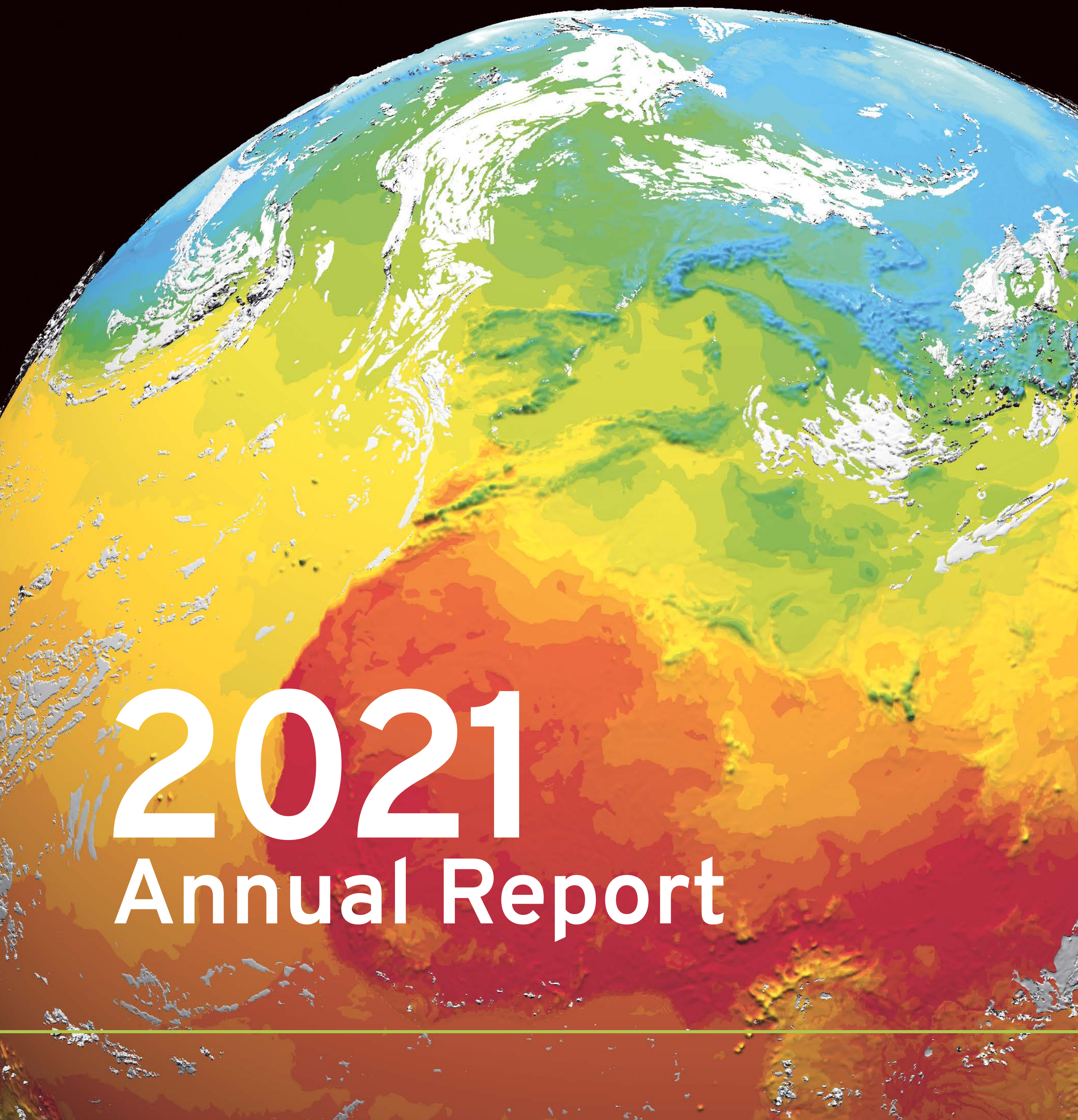
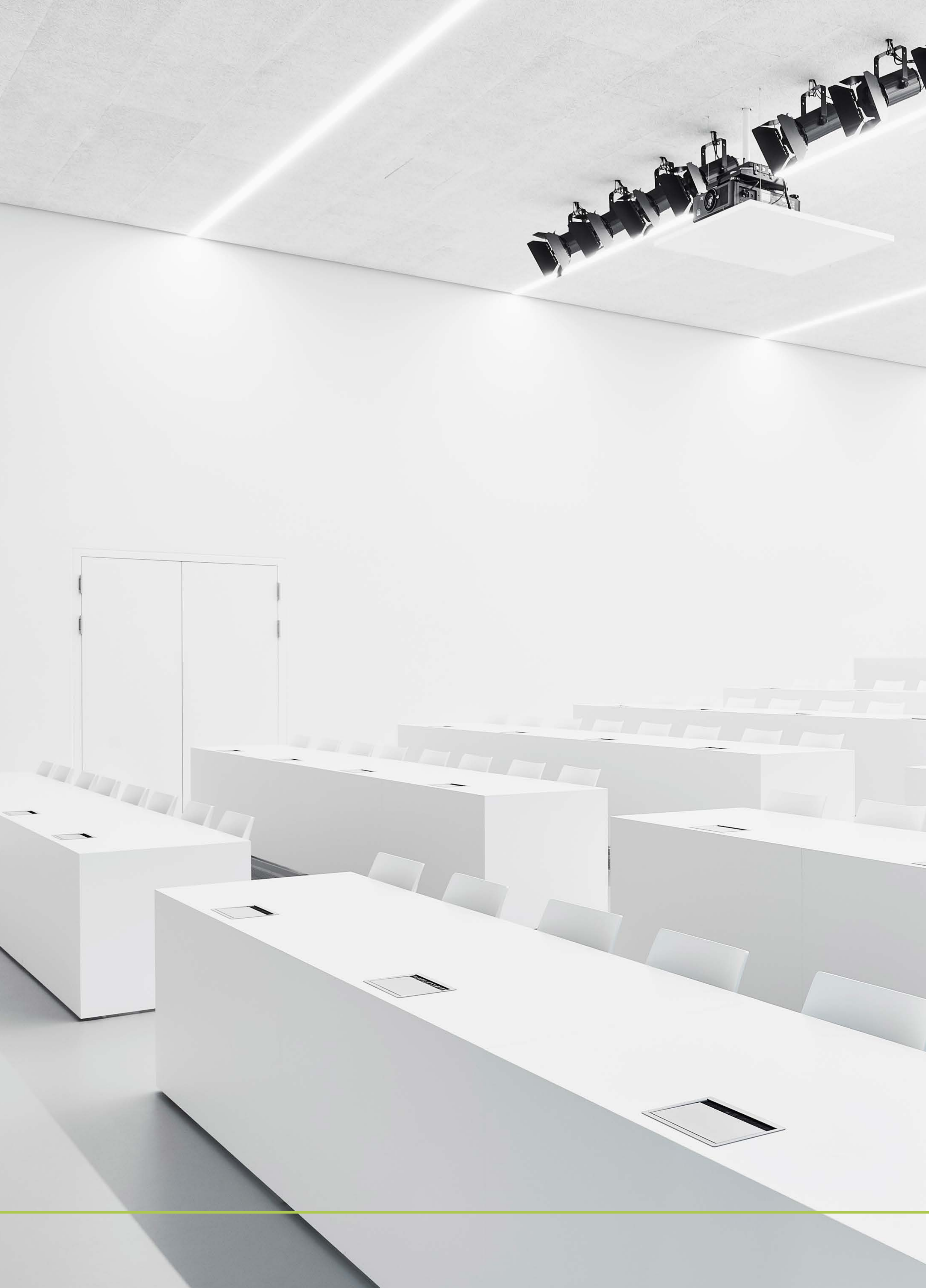
25 Years HLRS

