as finding ways to motivate students to study virtual automobile development and to select the best program of study.
The need for experts in simulation is constantly growing. By promoting young investigators and helping them to quickly become integrated into the development process, we can not only offer advantages for industry but also strengthen Baden-Württemberg as a center for research. We expect that this kind of cooperation will grow stronger in the future. *(CW)*

Student Dives into Data to Predict Train Delays

As a participant in the HLRS program Simulated Worlds, high school student Niklas Knöll used machine learning to investigate a common problem.

Smartphone apps from the Deutsche Bahn and Stuttgart's local transit networks can show delays of trains and buses in real-time. But wouldn't it be nice to know earlier whether there's time to stop at the bakery for a pretzel?
As a high school student living in Stuttgart, Niklas Knöll is very familiar with this problem. In 2018 he was one of eight scholars who participated in Simulated Worlds, an initiative of the Baden-Württemberg Ministry of Science, Research, and the Arts. Over the school year, students receive €1,000 to conduct a research project at HLRS, receiving supervision from HLRS employees. The aim is to prepare young people for the digital realm.
At HLRS students were encouraged to analyze big datasets. Niklas accessed public data from the Deutsche Bahn and learned to analyze it using the programming language Python and the programming framework Apache Spark, tools that are often used for solving big data problems on supercomputers. He developed models and trained them using machine learning algorithms to predict train departures to the minute. In 8 out of 10 cases his approach could clearly predict whether a city train would leave at least three minutes late.
From a strictly statistical point of view, this result was not fully satisfying because the database Niklas used

was too small for a big data problem. But Simulated Worlds' aspiration is not to produce scientific breakthroughs. Most importantly, it provides the participating scholars with advanced technical competencies and problem-solving skills. These skills were on display at an awards ceremony at HLRS on July 4, when Niklas and the other participating students presented their projects and results. According to Simulated Worlds project coordinator Doris Lindner, "Everyone was impressed by how thoroughly the students had studied their subject." *(LB)*

HLRS by the Numbers

Staff
155

Visiting Researchers
23

- 78 SCIENTISTS
- 49 NONSCIENTISTS
- 5 RESEARCH ASSISTANTS

System Usage

- 1.28 BILLION — CORE HOURS PRODUCED
- 107 — USER PROJECTS
- 36 — INDUSTRIAL CUSTOMERS
- 63 — USER PUBLICATIONS

Education and Training

41 CONTINUING EDUCATION COURSES
- 997 Participants
- 129 Course-Days

12 SCIENTIFIC WORKSHOPS
- 451 Participants
- 24 Days

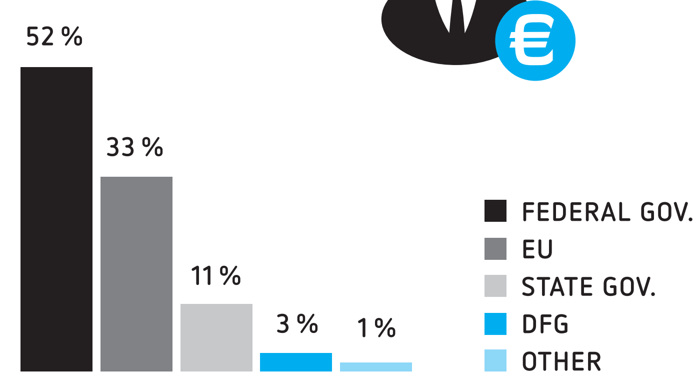
22 UNIVERSITY LECTURES
- 2,733 Participants
- 36 SWS

HL RS

Visitors at HLRS
2,142

Talks
44

Third-Party Funds
8,136,138



Staff Publications

- 20 PAPERS IN JOURNALS, BOOKS, AND CONFERENCE PROCEEDINGS
- 2 BOOKS

Enhanced User Support Improves Performance of HPC Systems

Providing personalized guidance to HPC users results in faster codes and more efficient use of computing resources.

Since 2007 the Gauss Centre for Supercomputing (GCS) — the network of Germany's national supercomputing centers that includes HLRS, the Jülich Supercomputing Centre, and the Leibniz Supercomputing Centre — has coordinated the installation and operation of world-class systems for high-performance computing. In 2018 it expanded in an important new direction, implementing enhanced user support services that will empower scientists to use these systems more efficiently.

"Every time you help individual users to utilize the machine more efficiently you enhance the capabilities of the computer as a whole," says Thomas Bönisch, leader of the HLRS user management team. "By ensuring that applications are optimized for the computing hardware they are run on, we can get a lot more science out of the same computing resources."

Enhanced user support involves more than helping users port codes or transfer data. Instead, scientists receive hands-on, personalized advice for improving their codes' performance on HPC resources. This can occur at several levels: selecting and optimizing the best algorithm for a particular problem and supercomputer, improving its ability to scale up to parallel computing networks, structuring it to take advantage of unique characteristics of the specific processors that make up the system, and eliminating bottlenecks in the movement of large datasets.

While some computational scientists develop their own computational tools for analyzing a scientific problem, others rely on community-built codes or open-source software. In either case, they can benefit from the help of HPC experts in selecting the best tools and optimizing their performance. This can make a big difference, making it possible to ask new, more computationally demanding kinds of scientific questions.

Since 2016 HLRS has held a biannual optimization workshop in which Hazel Hen users meet with support staff to identify opportunities for improving their codes' performance. These meetings have been very productive, resulting in improvements in runtime and data transfer speeds; in some cases, codes can end up running twice as fast, or faster.

With grants provided by the Baden-Württemberg Ministry of Science, Research, and Art, HLRS added new staff positions in 2018, each of which is dedicated to supporting specific user groups all year round. In this way, deeper collaborative relationships can develop in which experts in scientific domains and experts in high-performance computing regularly exchange ideas, working together to continually improve computational tools.

This enhanced user support initiative has also made it possible to improve coordination of user support activities between HLRS and its GCS partner institutions. Representatives of the three centers now meet regularly to share knowledge about their accomplishments in improving computational efficiency. This dialogue also enables the three centers to address the needs of users who compute at multiple GCS sites in a more coordinated way. In this way, the initiative promises to raise the performance of users' codes across Germany's entire national supercomputing infrastructure. *(CW)*

Attendees at an HLRS optimization workshop receive guidance on improving their codes.

EUXDAT: Taking Agriculture into the Cloud

High-performance data analytics holds enormous potential to improve efficiency in food production.

In the past, farmers consulted books like *The Farmer's Almanac* to know which crops to plant, when to plant them, and when to harvest them. As in other industries being transformed by the Internet of Things, however, digital tools have initiated new thinking about the future of agriculture. High-resolution weather and climate models and sensors for measuring soil moisture and composition, for example, offer rich sources of data that could make farming more productive. The challenge now is to design systems to integrate, interpret, and apply this information.

As part of a multidiscplinary European Union-funded innovation project called EUXDAT (European e-Infrastructure for Extreme Data Analytics in Sustainable Development), researchers at HLRS are developing a software platform to address this need. The goal is to create an off-the-shelf product hosted in the cloud that could make big data analytics available to anyone in agriculture. In cases where analysis of extremely large datasets is needed, users could access high-performance computing resources at HLRS through the web. Having access to such a product could, for example, enable farmers to identify the optimal time to fertilize their crops to produce the best harvest.

Atos, a European provider of business technology, invited HLRS to join the project because of its expertise in high-performance computing, cloud computing, and big data analytics. According to Dr. Michael Gienger, who heads the cloud computing research group at HLRS, "For us, this is the best of all possible projects, because it combines many key areas of expertise at HLRS, while offering an opportunity to test new approaches for integrating cloud and HPC technologies in a field that could really benefit from it." *(CW)*

Learn more about how data analytics and cloud computing can support agriculture at www.euxdat.eu.

PhD Graduates 2018

Three students completed their doctoral studies at HLRS in 2018. Read more about their dissertation topics below.

Björn Bliese

An Augmented Reality System Suitable for Geometric Analysis in Product Development

Augmented reality offers the potential to perform geometric analyses between physical and virtual models in product development and production planning, although today it is rarely used in practice. Bliese's thesis defines basic requirements for a usable AR system for geometric analyses and improves upon the chosen system components. It provides a process-driven user interface to guide a user through an AR-assisted investigation. The developed AR system is finally evaluated within a usability study.

Marius Feilhauer

Simulation-Supported Safeguarding of Driver Assistance Systems

In theory, ensuring that an autonomous vehicle drives safely would require programming it to recognize all possible situations, including various traffic or lighting conditions. This is impossible, however. In his thesis, Feilhauer proposes an expandable catalog of traffic scenarios that would grow as it incorporates lessons learned based on real or virtual driving test data. Driving scenarios could be investigated in virtual test drives on computers, with the results being fed back into the catalog. Such a resource would improve iteratively, benefiting the training of machine learning applications for autonomous driving.