HLRS

High-Performance Computing Center Stuttgart



2021 Annual Report



2021 Annual Report

The High-Performance Computing Center Stuttgart 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 comprehensive HPC services to academic users and industry. HLRS operates one of Europe's most powerful supercomputers, provides advanced training in HPC programming and simulation, and conducts research to address key problems facing the future of supercomputing. Among HLRS's areas of expertise are parallel programming, numerical methods for HPC, visualization, grid and cloud computing concepts, data analytics, and artificial intelligence. Users of HLRS computing systems are active across a wide range of disciplines, with an emphasis on computational engineering and applied science.

Director’s Welcome

Grußwort

Prof. Dr.-Ing. Michael M. Resch, Director, HLRS

Welcome to the 2021 annual report of the High-Performance Computing Center Stuttgart (HLRS), presenting recent accomplishments and activities from across our organization. We are pleased to be able to share these highlights with you.

Willkommen zum Jahresbericht 2021 des Höchstleistungsrechenzentrums Stuttgart (HLRS), in dem aktuelle Leistungen und Aktivitäten unserer Organisation vorgestellt werden. Wir freuen uns, dass wir diese Highlights mit Ihnen teilen können.

This annual report concludes a central story for us in 2021: our celebration of the 25th anniversary of HLRS’s founding as Germany’s first national high-performance computing center. In October we invited longtime partners, supporters, colleagues, and friends to reflect not only on HLRS’s history, but also on its evolution and continuing importance in the German, European, and international supercomputing communities. In the panel discussions and formal ceremony that took place, I was struck not only by the high esteem with which HLRS is held by so many in the community, but also — more importantly — by the shared sense that the remarkable computing resources, solutions, and expertise that HLRS provides are only growing in their relevance for scientific discovery, industrial competitiveness, and the solution of many challenges facing society in the coming decades.

In this annual report we present a timeline of key events in HLRS’s history, as well as an interview with Dr. Monica Wierse, Manager of Methods and Model Based Systems Engineering at Porsche and a witness to HLRS’s growth over many years. In the conversation she describes how HLRS’s HPC resources have supported automobile development at Porsche and how artificial intelligence (AI) is opening new opportunities for technology development.

HLRS’s growing engagement with AI is also a leitmotif of this year’s annual report. In September our supercomputer Hawk was expanded through the addition of graphic processing units, meaning that we now offer substantial resources for machine learning, deep learning, AI, and high-performance data analyitcs. December saw the start of IKILeUS, a project that HLRS is coordinating to improve the integration of AI into instruction across the entire University of Stuttgart campus. This effort will help to ensure that graduates enter the workplace with the skills they need for 21st century careers. In addition, I was delighted to see the start of a new collaboration facilitated by our Media Solution Center, in which the Stuttgart Chamber Orchestra and ZKM are exploring how neural networks could be used to compose music. I look forward to hearing the results.

Dieser Jahresbericht bildet den Abschluss eines für uns zentralen Ereignisses im Jahr 2021: die Feierlichkeiten anlässlich des 25-jährigen Bestehens des HLRS als erstes Bundeshöchstleistungsrechenzentrum Deutschlands. Im Oktober haben wir langjährige Partner, Unterstützer:innen, Kolleg:innen und Freunde eingeladen, nicht nur über die Geschichte des HLRS zu reflektieren, sondern auch über dessen Fortentwicklung und Bedeutung in der Supercomputing-Community auf deutscher, europäischer und internationaler Ebene. Während der Podiumsdiskussionen und der feierlichen Zeremonie war ich nicht nur von der hohen Wertschätzung beeindruckt, die so viele Mitglieder der Community dem HLRS entgegenbringen. Noch viel wichtiger war das gemeinsame Gefühl, dass die bemerkenswerten Rechenressourcen, Lösungen und Fachkenntnisse, die das HLRS bereitstellt, in den kommenden Jahrzehnten noch bedeutender für wissenschaftliche Entdeckungen, industrielle Wettbewerbsfähigkeit und die Lösung vieler gesellschaftlicher Herausforderungen wird.

In diesem Jahresbericht präsentieren wir einen Zeitstrahl der wichtigsten Ereignisse in der Geschichte des HLRS sowie ein Interview mit Dr. Monica Wierse, Leiterin des Bereichs Methoden und Model-based System Engineering bei Porsche und Zeugin des Wachstums des HLRS über viele Jahre hinweg. In dem Gespräch beschreibt sie, wie die HPC-Ressourcen des HLRS die Automobilentwicklung bei Porsche unterstützt haben und wie künstliche Intelligenz (KI) neue Möglichkeiten für die Technologieentwicklung eröffnet.

Das wachsende Engagement des HLRS hinsichtlich künstlicher Intelligenz ist auch ein Leitmotiv des diesjährigen Jahresberichts. Im September wurde unser Supercomputer Hawk um Grafikeinheiten erweitert, sodass wir nun über umfangreiche Ressourcen für maschinelles Lernen, Deep Learning, KI und Höchstleistungsdatenanalyseanwendungen verfügen. Im Dezember startete das vom HLRS koordinierte Projekt IKILeUS mit dem Ziel, KI besser in die gesamte Lehre der Universität Stuttgart zu integrieren. Damit soll sichergestellt werden, dass Absolvent:innen mit den Fähigkeiten in die Arbeitswelt eintreten, die sie für eine

In a year when Germany witnessed severe flooding and continuing disruptions resulting from the COVID-19 pandemic, another important question in 2021 was how high-performance computing could help public administration to prepare for and manage future crisis situations. Through a new project called CIRCE, HLRS has begun meeting with government agencies to identify ways in which simulation could help decision making in crisis situations. Much work is needed to identify potential collaborations with government agencies and to determine what data could form a basis for simulations, but our goal is to put HLRS in a position where it is able to respond quickly in case of an emergency.

In addition to celebrating the anniversary of its founding, HLRS this year also marked the 10th anniversary of its sustainability strategy. Far from resting on our laurels, though, we launched two new projects that we anticipate will lead to even better environmental performance. ENRICH and DEGREE will explore how we could improve energy efficiency and resource management at the center and will establish contacts with industry to help improve sustainability in data centers across Baden-Württemberg. The knowledge gained will also help us in planning for the construction of a new building for our next generation supercomputer, which we currently anticipate should open in 2026.

This year we were once again glad to see strong results in our key performance indicators. Our third-party funding saw an increase over last year, while income from industrial users of our HPC systems was again at a high level. Our HPC training program also bounced back better than ever after disruptions due to COVID in 2020, with our highest ever number of course participants, strong international participation through our increased use of online courses, and the transformation of our Supercomputing Academy into a self-sustaining business model. Reading the science stories and list of publications by our users found in this annual report, it is also clear that our computing resources have been enabling excellent research.

Karriere im 21. Jahrhundert benötigen. Darüber hinaus habe ich mich über den Beginn einer neuen Kollaboration gefreut, die von unserem Media Solution Center gefördert wird. In diesem Projekt erforschen das Stuttgarter Kammerorchester und das Zentrum für Kunst und Medien (ZKM), wie neuronale Netze für die Komposition von Musik eingesetzt werden können. Ich bin gespannt auf die Ergebnisse.

In einem Jahr, in dem Deutschland von schweren Überschwemmungen und anhaltenden Beeinträchtigungen aufgrund der COVID-19-Pandemie betroffen war, stellte sich eine weitere wichtige Frage: Wie können Höchstleistungsrechner und verwandte Technologien die öffentliche Verwaltung bei der Vorbereitung auf künftige Krisensituationen und deren Bewältigung unterstützen? In einem neuen Projekt mit der Bezeichnung CIRCE hat das HLRS den Austausch mit Regierungsbehörden begonnen, um herauszufinden, wie Simulationen die Entscheidungsfindung in Krisensituationen unterstützen könnten. Es wird viel Arbeit erfordern, potenzielle Kooperationsmöglichkeiten mit Regierungsbehörden zu ermitteln und festzustellen, welche Daten als Grundlage für Simulationen dienen könnten. Unser Ziel ist es definitiv, dass wir als Zentrum im Ernstfall schnell reagieren können.

Das HLRS feierte in diesem Jahr nicht nur den Jahrestag seiner Gründung, sondern darüber hinaus das zehnjährige Bestehen seiner Nachhaltigkeitsstrategie. Wir ruhen uns jedoch nicht auf unseren Lorbeeren aus, sondern haben zwei neue Projekte gestartet, von denen wir uns eine noch bessere Umweltleistung versprechen: ENRICH und DEGREE werden erforschen, wie wir die Energieeffizienz und das Ressourcenmanagement des Zentrums verbessern können. Parallel dazu möchten wir Kontakte zur Industrie knüpfen, um Fortschritte im nachhaltigen Betrieb von Rechenzentren in ganz Baden-Württemberg zu erzielen. Die aus den Projekten gewonnenen Erkenntnisse werden uns auch bei der Planung eines neuen Gebäudes für unseren Supercomputer der nächsten Generation helfen, dessen Eröffnung wir derzeit für das Jahr 2026 vorsehen.

As always, I extend my thanks to the supporters and funders who have made HLRS's successes possible, not just this year but throughout our 25-year history. We look forward to continuing to work with you to find innovative ways of using HPC and other advanced digital technologies to address the most pressing challenges facing science, industry, the HPC community, and society at large.

As I write this letter in late March 2022, the war in Ukraine weighs heavy on our minds, and our thoughts and sympathies are with everyone affected by it. Let us hope for peace.

With best regards,

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

Auch in diesem Jahr konnten wir uns über gute Ergebnisse bei unseren Key Performance Indicators freuen. Die Drittmitteleinnahmen sind im Vergleich zu letztem Jahr gestiegen, und die Einnahmen von industriellen Nutzern unserer HPC-Systeme bewegten sich erneut auf hohem Niveau. Auch unser HPC-Schulungsprogramm hat sich von den coronabedingten Unterbrechungen im Jahr 2020 mit der bisher höchsten Zahl an Kursteilnehmer:innen, einer starken internationalen Beteiligung dank des verstärkten Einsatzes von Online-Kursen und der Umwandlung unserer Supercomputing-Akademie in ein selbsttragendes Geschäftsmodell besser denn je erholt. Die wissenschaftlichen Berichte und die Liste der Veröffentlichungen unserer Nutzer:innen in diesem Jahresbericht verdeutlichen, dass unsere Rechenressourcen exzellente Forschung ermöglicht haben.

Auch in dieser Ausgabe möchte ich mich bei den Unterstützer:innen und Förder:innen bedanken, die die Erfolge des HLRS nicht nur in diesem Jahr, sondern in unserer 25-jährigen Geschichte ermöglicht haben. Wir freuen uns darauf, weiterhin mit Ihnen zusammenzuarbeiten, um innovative Wege für die Verwendung von HPC und anderen fortschrittlichen digitalen Technologien zu finden und so die globalen Herausforderungen zu bewältigen, vor denen die Wissenschaft, Industrie, die HPC-Gemeinschaft und die Gesellschaft im Allgemeinen stehen.

Während ich diesen Brief Ende März 2022 schreibe, lastet der Krieg in der Ukraine schwer auf unseren Seelen, und unsere Gedanken und unser Mitgefühl gelten allen, die von ihm betroffen sind. Hoffen wir auf den baldigen Frieden.