Matthias Nachtmann

Model-Centric Task Debugging at Scale

With the increasing complexity of HPC hardware and software, there is a need for tools to support computer scientists and engineers in efficiently porting and optimizing their computational codes regardless of what system they are using. In addition, researchers want to be able to debug their applications within their respective programming models. In his thesis, Nachtmann focuses on further developing this "model-centric" debugging approach, spearheading the redevelopment of the backend of the HLRS-developed TEMANEJO graphical debugging tool.

Looking Inside Simulation's "Black Box"

Visiting scholars in the HLRS Department of Philosophy of Computer Simulation work toward a clearer understanding of computational research and its limitations

Simulation and other applications of high-performance computing have become indispensable tools for research in the basic and applied sciences. Employing HPC has had many positive impacts, helping to strive for a deeper understanding of our world and enabling the development of new technologies. As our reliance on computer simulation grows, however, many wonder how it is changing science, technology, politics, and society, and how we should react.

As a supercomputing center, HLRS is unusual in that for many years it has prioritized discussion about such issues. Through its Department of Philosophy of Simulation, HLRS promotes interdisciplinary dialogue among simulation scientists, philosophers, historians of science, sociologists, and other scholars whose insights enable reflection on the nature of simulation.

In 2018, the Department of Philosophy of Simulation hosted two visiting scholars — PD Dr. Johannes Lenhard (Philosophy Department, University of Bielefeld) and Prof. Dr. Nicole J. Saam (Institute for Sociology, Friedrich-Alexander-Universität Erlangen-Nürnberg). Their research highlights some key questions facing the philosophy of simulation today, and their experiences at HLRS show the benefits of promoting multidisciplinary discourse.

Simulation yesterday and today

Johannes Lenhard initially trained as a mathematician, but in 2001 became captivated by philosophical and historical questions related to the growing use of computing across many scientific disciplines. He realized that a conceptual framework was needed for discussing the deeper implications of this trend, "For philosophers of science," Lenhard says, "one important problem is what it means for a scientist to know something. In the case of computer simulation, is the knowledge it produces different from that produced by older methods? If so, how? As a historian, one can also ask how the conditions in which computer simulation is used have changed over the years. This gives us a better understanding of how simulation is used today." In his research Lenhard has written about features that distinguish today's computer simulation from earlier mathematical modelling.

One example is the change in experiments using simulation. Supercomputers enable scientists to easily adjust a mathematical model's parameters so that it approaches observed data. Deep learning algorithms using neural networks are perhaps the best examples of this approach; by adjusting parameters, scientists gain the ability to model almost any behavior. But although such a capability can be useful, Lenhard asks, is it still science?

"The idea that general laws can reveal order in chaos is historically connected to the idea that these laws can be formulated mathematically," Lenhard says. "But newer kinds of computer modelling have nothing to do with finding such general laws. Today, we hope to describe and manage things in a predictable way, even if we don't have a law for it." In this sense, computer simulation is different from some earlier scientific approaches, but offers completely new options.


Nicole J. Saam


Johannes Lenhard

The opacity of simulation

Perhaps the most interesting philosophical problem in computer simulation is the result of what philosophers call its "opacity." Often, a computer simulation behaves in unexpected ways. In many cases it is impossible to determine why, because it is impossible to mechanistically observe how an algorithm functions. "This turns the idea of mathematical modeling on its head," Lenhard says, "because we used to think that mathematical models should be able to make the causes of a behavior crystal clear."

During her residency at HLRS, Nicole J. Saam has been developing a systematic method for defining, categorizing, and measuring such opacity. Although her project is still evolving, such a model might address factors such as instability in the numerical model itself, methods to simplify a model to reduce computational effort, and the number of different research teams involved in developing a model, each of whom only understands a small piece of the project. Such criteria address the fact that opacity in computer simulation can have technical, mathematical, and social origins.

After defining the dimensions of opacity, Saam has developed a scientific framework and questionnaire. Her team has started conducting interviews with groups of scientists who run their simulations at HLRS in order to gain a more precise understanding of opacity in all of its different forms.

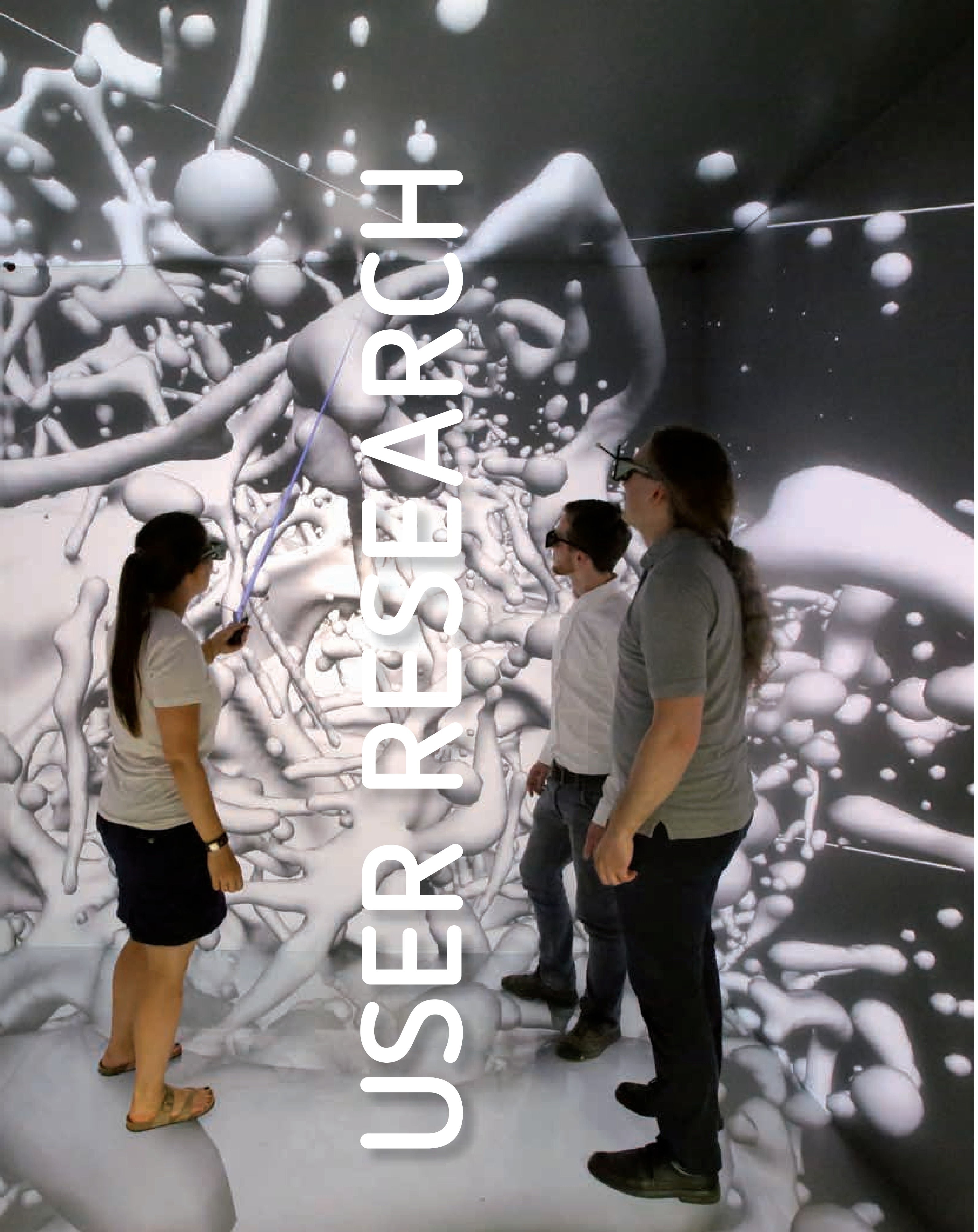
"Opacity can look quite different from the perspective of a principal investigator in comparison with that of a graduate student," Saam points out. "Because of each's degree of experience, their perceptions of opacity can be different. Is opacity an objective condition of simulation, or is it a subjective experience that varies from individual to individual? As defined now, opacity is a relational concept. We would love to have a way to measure this."

Saam also anticipates a practical use for such a tool. "If one could know in advance which kinds of simulation models typically suffer from specific problems due to opacity," she suggests, "one might be able to identify and avoid typical problems early in the process of implementing a model." What might at first seem to be a theoretical issue could thus enable tangible improvements in how simulation is done.

The value of interdisciplinary dialogue

Bridging the conceptual divides between scientists and researchers in the humanities and social sciences is not easy, but Saam's project suggests why it is important to make the effort. "Sometimes it can take years or even decades to get scientists and researchers from diverse disciplines such as natural sciences, engineering sciences, humanities, or the social sciences to have a productive conversation," Saam remarks. "The opportunity for me to work directly with simulation scientists here at HLRS is very unusual."

Lenhard agrees. "I find it wonderful that HLRS has a group whose job it is to talk with interested scientists about their work, and to promote greater self-reflection about what they are doing," he observes. "It is something that the scientific community and society in general need to do more often." *(CW)*



Supercomputer Enables Sound Prediction Model for Noise Control

Combining principles from computational fluid dynamics and acoustics, researchers at the TU Berlin have developed a model that could simplify the process of designing noise cancelling structures for airplanes, ships, and ventilation systems.

Noise-cancelling headphones have become a popular accessory for frequent flyers. By analyzing the background frequencies produced by an airplane in flight and generating an "anti-noise" sound wave that is perfectly out of phase, such headphones eliminate disturbing background sounds. Although the headphones can't do anything about the cramped seating, they can make watching a film or listening to music in flight nearly as enjoyable as at home.

To minimize the disturbing noise caused by loud machines like cars, ships, and airplanes, acoustic engineers use many strategies. One technology, called a Helmholtz cavity, is based on a similar concept to that used in noise-cancelling headphones. Here, engineers build a resonating box that opens to a slit on one side. As air passes over the slit, the box vibrates like a church organ pipe, producing a tone. By adjusting the size and shape of the cavity and its slit, acoustic engineers can tune it to produce a specific tone that — like the headphones — cancels a dominant, irritating sound produced by machinery.

Historically, the process of tuning a Helmholtz cavity was a brute force undertaking involving costly and time-consuming trial and error. Engineers had no other choice but to physically build and test many different geometries experimentally to find an optimal shape for a specific application, especially in an environment of turbulent flow. Today, however, high-performance computing offers the potential to undertake such tests virtually, making the design process faster and easier.

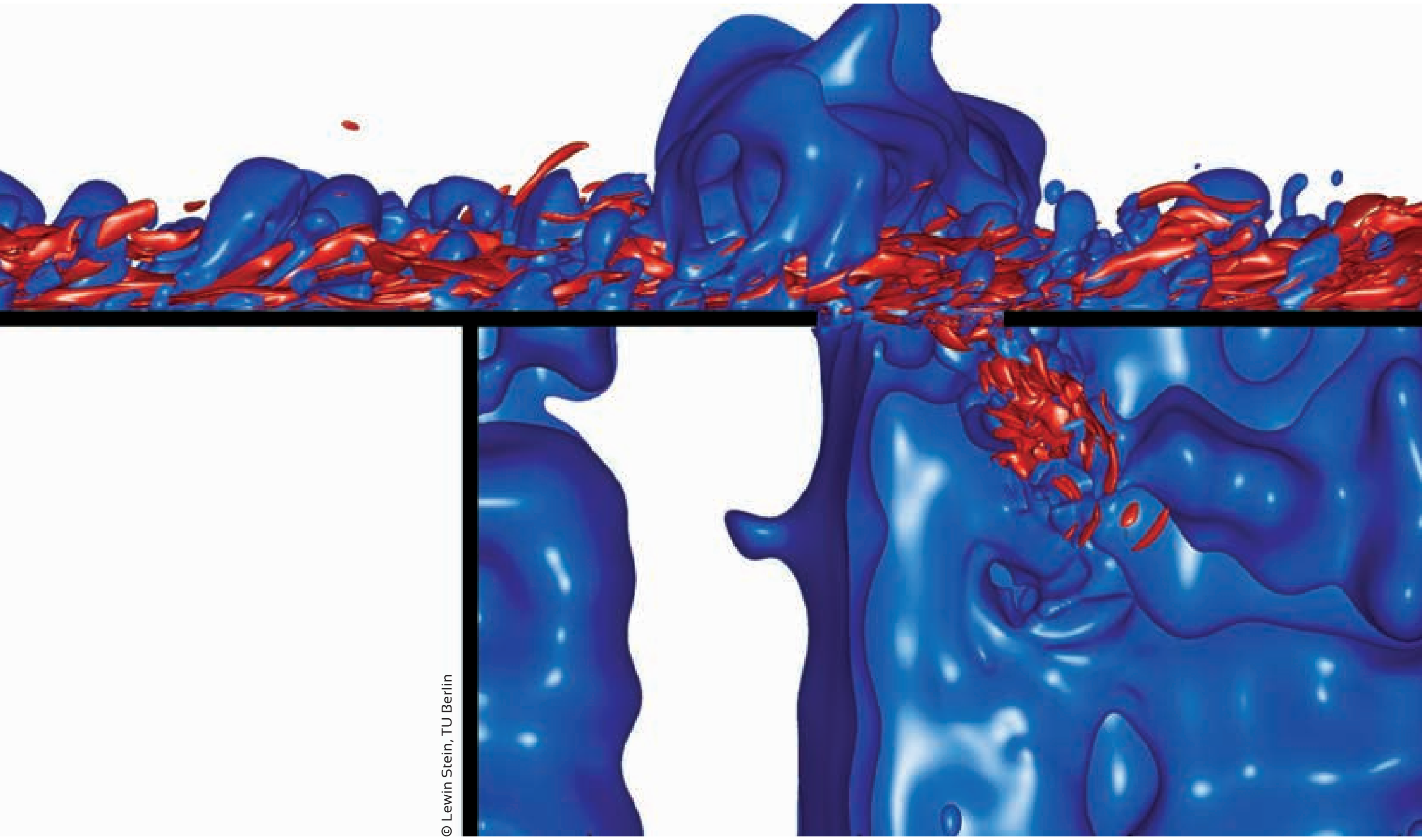
In a paper published in the journal *Acta Mechanica*, Lewin Stein and Jörn Sesterhenn of the TU Berlin describe a new analytical model for sound prediction that could make the design of Helmholtz cavities cheaper and more efficient. The development of the model was facilitated by a dataset produced using direct numerical simulation at the High-Performance Computing Center Stuttgart (HLRS).

The analytical model can predict, in a way that is more generally applicable than before, a potential Helmholtz cavity's sound spectrum as turbulent air flows over it. The authors suggest that such a tool could potentially be used to tune Helmholtz cavities to cancel out or to avoid any frequency of interest.

Simulation approaches all the scales of nature

When moving air passes over the slit of a Helmholtz cavity, its flow becomes disrupted and turbulence is enhanced. Vortices typically arise, detaching from the slit's upstream edge. Together they form a sheet of vortices that covers the slit and can interact with the acoustic vibrations being generated inside the cavity. The result is a frequency-dependent damping or excitation of the acoustic wave as air passes through this vortex sheet.

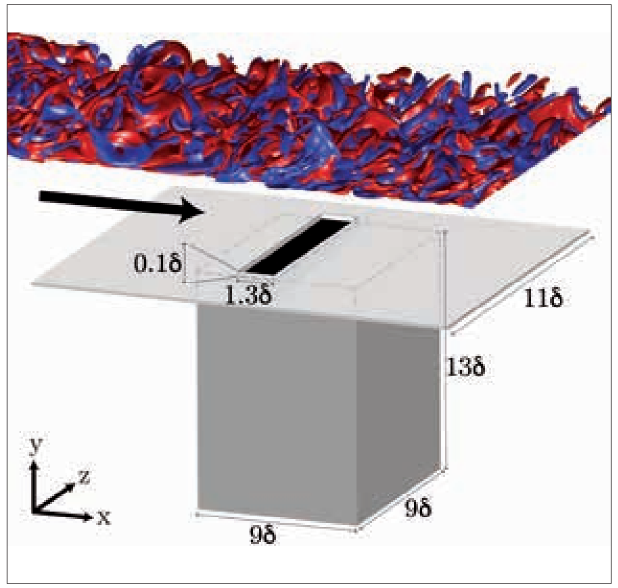
In the past it was difficult to study such interactions and their effects numerically without making crude approximations. For the first time, Stein's simulation realistically integrates turbulent and acoustic phenomena of a Helmholtz cavity excited by a turbulent



flow passing over its slit. At an unprecedented resolution, it makes it possible to track the flow–acoustic interaction and its implications for the cavity's resonance.

This achievement is possible using a method called direct numerical simulation (DNS), which describes a gas or liquid at a fundamental level. "I'm using the most complex form of fluid equations — called the Navier–Stokes equations — to get as close as possible to the actual phenomenon in nature while using as little approximation as necessary," Stein says. "Our DNS enabled us to gain new insights that weren't there before."

Stein's direct numerical simulation divides the system into a mesh of approximately 1 billion grid points and simulates more than 100 thousand time steps, in order to fully resolve the system dynamics for just 30 milliseconds of physical time. Each run of the numerical model on HLRS's Hazel Hen supercomputer required approximately four 24-hour days, using some 40,000 computing cores. Whereas a physical experiment is spatially limited and can only track a few physically relevant parameters, each individual DNS run provides a 20-terabyte dataset that documents all flow variables at all time steps and spaces within the mesh, delivering a rich resource that can be explored



in detail. Stein says that running the simulation over this time period provided a good compromise between being able to set up a reliable database and getting results in a practical amount of time.

Moving toward a general sound prediction model

Once the details of the acoustic model were developed, the next challenge was to confirm that it could


Lewin Stein

predict acoustic properties of other Helmholtz cavity geometries and airflow conditions. By comparing the extrapolated model results with experimental data provided by Joachim Golliard at the Centre de Transfert de Technologie du Mans in France, Stein found that the model did so with great accuracy.