25 Years HLRS

HLRS Director Michael Resch welcomed visitors to the anniversary celebration.

25 Years of Innovation at the High-Performance Computing Center Stuttgart

A special anniversary celebration offered an opportunity to reflect on milestones in HLRS's history and the challenges that will shape its evolution over the coming decade.

Founded in 1996 as Germany's first national high-performance computing (HPC) center, the High-Performance Computing Center Stuttgart (HLRS) has grown to become not just a key facility of the University of Stuttgart but also an internationally prominent center for research involving simulation, visualization, and data analytics. In 2021 HLRS marked the 25th anniversary of its creation, hosting a full-day event in which friends and partners from across the HLRS community gathered to reflect on the center's evolving role in powering scientific discovery, supporting industrial competitiveness, and addressing global challenges.

The event featured panel discussions considering key aspects of HLRS's history and activities, followed by a formal anniversary in the late afternoon. Guests of honor (either present or delivering greetings online) included University of Stuttgart Rector Prof. Wolfram Ressel, Federal Minister of Education and Research Anja Karliczek, and Baden-Württemberg Ministry of Science, Research, and Art Ministerial Director Dr. Hans Reiter. Representatives of the European Union, including Gustav Kalbe from the European Commission Directorate-General for Communications Networks, Content, and Technology (CNECT), and EuroHPC Joint Undertaking Managing Director Anders Dam Jensen recognized HLRS's contributions at the European level.

The ceremony was capped by short lectures by senior representatives of several of HLRS's international partners, focusing on questions that the HPC community will address in the coming years. These included Prof. Dr. Jesús Labarta (Barcelona Supercomputing Center, Spain), Prof. Horst Simon (Lawrence Berkeley National Laboratory, USA), and Prof. Dr. Hiroaki Kobayashi (Tohoku University, Japan).

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

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

A panel discussion focusing on HLRS's engagement with industry included (l-r) Matthias Hauser (Media Solution Center Baden-Württemberg), Alexander Walser (Automotive Solution Center for Simulation e.V.), Benedetto Risio (RECOM Services GmbH), Andreas Wierse (SICOS BW), Alfred Geiger (T-Systems and HWW), and Christoph Gümbel (future matters AG).

A History of High Performance

The founding of the High-Performance Computing Center Stuttgart in 1996 firmly established the city and surrounding region as a center for advanced computational research in Germany. Since then, HLRS has seized opportunities offered by increasingly powerful technologies, enabling new applications of supercomputing for scientific discovery, industrial innovation, and the solution of key challenges facing society.

Early History

1986
Baden-Württemberg Prime Minister Lothar Späth approves funding for a Cray 2 supercomputer, establishing Stuttgart's reputation as a center for high-performance computing (HPC).

Founding of the High-Performance Computing Center Stuttgart

1995
Baden-Württemberg Prime Minister Erwin Teufel and Edzard Reuter, Chairman of the Board at Daimler-Benz AG, establish Höchstleistungsrechner für Wissenschaft und Wirtschaft GmbH (HWW). HWW for the first time brings industry and science together in one company for the use of supercomputers.

1996
Prime Minister Teufel founds the High-Performance Computing Center Stuttgart (HLRS) at the University of Stuttgart as Germany's first national high-performance computing center. HLRS is a division within the Computing Center of the University of Stuttgart, and Prof. Roland Rühle is named director.
At the founding ceremony, HLRS announces the beginning of production of a new Cray supercomputer; at the time it is the 7th fastest supercomputer in the world.

Connecting Service and Research

1998
HLRS initiates the first European project for metacomputing (METODIS). Its success convinces the EU to create its own funding stream for metacomputing and grid computing, and establishes HLRS as a leading HPC research center at the European level.

1999
In partnership with the Pittsburgh Supercomputing Center (USA), HLRS for the first time connects two supercomputers to solve a simulation problem, receiving an award from the US National Science Foundation for Real Distributed Supercomputing.

Bringing Baden-Württemberg, Germany, and Europe together

2003
Prof. Rühle steps down as HLRS director and hands leadership to Prof. Michael Resch.

HLRS wins the HPC Challenge at the SC Supercomputing Conference in Phoenix, USA.

2004
Baden-Württemberg Prime Minister Günther Oettinger welcomes a new HLRS supercomputer, an NEC SX-8, and opens the center's new building on Nobelstraβe. For the first time, an HLRS computing system achieves performance at the teraflop scale.

2006
HLRS is cofounder of D-Grid, an initiative to network all German high-performance computing centers.

2007
The State of Baden-Württemberg and the German federal government finance HLRS for an amount € 133 million over 10 years under the PetaGCS project.

HLRS, the Leibniz Supercomputing Centre, and the Jülich Supercomputing Centre found the Gauss Centre for Supercomputing (GCS), the alliance of Germany's national supercomputing centers. GCS joins the Partnership for Advanced Computing in Europe (PRACE) and begins providing computing resources to scientists from across the EU.

At the state level, HLRS launches BW-Grid and finances supercomputers at six locations across Baden-Württemberg.

In 1996 Baden-Württemberg Prime Minister Erwin Teufel received a tour led by Prof. Roland Rühle.

Baden-Württemberg Prime Minister Günter Oettinger, HLRS Director Michael Resch and other attendees at the opening of HLRS's permanent building in 2004.

Inauguration ceremony for the opening of HLRS's new Training Building in 2017.

New Directions for HPC in Science, Industry, and Society

2007
HLRS participates in the University of Stuttgart's Excellence Cluster "Simulation Technology" (SimTech), with the center's director serving as a principal investigator.

2008
With the creation of the Automotive Solution Center for Simulation, HLRS founds its first Solution Center. This is followed in 2018 with the establishment of the Media Solution Center.

2010
In cooperation with the Karlsruhe Institute of Technology, HLRS founds SICOS BW to facilitate access to simulation technologies among small and medium-sized enterprises.

2011
HLRS's power and cooling building begins operation.

With support of the State of Baden-Württemberg, HLRS starts Simulated Worlds, an outreach project designed to bring the theme of simulation into schools.

2012
Baden-Württemberg Prime Minister Winfried Kretschmann celebrates the start of operation of a new Cray XE6 supercomputer at HLRS. The system is christened with the name Hermit (after the Hermit beetle) and for the first time at HLRS achieves a performance of 1 Petaflop. In the coming years, the system is expanded and renamed Hornet (2014) and Hazel Hen (2015).

HLRS opens its new research building.