The model reported in the paper is optimized for low speed airflows and for low frequencies, such as those found in ventilation systems. It is also designed to be modular so that a cavity that includes complex materials like foam instead of a hard wall can be investigated as well. Stein anticipates that gaining more computing time and access to faster supercomputers would enable him to numerically predict a wider range of potential resonator shapes and flow conditions. Having recently completed his PhD and now working as a postdoc at the Institute of Fluid Dynamics and Technical Acoustics in the group of Prof. Sesterhenn (TU Berlin), Stein foresees some attractive opportunities to cooperate with industrial partners and possibly to apply his model in real-life situations. "Although I studied theoretical physics," he explains, "it is fulfilling to work on problems that reach beyond pure academic research and can be applied in industry, where people can potentially profit from what you've accomplished. This latest paper is an opportunity to prove the utility and applicability of our work. It's a great moment after years of working on a PhD." *(CW)*

Using Computational Chemistry to Investigate New Semiconductor Technologies

University of Marburg researchers are exploring how functionalizing silicon with other compounds could make light-based signaling in semiconductors feasible.

As new methods have become available for understanding and manipulating matter at its most fundamental levels, researchers in the interdisciplinary field of materials science have successfully synthesized new kinds of materials. Often the goal is to design materials that incorporate properties that can be useful for performing specific functions. Such materials can, for example, be more chemically stable or resistant to physical breakage, have advantageous electromagnetic characteristics, or react in predictable ways to specific environmental conditions.

Dr. Ralf Tonner and his research group at the University of Marburg are addressing the challenge of designing functional materials in an unusual way — by applying approaches from computational chemistry. Using computing resources at HLRS, Tonner models phenomena that happen at the atomic and subatomic scale to understand how factors such as molecular structure, electronic properties, chemical bonding, and interactions among atoms affect a material's behavior.

Tonner and his group have highlighted the ability of computational chemistry and high-performance computing to reveal interesting phenomena that occur between organic molecules and surfaces, and have demonstrated how these interactions can be understood with respect to the molecular and solid state world. The knowledge they have gained could help design patterned surfaces, a goal of scientists working on the next generation of more powerful, more efficient semiconductors.

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Bringing computation to chemistry

Atoms bond together to form molecules and compounds when they approach one another and then trade or share electrons orbiting around their nuclei. The specific atoms involved, the physical shapes that the molecules take, their energetic properties, and how they interact with other nearby molecules are all properties that give a compound its unique properties. Such characteristics can determine whether compounds are likely to remain stable, or whether stresses such as changes in temperature or pressure could affect their reactivity.

Tonner uses a computational approach called density functional theory (DFT) to explore such characteristics at the quantum scale; that is, at the scale where Newtonian mechanics becomes replaced by the much stranger world of quantum mechanics. DFT uses information about variations in the density of electrons within a molecule — a quantity that can also be experimentally measured using x-ray diffraction — to derive the energy of the system. This, in turn, enables the researchers to infer interactions among nuclei as well as between electrons and nuclei, factors that are critical to understanding chemical bonds and reactions.

DFT can provide useful, though static, information about the energy profiles of the compounds they study. To gain a better understanding of how systems of molecules actually behave when interacting with a surface, Tonner's group also uses high-performance computing at HLRS to perform molecular dynamics simulations. Here, the scientists look at how the system of molecules develops over time, at the level of atoms and electrons and at time scales of picoseconds (one picosecond is one trillionth of a second).

"Increasing computing power has made it possible for computational chemistry and quantum chemistry to describe real molecular systems. Just 15-20 years ago, people could only look at small molecules and had to make rather strong approximations," Tonner explains. "The computational chemistry and solid state theory communities have now solved the problem of parallelizing their codes to operate efficiently on HPC systems. As supercomputers get bigger, we anticipate being able to develop increasingly realistic models for experimental systems in materials science."

Toward light-based semiconductors

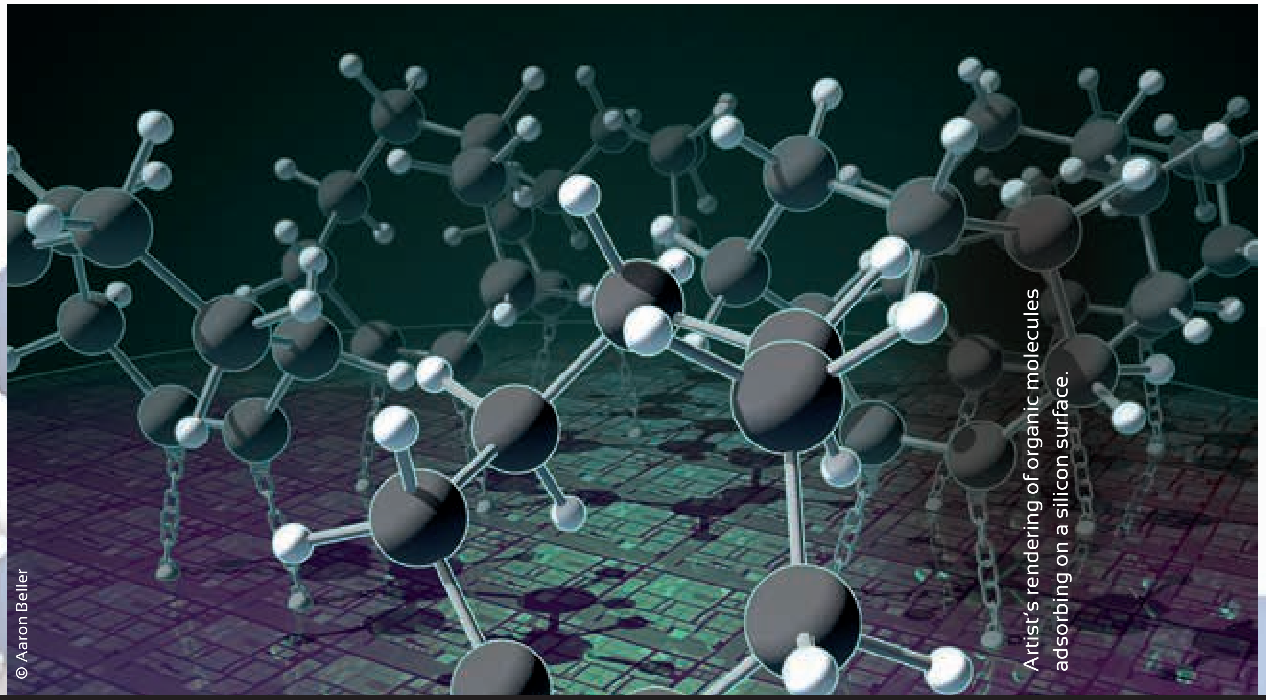
One area in which Tonner is currently using computational chemistry is to study ways to improve silicon for use in new kinds of semiconductors. This problem has gained urgency in recent years, as it has become clear that the microelectronics industry is reaching the limits of its ability to improve semiconductors using silicon alone.

Tonner and experimental colleagues have been investigating how functionalizing silicon with compounds such as gallium arsenide (GaAs) could enable the design of new kinds of semiconductors. This research posits that such new materials would make it possible to use light instead of electrons for signal transport, supporting the development of improved electronic devices.

"To do this," Tonner explains, "we really need to understand how the interfaces between silicon and these organic compounds look and behave. The reaction between these two material classes needs to proceed in a very controlled manner so that the interface is as perfect as possible. With computational chemistry we can look at the elemental details of these interactions and processes."

For example, to cover a slab of silicon, liquid precursor molecules for the constituent atoms of gallium arsenide are placed in a bubbler, where they are then brought into the gas phase; following a chemical process gallium and arsenide atoms attach to the silicon, forming a GaAs film. How atoms are arranged when they adsorb to a surface is determined by chemical bonding, though precisely how this takes place is an open question. Previously, it had been suggested that repulsive relationships among atoms is the most important factor in "steering" atoms into place when they adsorb on a surface. By using DFT and looking at intriguing features of how electrons are distributed, Tonner determined that the ability of atoms to steer other atoms into place on the surface can also result from attractive dispersive interactions.

Gaining a better understanding of these fundamental interactions should help designers of optically active semiconductors to improve adsorption of the precursor molecules onto silicon. This, in turn, would make it possible to combine light signal conduction with silicon based microelectonics, bringing together the best of both worlds in optical and electronic conduction. *(CW)*



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Artist's rendering of organic molecules adsorbing on a silicon surface.

Simulation and Machine Learning Could Make Power Plants More Efficient

Using high-performance computing and data-driven machine learning, University of Stuttgart researchers investigate whether carbon dioxide could replace water in power generation.

In conventional steam power plants, residual water is separated from power-generating steam. This process limits efficiency, and in early generation power plants could be volatile, leading to explosions. In the 1920s, Mark Benson realized that the risk could be reduced and power plants could be more efficient by bringing water to a supercritical state — when a fluid exists as both a liquid and gas at the same time. Though it was too expensive to use in practice during his day, the Benson Boiler offered the world its first glimpse of supercritical power generation.

Almost a century later, researchers at the University of Stuttgart's Institute of Nuclear Technology and Energy Systems (IKE) and Institute of Aerospace Thermodynamics (ITLR) are revisiting Benson's concepts to explore how it can improve safety and efficiency in modern power plants. Using high-performance computing, the researchers are developing tools that can make supercritical heat transfer more viable.