2014
HLRS commits itself to sustainability and starts its first state-funded sustainability project.

On the Way to Exascale

2015
HLRS creates a working group focusing on the theory of science and the societal relevance of simulation. A state-funded project on these themes begins in 2016.

2017
The State of Baden-Württemberg and German federal government agree to financing in the amount of €153 million for HLRS for the coming 10 years under the auspices of the project SiVeGCS.

HLRS celebrates the opening of its new HPC training building.

2018
HLRS establishes a Sociopolitical Advisory Board tasked with considering how HLRS could help to address new kinds of societal challenges.

HLRS leads European Centers of Excellence focused on the engineering sciences (EXCELLERAT) and global systems science (HiDALGO).

HLRS expands on its comprehensive HPC training program to co-found the Supercomputing-Akademie, which aims to improve HPC expertise in industry.

Honored guests at Hawk's inauguration in February 2020: State Secretary Gisela Splett, Representative Sabine Kurtz, Parliamentary State Secretary Michael Meister, Minister Theresia Bauer, Baden-Württemberg Prime Minister Winfried Kretschmann, HLRS Director Michael Resch, HPE Chief Sales Officer Heiko Meyer.

2020
Prime Minister Kretschmann inaugurates HLRS's next-generation supercomputer, an HPE Apollo system named Hawk.

HLRS is certified under the Blue Angel Ecolabel and the Eco-Management and Audit Scheme (EMAS) in recognition of its environmental management system.

HLRS is named coordinating center for EuroCC and CASTIEL projects, which promote the development of HPC expertise across Europe.

HLRS scientists work with the German Federal Institute for Population Research (BiB) to predict the impact of the COVID-19 pandemic on the nation's healthcare system. It is the first time that a federal ministry uses HPC for simulation.

2021
HLRS celebrates its 25th anniversary, reflecting on the history and future challenges of high-performance computing.

Supporters Congratulate HLRS on Its 25th Anniversary

Image: University Stuttgart/Max Kovalenko

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

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

* Anja Karliczek held this position until December 2021.

Image: MWK / Sabine Arndt

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

Book Documents History of Supercomputing in Stuttgart

Stuttgart has long been a prominent center for high-performance computing in Germany, but it wasn't inevitable that it would turn out that way. In the book *An der Grenzen der Berechenbarkeit: Supercomputing in Stuttgart* (Chronos Verlag), historians of science David Gugerli and Ricky Wichum tell the story of supercomputing's arrival in southwest Germany in the 1970s and of the factors that led to HLRS's establishment as the country's first national supercomputing center. The book was published in conjunction with HLRS's 25th anniversary.

Tracing the history of supercomputing from the founding of the Computing Center of the University of Stuttgart (Rechenzentrum der Universität Stuttgart, RUS) in 1972 to the present day, the book summarizes the crucial debates surrounding Stuttgart's emergence as a nationally and internationally prominent HPC center. These were driven not only by technological advances and scientific needs, but also by political, economic, and administrative considerations regarding the financing and mangement of such valuable resources. The authors also consider the establishment of HWW (Höchstleistungsrechner für Wissenschaft und Wirtschaft), an innovative public-private partnership that provides supercomputing for industry, as well as the influence of the needs of HLRS's system users on the evolution of the center's computing resources and services. *CW*

Image: Chronos Verlag

HLRS scientists in the project Cape Reviso are using simulation to identify strategies for reducing stress among cyclists, pedestrians, and other visitors at Stuttgart's Marienplatz.

News Briefs

In 2021 HLRS's flagship supercomputer gained new capabilities for AI and data analytics.

GPU Expansion of Hawk Goes into Operation

When initially installed in 2020, HLRS's flagship supercomputer began as a CPU-only system that was optimized for large-scale simulations. In response to the changing needs of its user community, the center in 2021 welcomed the addition of new graphic processing units (GPUs), offering an important upgrade in Hawk's capabilities. Twenty-four HPE Apollo 6500 Gen10 Plus systems containing 192 NVIDIA A100 GPUs based on the NVIDIA Ampere architecture now provide 120 petaflops of AI performance. The expansion gives users an ideal architecture for applications of machine learning, deep learning, high-performance data analytics, and artificial intelligence (AI). With the integration of GPUs into Hawk's existing CPU infrastructure, computer scientists at HLRS have also begun working with the center's users to develop new hybrid computing workflows that integrate traditional simulation methods and AI approaches. *CW*

Gathering Facilitates Communication between HLRS System Users and Staff

On April 22, nearly 100 users of HLRS's computing systems participated in an online meeting organized to provide updates on recent developments at the center that affect user research. The new format for exchanging ideas and insights within HLRS's user community addressed complications resulting from the ongoing COVID-19 pandemic, provided information about technical developments in HLRS's systems, and gave users a chance to ask questions regarding HLRS's resources and operations. Key topics included an update on the installation of the Hawk supercomputer, and new measures concerning scheduling, data storage, security, and power consumption. HLRS also invited users to work more closely with HLRS user support staff to improve performance of their codes on HLRS's systems. As HLRS's Thomas Bönisch pointed out, "Optimizing software so that it runs as efficiently as possible is something concrete that scientists can do to reduce our carbon footprint." *CW*

Participants in the eCulture Convention included Bernd Eberhardt (HdM), Bastian Koller (HLRS), Matthias Stroezel (SSC Services), Daria Tataj (Tataj Innovation), Matthias Hauser (MSC), Uwe Wössner (HLRS), Bernd Fesel (ECBN), Clara Gonçalves (CUNY Firefly Innovations), and Ellen Seehusen (Consultant).

eCulture Convention Explores Intersection of Art and Digital Technologies

In September HLRS hosted a three-day, international convention titled "The Economic and Cultural Impacts of the Digital Age." The event highlighted recent trends in art, culture, and the economy and provided the chance to discover state-of-the-art applications of computing technologies in the arts and culture industry. The event was organized by the Media Solution Center Baden-Württemberg (MSC), a nonprofit organization co-founded by HLRS in 2018 to address a growing need in the media arts industry for high-performance computing resources and expertise. Since then, the MSC has steadily built an international network of artists and cultural organizations interested in exploring this new territory, facilitating collaboration with scientists and engineers who can provide the technical expertise to help realize their visions. Held in a hybrid online/onsite format, the eCulture convention for the first time brought together many protagonists within the MSC network. *CW*

New Programming Course for Machine Learning

HLRS partnered with computer hardware manufacturer AMD to offer an online course focusing on the use of the ROCm™ software ecosystem, AMD's programming framework for machine learning using its AMD Instinct™ graphic processing units on high-performance computing systems. It was the first time that AMD had conducted a training course focused on programming in the ROCm environment in Europe. The course was organized as part of a collaboration between AMD, HLRS, and EXCELLERAT, the European Centre of Excellence for Engineering Applications, and held under the auspices of the bwHPC user support program. HLRS Managing Director and EXCELLERAT Project Coordinator Bastian Koller welcomed the collaboration, saying, "As the landscape of hardware for machine learning, deep learning, and artificial intelligence evolves, it is important that we help HPC users gain the necessary skills to use it." *CW*

The AMD/HLRS course was held online in January. Because of overwhelming demand, a second course was organized.

New Collaboration Begins with Institute of Advanced Studies, Brazil (IAS)

Building on complementary strengths in topics such as the digital transformation of society, the political implications of these changes, and emerging eCultures, HLRS and the IAS entered into a three-year agreement to develop joint programs for research and continuing education. Key topics for the collaboration include uses of computer simulation and machine learning in eCultures, problems of trust and disinformation, the history of adaptation and deception in technology and art, and the use of visualization in art. Leading the partnership are Lúcia Maciel Barbosa de Oliveira and José Teixeira Coelho Netto of the IEA Study Group on Computational Humanities at the University of São Paulo, along with HLRS Director Michael Resch and Andreas Kaminski, who heads the HLRS Department of Philosophy of Computational Sciences. The collaboration is the first for HLRS in South America, and expands on its international network of more than a dozen partner institutions in Asia, Europe, and the United States. *CW*

The Golden Spike Awards recognize outstanding research and optimal usage of HPC resources.

2021 Golden Spike Awards Announced at 24th Annual Results and Review Workshop

Due to the ongoing COVID-19 pandemic, this year's annual showcase for scientific research on HLRS's computing systems once again took place online. The program featured 27 short lectures and a virtual poster session with 22 posters provided as PDF files. At the conclusion of the event, Dr. Dietmar Kröner, a professor at the University of Freiburg and vice-chairman of the HLRS steering committee announced the winners of the 2021 Golden Spike Awards, which recognize excellence in research and innovative applications of HPC resources. This year's winners were Markus Scherer of the Karlsruhe Institute of Technology for simulations of flow and sediment patterns in streams, Jakob Dürrwächter of the University of Stuttgart for work on uncertainty quantification in high order computational fluid dynamics, and Daniel Mohler of GSI Helmholtzzentrum für Schwerionenforschung GmbH, Darmstadt, for research on hadronic contributions to the anomalous magnetic moment of the muon from lattice QCD. *CW*

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

First Stuttgart "Zukunftsrede" Explores Border Between Humans and Computers

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

IKILeUS to Integrate AI in University Education

HLRS is coordinating a new project funded by the German Federal Ministry for Education and Research (BMBF) that aims to better prepare University of Stuttgart graduates for the future of artificial intelligence. The project, called IKILeUS, is pursuing a holistic strategy that involves bringing both AI "for" teaching and AI "in" teaching to the entire student body. On the one hand, this means giving students the knowledge and skills needed to identify and implement potential applications of AI in their field. On the other, IKILeUS will introduce AI-based technologies at the University that can improve instruction, for example by automating the grading of assignments or making educational materials accessible to students with vision or hearing impairments. HLRS's contributions will also include teaching students to reflect on ethical questions surrounding AI, developing a continuing education course in AI for industry professionals, and providing computing resources. *CW*

Hardware Donation Supports COVID-Related Research

In April HLRS received delivery of 10 server systems from computing hardware manufacturer AMD that are dedicated for urgent computing needs. Donated as part of the AMD COVID-19 High Performance Computing Fund, the new hardware is being used for research at the German Federal Institute for Population Research to predict intensive care unit demand caused by the COVID-19 pandemic. In the future it will support HLRS's activities in the field of global systems science and offer dedicated computing power for responding to crisis situations. "The COVID-19 pandemic has been a big wakeup call in Germany and across Europe, showing that new challenges can arise very suddenly and have widespread impacts across societies," said HLRS Director Michael Resch. "Because simulation and data analytics are increasingly important in scientific disciplines that address such challenges, HPC centers must have sufficient supercomputing capacity to react to sudden and urgent surges in need." *CW*

Installation of HLRS's new system for COVID-related research.

Artificial Intelligence in Music Composition

As machine learning tools become more widespread, musicians and composers have begun to explore what new kinds of opportunities they could offer for writing music, and perhaps even what new types of musical forms they could produce. In an ongoing collaboration facilitated by the Media Solution Center Baden-Württemberg, HLRS scientists have been contributing expertise and computing resources to an innovative project involving the Stuttgart Chamber Orchestra (SKO) and the Hertz-Laboratory of the Center for Art and Media in Karlsruhe (ZKM). Using a neural network approach running on HLRS's systems, the team has been training a machine learning algorithm to compose music that combines the styles of classical composer Wolfgang Amadeus Mozart and serial music composer Luigi Nono. The SKO plans to perform the resulting compositions, which will emerge from a unique interaction between humans and powerful supercomputers. *CW*

AMD Corporate Vice President EMEA Mario Silveira and HLRS Managing Director Bastian Koller take a short break during the Hand in Hand Spendenlauf.