Sandeep Pandey, a PhD candidate at IKE, and Dr.-Ing. Xu Chu of ITLR are leading the computational aspects of this research. In cooperation with computer science researchers at the Singapore Institute of Technology (SIT), they are employing machine learning techniques informed by high-fidelity simulations. They are also developing a tool that can be easily used on commercial computers.

To achieve these goals, the team needed to run computationally intensive direct numerical simulations (DNS), which is only possible using high-performance computing. HLRS's Hazel Hen supercomputer enabled the high-resolution fluid dynamics simulations they required.

The heat of the moment

Water is often used in power generation and heat transfer because it is easily accessible, well-understood on a chemical level, and predictable under a wide range of temperature and pressure conditions. That said, in order to become supercriticial. water must be heated to 374°C and placed under extremely high pressure. Further, when a material enters its critical state, even slight changes to temperature or pressure can have a large impact. For instance, supercritical water does not transfer heat as efficiently as it does in a purely liquid state, and the extreme heat needed to reach supercritical levels can lead to degradation of piping and, in turn, catastrophic accidents.

Although using carbon dioxide (CO_2) to make power plants cleaner may sound like an oxymoron, Pandey and his colleagues are investigating its use as an alternative. The common molecule offers a number of advantages, chief among them being that it reaches supercriticality at just over 31°C, making it far more efficient than water. In addition, supercritical CO_2 (sCO_2) needs far less space and can be compressed with far less effort than subcritical water. This, in turn, means that it requires a smaller power plant.

In order to replace water with carbon dioxide, though, engineers need to understand its properties on a fundamental level, including how the fluid's turbulence transfers heat and in turn, interacts with machinery. To do so, the team turned to a method called direct numerical simulation, which is very computationally expensive and requires HPC resources.

Neural networks for commercial computers

Using the stress and heat transfer data coming from its high-fidelity DNS simulations, the team worked with SIT's Dr. Wanli Chang to train a deep neural network (DNN), a machine learning algorithm modeled roughly after networks of neurons in the brain.

Using Hazel Hen, the team ran 35 DNS simulations, each focused on one specific operational condition, and then used the generated dataset to train the DNN. The team uses inlet temperature and pressure, heat flux, pipe diameter, and heat energy of the fluid as inputs, and generates the pipe's wall temperature and wall shear stress as output. Eighty percent of the data generated in the DNS simulations is randomly selected to train the DNN, while researchers use the other 20 percent of data for simultaneous, but separate, validation.

After the team felt confident with the agreement, they used the data to start creating a tool for commercial use. Using the outputs from the team's recent work as a guide, they were able to use their DNN to simulate the heat energy of specific operational conditions in 5.4 milliseconds on a standard laptop computer.

Critical next steps

To date, the team has been using OpenFOAM, a community code, for its DNS simulations. While OpenFOAM is a well-established code for a variety of fluid dynamics simulations, Pandey indicated that the team wanted to use a higher-fidelity code. The researchers are working with a team from University of Stuttgart's Institute of Aerodynamics and Gas Dynamics (IAG) to use its FLEXI code, which offers higher accuracy and can accommodate a wider range of conditions.

Pandey also mentioned he is using a method called implicit LES in addition to the DNS simulations. While implicit LES simulations do not have quite the same high resolution as the team's DNS simulations, it does allow them to run simulations with higher Reynolds numbers, meaning it can account for a wider range of turbulence conditions.

The team wants to continue to enhance its database in order to further improve its DNN tool. Further, it is collaborating with IKE experimentalists to conduct preliminary experiments and to build a model supercritical power plant in order to test the agreement between experiment and theory. The ultimate prize will be if the team is able to provide an accurate, easy-to-use, and computationally efficient tool that helps engineers and power plant administrators generate power safer and more efficiently.

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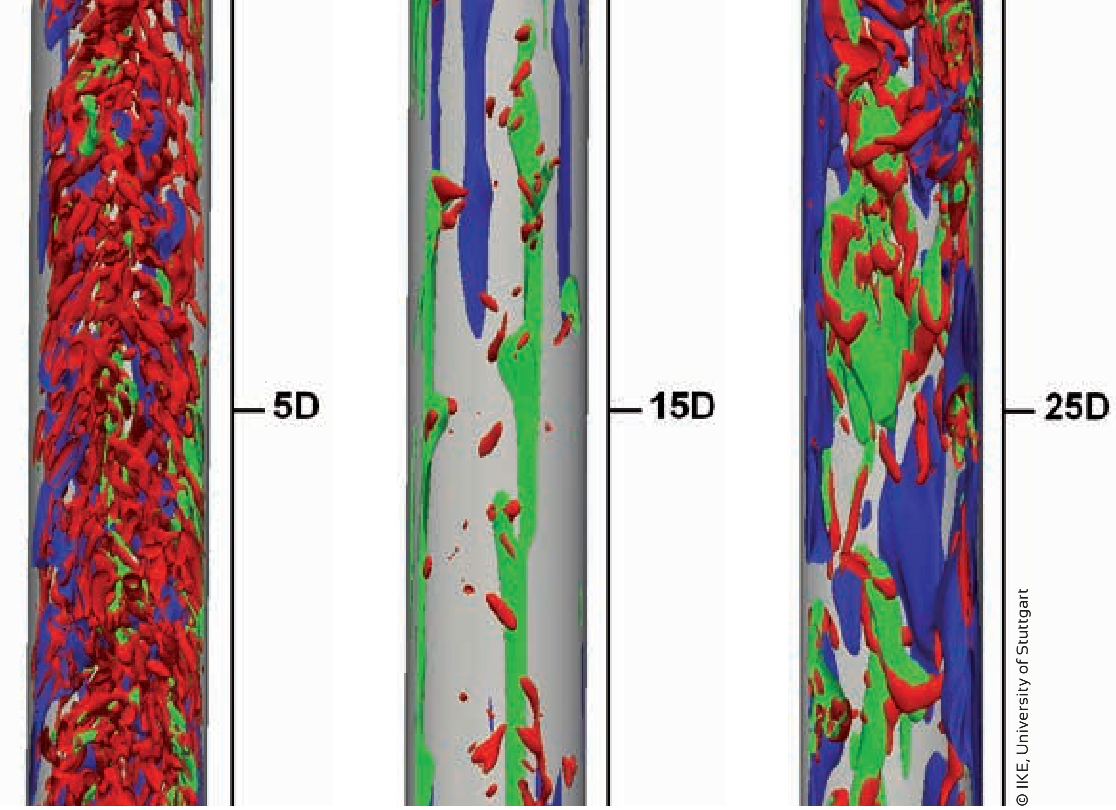

The simulation shows the structure and the (red) high and (blue) low speed streaks of the fluid during a cooling process. The researchers observed a major difference in turbulence between downward flowing (left) and upward flowing (right) supercritical carbon dioxide.

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Inside Our Computing Room

Cray XC40 Hazel Hen

Hazel Hen is at the heart of HLRS's HPC system infrastructure. With a peak performance of 7.42 Petaflops, it is one of the most powerful HPC systems in the world (position 30 in the TOP500, November 2018). Hazel Hen entered operation in October 2015, is based on the Intel Haswell Processor and the Cray Aries network technologies, and is designed for sustained application performance and high scalability.

CPU	Intel® Xeon CPU E5-2680 v3 12 core @ 2.5 GHz
Number of nodes / cores	7,712 / 185,088
Peak performance	7.42 PFLOPS
Memory	128 GB/node
Disk storage	15 PB

Cray Urika-GX

Increasingly, projects running on the Cray XC40 Hazel Hen generate large amounts of data. To provide a powerful tool for analyzing such results, HLRS installed a specialized Data Analytics Platform in December 2016. This research project gives users the ability to adapt data analytics methods for engineering applications.

Optimized software for	Spark Hadoop CGE (CrayGraph Engine)
Number of nodes	48 + 16
Cooperation with academic and industrial partners	Daimler, Porsche, Sicos BW, among others

NEC SX-ACE

The NEC SX-ACE is a vector computer optimized for applications demanding vector operations and high memory bandwidth.