HLRS and AMD Team Up for Charity Run

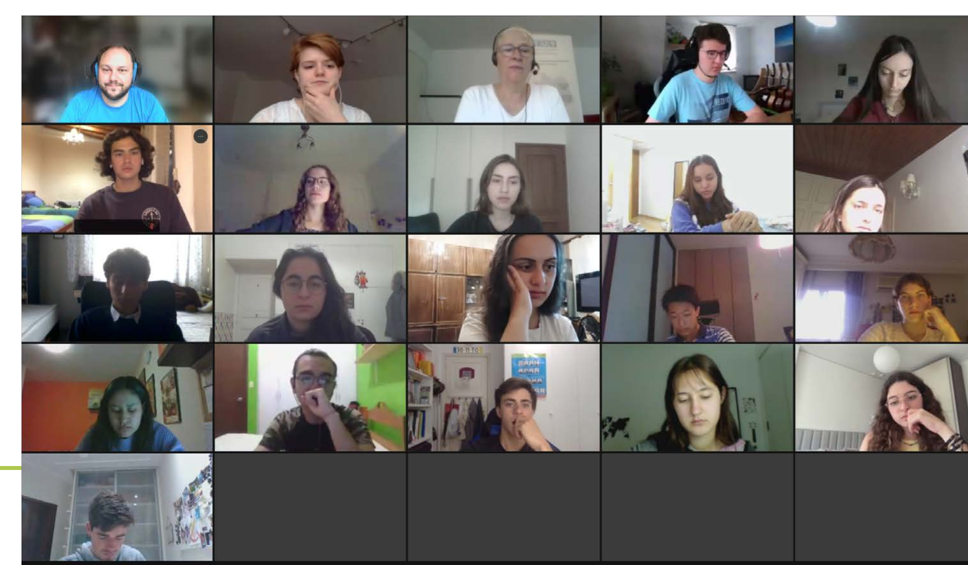
In July, HLRS once again participated in the Hand in Hand Spendenlauf, an annual fundraiser organized to benefit the Stuttgart Hospice for Children and Youth. This year HLRS runners were pleased to welcome employees at HPC hardware manufacturer AMD as teammates. Running under the name Core Performance Unit (CPU), the runners together achieved second place in the team ranking, completing the equivalent of 1,948 laps, approximately a third more than in 2020. A total of 78 team members from AMD and HLRS participated in the run, and 3 runners placed among the top 10 in the individual rankings. Together, the team raised € 2,000 for the Hospice, money that will contribute to the maintenance of programs and facilities supporting severely ill children and their families. *CW*

Industrial HPC Users Gather for 5th iHURT Symposium

In December more than 30 representatives of companies that use high-performance computing (HPC) gathered for the 5th iHURT Symposium. Organized by SICOS BW and HLRS, the event offered a closed forum in which HPC users from large and small companies could discuss the challenges they face in using HPC, simulation, and data analytics in industrial R&D. Gunther Mayer of Volkswagen, Dr. Susanne Kilian of hhpberlin, Haymo Kutschbach of ILNumerics, and Darko Brodarac of Robert Bosch GmbH all presented talks focusing on recent HPC applications at their companies. In addition, staff scientists at HLRS including Dr. Thomas Bönisch, Dennis Hoppe, and Dr. Dmitry Khabi discussed recent developments at HLRS related to new HPC technologies, Big Data and AI, and quantum computing. The event closed with a round table discussion moderated by SICOS BW's Dr. Andreas Wierse that addressed issues related to cloud computing, sustainability, software licenses, and the need for continuing education programs in HPC. *CW*

Simulated Worlds Program Extended

Recognizing the success of HLRS's educational enrichment activities, the Baden-Württemberg Ministry of Science, Resarch, and Art in 2021 renewed funding for the project Simulated Worlds for the fourth time. This support will enable the program to continue offering school-age students early experiences with the simulation sciences. This year, Simulated Worlds also welcomed the Pädagogische Hochschule Ludwigsburg as a new project partner, a collaboration that will expand the reach of the program into additional types of schools, including Gemeinschaftsschulen and Realschulen. In September Simulated Worlds designed a workshop held at the TU9-Ing Woche (STEM Study Exploration Week), designed for students from across the globe interested in studying MINT subjects in Germany. The workshop (do-IT Day) focused on the modeling of heat diffusion and promoted the Simulation Technology program at the University of Stuttgart. *CW*



Students from around the world attended an online workshop presented by Simulated Worlds.

News Highlights

Image: Brian McGowan for Unsplash

CIRCE Project to Improve Capabilities for Urgent Computing

Supercomputing infrastructure and expertise could support government agencies in quickly reacting to future pandemics, extreme weather events, and other crises.

In a new project called CIRCE (Computational Immediate Response Center for Emergencies), HLRS, under the auspices of the Gauss Centre for Supercomputing, will undertake a study to assess the need for and potential applications of high-performance computing (HPC) in crisis situations. The three-year project will identify situations such as pandemics, natural disasters, and migration events in which simulation, high-performance data analytics, and artificial intelligence could support decision making in government. It will also determine what organizational procedures are needed to ensure that HPC resources are immediately available at HLRS when emergency situations arise.

The need for a project like CIRCE became evident during the COVID-19 pandemic, when HLRS worked together with simulation experts in the Federal Institute for Population Research (Bundesinstitut für Bevölkerungsforschung, BiB) to quickly implement a model on HLRS's supercomputer that predicts demand for intensive care units across Germany up to 4 weeks in advance. This tool, which continues to run on HLRS's Hawk supercomputer and delivers daily information to the federal government once every week, has helped policy makers in decision making concerning public health management related to the pandemic. CIRCE also builds on expertise that HLRS has gathered in the HIDALGO project, a European Center of Excellence focused on developing HPC and big data technologies to address global challenges.

In the CIRCE project, HLRS will identify and communicate additional needs for high-performance computing and data analytics resources for crisis management. Through workshops, interviews, and focus groups, the center will build contacts with potential partners at the federal and state levels. These exploratory meetings will enable HLRS to better understand how simulation could help address the needs of public authorities and what specific kinds of forecasting tools would provide the greatest benefit. Discussions will also focus on what data government agencies have available and could provide as a basis for predictive tools running on HLRS's systems.

CIRCE will also investigate specific scenarios in which high-performance computing, high-performance data analytics, and artificial intelligence could be implemented during crises. This will include conducting proof-of-concept tests focusing on representative applications of HPC in emergencies. Through these efforts, HLRS intends to gain a better understanding of what activities and procedures are needed to quickly address urgent computing needs, and what current gaps in preparedness currently exist.

CIRCE is co-financed by the German Federal Ministry for Science and Education (BMBF) and the State of Baden-Württemberg Ministry for Science, Research and Art (MWK). *CW*

A dedicated cooling facility behind the HLRS main building keeps the center's computing systems from overheating.

Sustainability at HLRS: With Great Performance Comes Great Responsibility

HLRS celebrated 10 years of its sustainability strategy and launched two new projects to improve energy efficiency in IT.

At HLRS, running one of Europe's fastest supercomputers also means operating its infrastructure in a sustainable manner. Ten years ago, the center began an intensive engagement with environmental protection, leading to multiple official certifications. Nevertheless, the center shows no sign of resting in its efforts to make additional gains in environmental protection.

"Sustainability and climate protection are central concerns of the state government — this also applies to the IT sector," said Baden-Württemberg Minister of Science Theresia Bauer in a press release celebrating the 10-year milestone. "The fact that an international beacon like HLRS is living its sustainability concept in such an exemplary way is especially valuable considering the importance of climate protection in digitalization and AI."