CPU	NEC Vector CPU, 4 cores @ 1.0 GHz
Number of nodes / cores	64 / 256
Peak performance	~16 TFLOPS
Memory	4 TB
Memory BW per node	220 GB/s (single core), 256 GB/s (4 cores)
Interconnect	NEC IXS

NEC Cluster

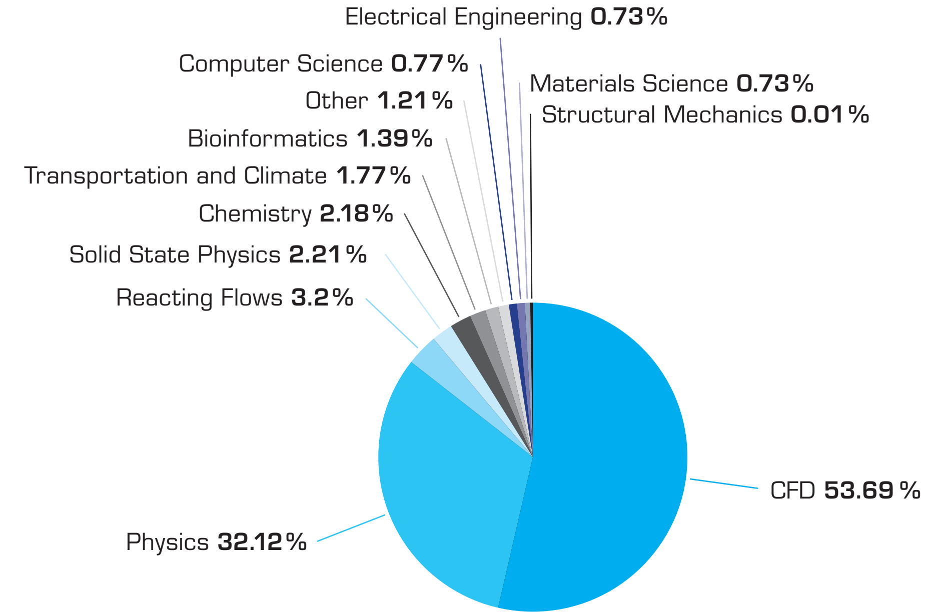
This standard PC cluster was installed in spring 2009. To meet increasing demands for compute resources, its configuration has been constantly adapted. The current configuration is as follows:

Node type	Intel Xeon E5-2670 (SandyBridge)	124
Node type	Intel Xeon E5-2660 v3 @ 2.6 GHz (Haswell)	88
Node type	Intel Xeon E5-2680 v3 @ 2.5 GHz (Haswell)	360
Memory per node	32 / 64 / 128 / 256 GB	
Interconnect	Infiniband QDR/FDR	

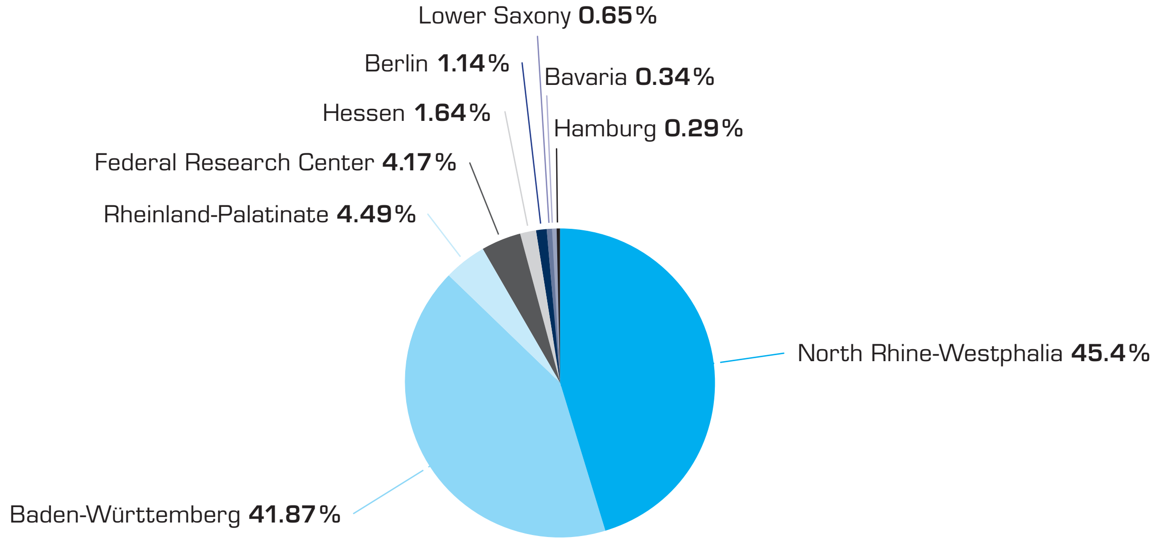
User Profile

In 2018 the Gauss Centre for Supercomputing approved 10 new large-scale projects for Hazel Hen (each project requiring more than 35 million core hours within one year), for a total of 766 million core-hours. The Partnership for Advanced Computing in Europe (PRACE) also approved 4 international simulation projects for HLRS, for a total of 113 million core-hours. In total, 129 projects were active on Hazel Hen in 2018 with 1.28 billion core-hours used.

System Usage by Scientific Discipline



System Usage by State



Third-Party Funded Research Projects

In addition to providing supercomputing resources for scientists and engineers in academia and industry, HLRS conducts its own funded research on important topics relevant for high-performance computing. These activities, many of which are conducted in collaboration with investigators at other institutes, are designed to address key challenges and opportunities in the field. The following is a list of funded projects that operated in 2018.

For more information about our current projects, visit **www.hlrs.de/about-us/research/current-projects/**

Project	Duration	Funded by
BEAM-ME	**December 2015 - November 2018**	**BMBF**

→ BEAM-ME is exploiting the potential of parallel and high-performance computing using distributed memory for high-resolution optimization models in energy system analyses.

bw Naha 2	**January 2017 - December 2019**	**MWK**

→ This project supports implementation of an energy management system (ISO 50001) and an environmental management system (EMAS), which will reduce consumption, improve environmental performance, and contribute to the realization of HLRS's sustainability strategy.

BW Stiftung II	**October 2016 - September 2019**	**MWK**

→ BW Stiftung supports universities and other nonprofit research institutions in Baden-Württemberg in using HLRS computers and advises them on issues related to optimization.

bwHPC-S5	**July 2018 - December 2020**	**MWK**

→ BwHPC coordinates support for HPC users in Baden-Württemberg and the implementation of related measures and activities, including data intensive computing and large scale scientific data management.

bwVisu II	**August 2014 - October 2020**	**MWK**

→ bwVisu is developing a service for remote visualization of scientific data, ensuring high scalability through cloud technologies.

CATALYST	**October 2016 - September 2019**	**MWK**

→ CATALYST researches methods for analyzing modelling and simulation data with the goal of implementing a framework that unites HPC and data analytics.

Leadning European HPC centers	**December 2018 - November 2021**	**EU**

→ In ChEESE, leading European HPC centers, academia, hardware developers, alongside SMEs, industry and public governance bodies such as civil protection are working together to prepare European flagship codes for upcoming pre-exascale and exascale supercomputing systems to tackle global challenges in the domain of solid earth.

DIPL-ING	**April 2017 - March 2019**	**BMBF**

→ The project is researching solutions for efficiently managing the high amounts of data emerging from engineering education programs at the University of Stuttgart.

EOPEN	**November 2017 - October 2020**	**EU**

→ EOPEN is tackling technical barriers that result from massive streams of Earth observation data and seeks to ensure that methods for data harmonization, standardization, fusion, and exchange are scalable.

EuroLab-4-HPC 2	**May 2018 - April 2020**	**EU**

→ EuroLab-4-HPC aims to establish a European Research Center of Excellence for HPC systems.

EUXDAT	**November 2017 - October 2020**	**EU**

→ EUXDAT provides a platform that unites HPC and cloud infrastructures to manage and process high amounts of heterogeneous data. Its focus is to support sustainable development in agriculture.

ExaFLOW	**October 2015 - September 2018**	**EU**

→ ExaFLOW is addressing key algorithmic challenges in computational fluid dynamics that will need to be solved to enable simulation at exascale. It is guided by use cases of industrial relevance and will provide open-source pilot implementations.

Exasolvers	**May 2016 - April 2019**	**DFG**

→ The exascale computers of the future are characterized by extreme parallelism. Exasolvers is combining crucial aspects of extreme scale solving, developing methods that scale perfectly and have optimal complexity.

EXCELLERAT	**December 2018 - November 2021**	**EU**

→ EXCELLERAT's goal is to facilitate the development of important codes for high-tech engineering, including maximizing their scalability to ever larger computing architectures and supporting the technology transfer that will enable their uptake within the industrial environment.

EXPERTISE | **March 2017 - February 2020** | **EU**

➜ EXPERTISE is a European training network (ETN) for the next generation of mechanical and computer science engineers. Its objective is to develop advanced tools for analyzing fluid dynamics in large-scale models of turbine components and to eventually enable the virtual testing of an entire machine.

FocusCoE | **December 2018 - November 2021** | **EU**

➜ FocusCoE supports EU-funded Centres of Excellence to more effectively exploit the tangible benefits of extreme scale applications for addressing scientific, industrial or societal challenges by creating a platform for the CoEs to coordinate strategic collaboration and outreach.

FORTISSIMO 2 | **November 2015 - December 2018** | **EU**

➜ FORTISSIMO 2 supports small and medium-sized enterprises (SMEs) in accessing simulation tools on supercomputers, promoting an expansion of their business and improvements in their competitiveness.

HiDALGO | **December 2018 - November 2021** | **EU**

➜ HiDALGO enables the assessment of Global Challenges problem statements by enabling highly accurate simulations, data analytics, artificial intelligence and data visualization, but also by providing knowledge on how to integrate the various workflows and the corresponding data.

HPC-Europa 3 | **May 2017 - March 2020** | **EU**

➜ HPC-Europa 3 fosters transnational cooperation among EU scientists (especially junior researchers) who work on HPC-related topics such as applications, tools, and middleware.

HyForPV | **October 2018 - September 2021** | **BMWi**

➜ The overall aim of HyForPV is to develop and operationalize new prediction products for the system integration of photovoltaics (PV) into the energy market and smart grids by delivering highly detailed simulations of PV power output with very high resolution in space and time.

InHPC-DE | **November 2017 - September 2021** | **BMBF**

➜ This collaboration aims to lay the groundwork for a standardized and distributed HPC ecosystem that integrates Germany's three Tier-1 supercomputing centers. It provides funding for 100 Gbit networking and opportunities for high-speed data management and visualization.

MoeWe | **July 2016 - December 2020** | **ESF, MWK**

➜ To address the long-term demand for supercomputing experts, particularly in industry, MoeWe has been developing a modular, flexible training program called the Supercomputing-Akademie.

MontBlanc 3 | **October 2015 - September 2018** | **EU**

➜ MontBlanc 3 aims to design a new type of computer architecture capable of setting future HPC standards. The approach is based on energy efficient solutions used in embedded and mobile devices.

MWK CoE: Automotive Simulation Exzellenzcluster 2 | **March 2016 - June 2018** | **MWK**

➜ This project is establishing and strengthening concepts for using simulation and HPC in the automotive industry. The center of excellence will be developed with the support of international networks and the analysis of funding opportunities.

OpenForecast | **September 2019 - August 2020** | **EU**

➜ The overall goal of OpenForecast is to deliver a novel generic service of high quality and efficiency for the Public Open Data Digital Service Infrastructure. This generic service combines public open data sources and high-performance computing (HPC) to establish a new generation of services.

OSCCAR | **Juni 2018 - Mai 2021.** | **EU**

➜ The EU Horizon 2020 research project OSCCAR — Future Occupant Safety for Crashes in Cars — is developing a novel, simulation-based approach to safeguard occupants involved in future vehicle accidents.

PetaGCS | **January 2010 - December 2019** | **BMBF / MWK**

➜ PetaGCS has been supporting the procurement and operation of next-generation supercomputers at HLRS from 2011 to 2019. Acquisitions are coordinated by the Gauss Centre for Supercomputing.

PHANTOM | **December 2015 - November 2018** | **EU**

➜ This project is addressing challenges in the development of energy-efficient parallel infrastructures in domains such as the Internet of Things and high-performance computing, using acceleratable hardware such as GPU and CPU.

Pop-CoE October 2015 - November 2018 EU

→ POP-CoE assesses the performance of computing applications, identifying issues affecting code performance as well as the best ways to address them.

PRACE May 2017 - April 2019 EU

→ PRACE supports high-impact scientific discovery and engineering R&D to enhance European competitiveness for the benefit of society.

Reallabor Stadt:quartiere 4.0 January 2016 - December 2018 MWK

→ Reallabor is exploring new methods and technologies that support participatory town planning and sustainable development, resulting in the development of a digital twin and a planning and decision support tool.

SimTech December 2018 - May 2022 DFG

→ SimTech aims at developing simulation technologies towards an integrative system science based on data integrated modelling. Within the project, HLRS supports the development of efficient methods for uncertainty quantification and management.

Simulated Worlds February 2011 - June 2018 MWK

→ Despite its importance in R&D, simulation is not widely understood. Simulated Worlds aims to bridge this gap by making it accessible to students, the next generation of scientists.

SiVeGCS January 2017 - December 2025 BMBF / MWK

→ Coordinates and ensures the availability of HPC resources of the Gauss Centre for Supercomputing, addressing issues related to funding, operation, training, and user support across Germany's national HPC infrastructure.

Smart-DASH May 2016 - April 2019 DFG

→ Smart-DASH is continuing development of the C++ template library DASH, which offers distributed data structures with flexible data partitioning schemes and a set of parallel algorithms.

TalPas January 2017 - December 2019 BMBF

→ TalPas is developing a self-optimizing, task-based approach to high-performance particle simulations.

TranSim January 2016 - December 2018 MWK

→ The goal of the project Transforming Society – Transforming Simulation is to explore how computer simulation is transforming science and the worlds of work, knowledge, and values.

VirMuDeKo März 2018 - Februar 2019 MWK

→ The goal of this project is to develop a pilot and demonstration framework through which virtual reality and augmented reality can support scientific collaboration in spatially distributed projects.

Visdral May 2016 - December 2018 BMWi

→ Visdral is testing the use of 3D laser scanning and simulation technologies to virtually document and investigate traffic accidents.

Funder Abbreviations

BMBF	Federal Ministry of Education and Research
BMWi	Federal Ministry for Economic Affairs and Energy
DFG	German Research Foundation
ESF	European Social Fund
EU	European Union
MWK	Baden-Württemberg Ministry for Science, Research, and Art

HPC Training Courses in 2018

HLRS offered 41 courses in 2018, providing continuing professional education on a wide range of topics relevant for high-performance computing. The courses took place over 129 course-days in Stuttgart and at other locations in Germany and internationally. Approximately 1,000 trainees participated in these activities. For a current listing of upcoming courses, please visit **www.hlrs.de/training/**.

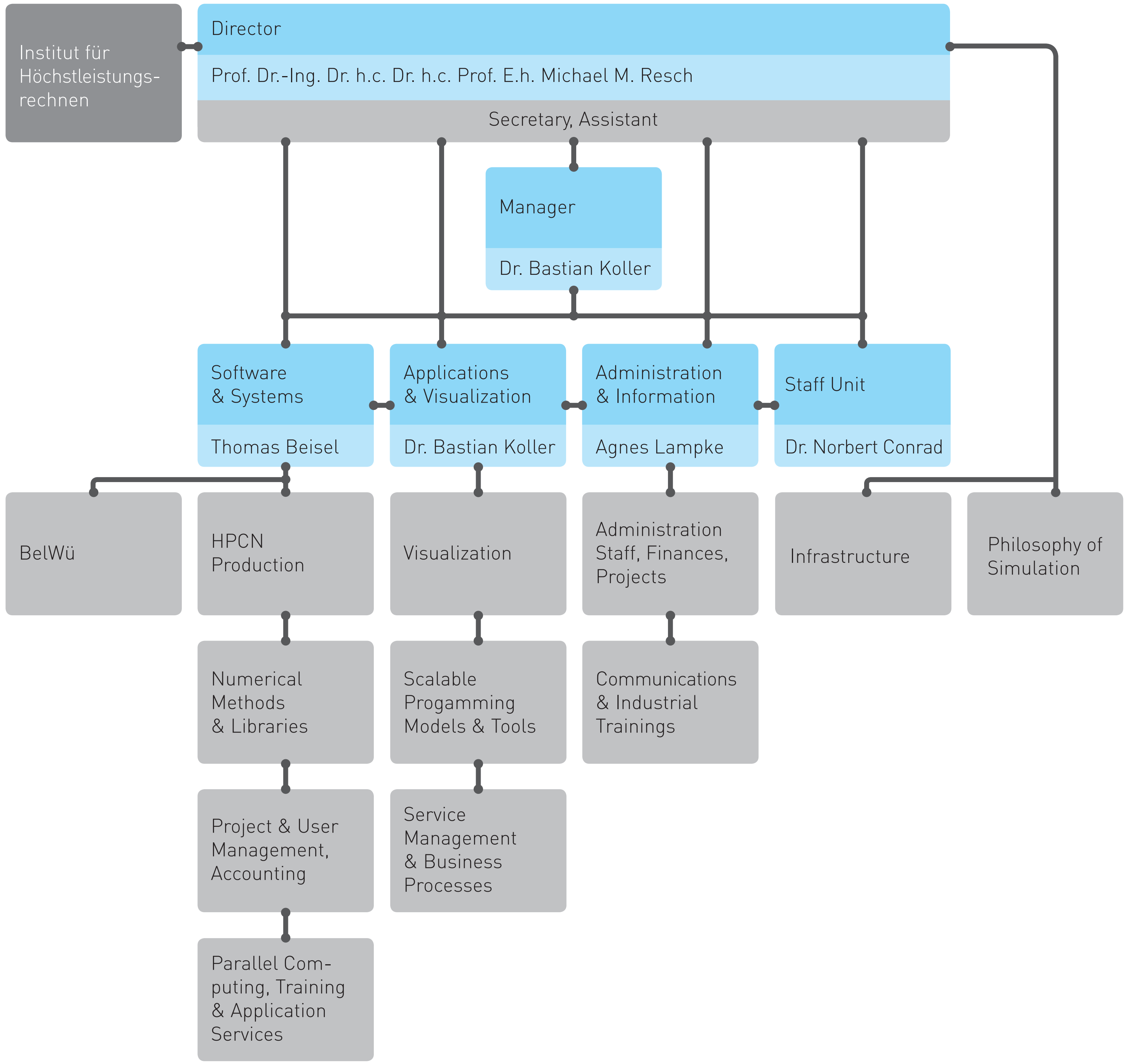
Date	Location	Topic
Jan 18	Garching	Introduction to Hybrid Programming in HPC (MPI+X) *
Feb 5-7	Paderborn	Parallel Programming with MPI and OpenMP
Feb 5-7	Amsterdam	Parallel Programming with MPI and OpenMP
Feb 12-16	Dresden	Parallel Programming & Parallel Tools
Feb 19-23	Siegen	Computational Fluid Dynamics
Mar 5-9	Stuttgart	CFD with OpenFOAM®
Mar 12-13	Stuttgart	OpenMP + OpenACC GPU Directives for Parallel Accelerated Super computers *
Mar 19-23	Stuttgart	Iterative Linear Solvers and Parallelization
Apr 9-12	Mainz	Parallel Programming with MPI and OpenMP
Apr 9-13	Stuttgart	Fortran for Scientific Computing *
Apr 11-13	Innsbruck	Parallel Programming with MPI and OpenMP
Apr 23-26	Stuttgart	Optimization of Scaling and Node-Level Performance on Hazel Hen
Apr 26-27	Vienna	Parallel Programming with MPI and OpenMP
May 7-8	Stuttgart	Scientific Visualization
May 14-17	Stuttgart	Advanced C++ with Focus on Software Engineering
May 15-17	Vienna	Parallel Programming with MPI and OpenMP
Jun 6-7	Vienna	Introduction to Hybrid Programming in HPC (MPI+X)
Jun 12-13	Stuttgart	Fortran Modernization Workshop
Jun 14-15	Stuttgart	Node-Level Performance Engineering *
Jun 19	Stuttgart	Introduction to Hybrid Programming in HPC (MPI+X)
Jun 20-21	Stuttgart	Cluster Workshop
Jul 2-3	Stuttgart	Concepts of GASPI and Interoperability with Other Communication APIs *
Jul 5-6	Stuttgart	Introduction to UPC and Co-Array Fortran *
Jul 10-13	Stuttgart	Advanced C++ with Focus on Software Engineering
Aug 20-23	Zürich	Parallel Programming with MPI and OpenMP
Sep 10-11	Innsbruck	Parallel Programming with MPI and OpenMP
Sep 10-14	Garching	Iterative Linear Solvers and Parallelization
Sep 10-14	Stuttgart	Computational Fluid Dynamics
Sep 12-14	Innsbruck	Parallel Programming with MPI and OpenMP
Sep 19	Stuttgart	Deep Learning Workshop
Sep 24-28	Siegen	CFD with OpenFOAM®
Oct 15-19	Stuttgart	Parallel Programming and Advanced Topics in Parallel Programming *
Oct 25-26	Stuttgart	Scientific Visualization
Nov 5-6	Vienna	Parallel Programming with MPI and OpenMP
Nov 5-9	Stuttgart	Optimization of Scaling and Node-Level Performance on Hazel Hen
Nov 7-9	Vienna	Parallel Programming with MPI and OpenMP
Nov 19-22	Stuttgart	Advanced C++ with Focus on Software Engineering
Nov 26-28	Jülich	Advanced Parallel Programming with MPI and OpenMP
Nov 27 + 30	Heverlee	Parallel Programming with MPI and OpenMP
Dec 3-7	Stuttgart	Fortran for Scientific Computing
Dec 13	Heverlee	Parallel Programming with MPI and OpenMP

* PRACE courses: HLRS is a member of the Gauss Centre for Supercomputing (GCS). GCS is one of ten PRACE Training Centres in the EU. The marked courses are in part sponsored by PRACE and are part of the PRACE course program.

Workshops and Conferences 2018

Date	Location	Partners	Topic
Mar 9-10	Erlangen	FAU Institute for Sociology	Simulation in the Social Sciences and the Sociology of Simulation
Apr 16-18	Stuttgart		17th HLRS/hww Workshop on Scalable Global Parallel File Systems
Apr 23-26	Kaliningrad	Russian Academy of Sciences, Keldysh Institute	Third Annual German-Russian Workshop
June 7-8	Stuttgart		Nachhaltigkeitstage (Sustainability Days)
Sep 17	Stuttgart	ZIH, TU Dresden	12th International Parallel Tools Workshop
Oct 1-2	Stuttgart	Hyperion Research	HPC User Forum
Oct 4-5	Stutgart		High-Performance Computing in Science & Engineering: 21st Results and Review Workshop
Oct 9-10	Stuttgart	Tohoku University	28th Workshop on Sustained Simulation Performance
Oct 23-24	Stuttgart		Workshop on Sustainable HPC Infrastructure
Nov 26-27	Stuttgart	HPC-Europa3, SICOS-BW	1st HPC-Europa Workshop for Small and Medium Enterprises
Nov 28-30	Stuttgart		Science and Art of Simulation Workshop 2018
Dec 11	Stuttgart	SICOS-BW	2nd Industrial HPC User Roundtable

Structure



Divisions and Departments

Administration and Information

➜ Leader: Agnes Lampke

Administration
Leader: Agnes Lampke

Manages issues related to the day-to-day operation of HLRS. Areas of responsibility include financial planning, controlling and bookkeeping, financial project management and project controlling, legal issues, human resources development, personnel administration, procurement and inventory, and event support.

Communications and Industrial Trainings
Leader: Dr. Jutta Oexle

Supervises and executes HLRS's communication to the general public and the media. It is the central point of contact for all questions regarding the center and its scientific work, and promotes new findings, achievements, and other news from around the center. In addition, the department designs and offers training courses and workshops for the industrial and service sectors, expanding interest in and accessibility of HPC technologies and solutions beyond its traditional community of scientific users.

Applications and Visualization

➜ Leader: Dr. Bastian Koller

Visualization
Leader: Dr.-Ing. Uwe Wössner

Supports engineers and scientists in the visual analysis of data produced by simulations on high-performance computers. By providing technologies capable of immersing users in visual representations of their data, the department enables users to interact directly with it, reducing analysis time and enabling new kinds of insights. The department has expertise in tools such as virtual reality, augmented reality, and has designed a method for integrating processing steps spread across multiple hardware platforms into a seamless distributed software environment.

Scalable Programming Models and Tools
Leader: Dr. José Gracia

Conducts research into parallel programming models and into tools to assist development of parallel applications in HPC. Currently the focus is on transparent global address spaces with background data transfers, task-parallelism based on distributed data-dependencies, collective off-loading of I/O operations, and parallel debugging. As a service to HLRS users, the group also maintains part of the software stack related to programming models, debugging, and performance analysis tools.

Service Management and Business Processes
Leader: Michael Gienger

Works on the development and operation of dynamic and scalable cloud computing services, particularly in a business context. The group conducts research focusing on performance and availability monitoring, elastic workflow management, and energy-efficient operation for federated cloud environments. It also works on issues related to the establishment of high-performance computing clouds, particularly for data intensive applications.

Software and Systems

➜ Leader: Thomas Beisel

High-Performance Computing Network – Production (HPCN Production)
Leader: Thomas Beisel

Responsible for the operation of all platforms in the compute server infrastructure. This department also operates the network infrastructure necessary for HPC system function and is responsible for security on networks and provided platforms.

Numerical Methods and Libraries
Leader: Dr.-Ing. Ralf Schneider

Provides numerical libraries and compilers for HLRS computing platforms. The department has expertise in implementing algorithms on different processors and HPC environments, including vectorization based on the architecture of modern computers. Department members also conduct research related to the simulation of blood flow and bone fracture in the human body, and are responsible for training courses focused on programming languages and numerical methods that are important for HPC.

Project and User Management, Accounting
Leader: Dr.-Ing. Thomas Bönisch

Responsible for user management and accounting, including creating and maintaining web interfaces necessary for (federal) project management and data availability for users. The department also conducts activities related to the European supercomputing infrastructure (PRACE) and data management. This involves operating and continually developing high-performance storage systems as well as conceiving new strategies for data management for users and projects working in the field of data analytics.

Parallel Computing, Training and Application Services
Leader: Dr. Rolf Rabenseifner

Organizes HLRS's academic continuing education program in high-performance computing, with emphases on parallel programming, computational fluid dynamics, performance optimization, scientific visualization, programming languages for scientific computing and data in HPC. The department also organizes the review process for simulation projects running at the national supercomputing center and participates in service provision for industrial clients. Additionally, it provides installation and software support for academic researchers in structural mechanics and chemistry.

Staff Units: Related Research

Philosophy of Science and Technology of Computer Simulation
Leader: Dr. Andreas Kaminski

Examines both how computer simulation changes science and technology development and how society and politics react to it: Does simulation change our understanding of knowledge and how we justify scientific results? How can simulation help to overcome uncertainties about the future? And how do we deal with the uncertainties of simulation itself?

Infrastructure
Leader: Marcel Brodbeck

Responsible for planning and operating facilities and infrastructure at HLRS. This division ensures reliable and efficient operation of the HLRS high-performance computing systems, provides a comfortable working environment for HLRS staff, and fosters all aspects of energy efficient HPC operation. It is also responsible for HLRS's sustainability program, which encourages and supports the entire HLRS staff in acting according to principles of sustainability.

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