HLRS was the first high-performance computing center of its size to be certified by EMAS — the world's most demanding program for environmental management — and by the Blue Angel ecolabel for Energy-Efficient Data Center Operation. The center's comprehensive environmental management plan ensures that its computing and cooling systems are operated as efficiently as possible and that it strives to continually improve its environmental performance.

Certification also means that HLRS takes efforts to share its expertise with other data centers. "With increasing digitalization it is becoming increasingly important that HLRS not only continue to develop its ambitious improvement process, but also to help other organizations to become more sustainable," said HLRS Director Michael Resch.

Improving energy efficiency in the IT sector

In 2021, HLRS started two new research projects that will focus on improving sustainability both in its own operation and in other data centers. The first, a collaboration between the University of Stuttgart and private industry called ENRICH, will develop a digitalization atlas to forecast the growth of the IT sector in Baden-Württemberg and identify opportunities for increasing energy efficiency across the state. HLRS will also conduct studies looking at key sustainability issues in computing centers such as supply chain management, the life cycle of digital technologies, and strategies for improving energy efficiency.

The second project, called DEGREE, is a collaboration between HLRS and the University of Stuttgart's Institute for Building Energetics, Thermotechnology and Energy Storage to test a new approach for reducing energy in the cooling of large supercomputers. The strategy involves dynamically regulating the mixture of energy-efficient free cooling and more energy-intensive active cooling to maximize the usage of free cooling while simultaneously optimizing the performance of the computing system.

The Baden-Württemberg Ministry for Science, Research and Art has provided funding for the ENRICH project, and supported the development of HLRS's environmental management system under the auspices of the project Sustainability in HPC Centers. DEGREE is funded by the German Federal Environmental Foundation.

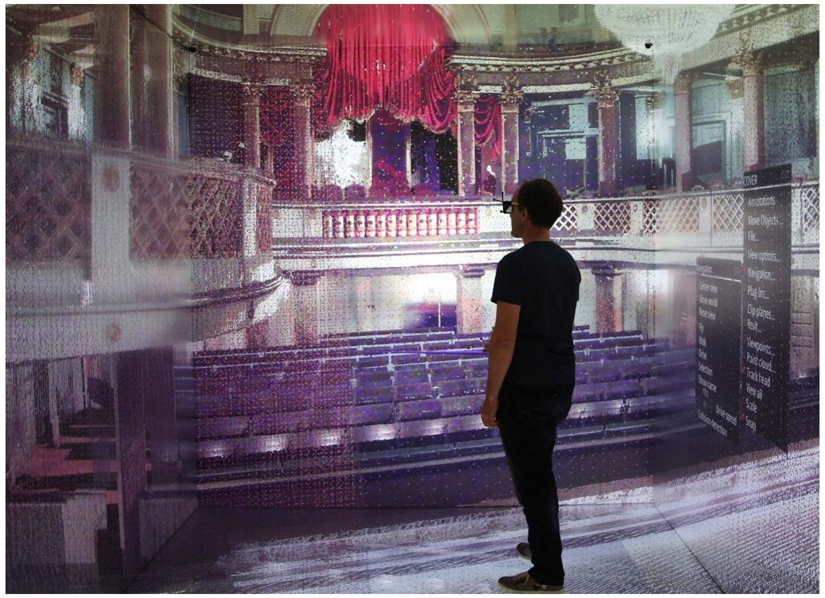
Sustainability integral in planning of new HLRS building

Sustainability is also a central concern in the design of a new computing building at HLRS, which is currently in its planning phase and whose opening is envisioned for 2026. Among the key issues being considered are the optimization of the building's energy supply, its cooling system, and the recycling of its waste heat for other uses. *CW*

HLRS continues to investigate new opportunities to improve its energy efficiency, including in the operation of its cooling system.

Digital Twin of Historic Ludwigsburg Theater

A comprehensive model of the theater in virtual reality will preserve and support study of the landmark, home to the oldest functional stage machinery in the world.

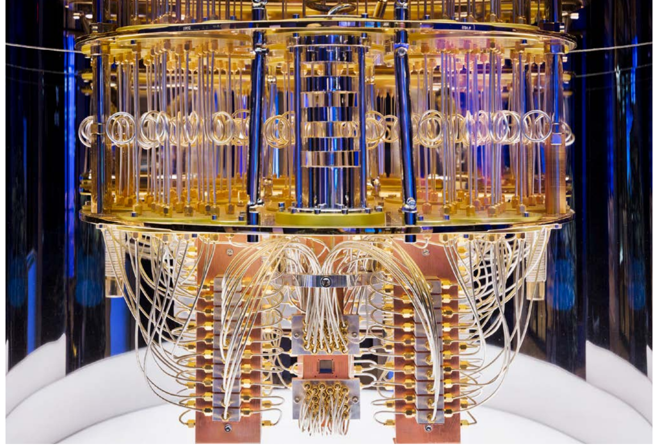


HLRS Visualization Department Head Uwe Wössner demonstrates a digital twin of the Ludwigsburg Palace Theater in the CAVE.

Built in the first half of the 18th century, the Palace Theater at the Ludwigsburg Residential Palace is significant not only for its opulent Baroque interior but also for the innovative technology built into its stage. Designed by engineer Johann Christian Keim, machinery constructed from wood and ropes made it possible for a single person located beneath the stage to automatically move background scenery without closing the curtain. Audiences are said to have watched in astonishment as stage settings changed without any visible human intervention.

To support the preservation and study of the theater, members of the HLRS Visualization Department used a 3D scanner to systematically capture a data set representing its entire interior. The researchers then used HLRS's high-performance computing facilities to integrate the scans into a comprehensive model called a digital twin, which reproduces the physical theater in virtual reality in extremely high detail. When displayed in HLRS's CAVE facility, visitors can experience the illusion of moving through the space as it might have looked in the 18th century and observe how the mechanical stage machinery worked.

In a press release Stephan Hurst, administrative director of the Ludwigsburg Palace, said, "We can learn a great deal about how the technology functioned and about the interaction of its many parts without having to actually touch anything. This will help to protect this one-of-a-kind monument." He also anticipates that visitors will find great benefit in the virtual model. "The virtual model will support new kinds of demonstrations that are not possible due to the fragility of the original." Hurst also predicts that the model will be of great interest to researchers who are continually learning more about the castle and developing new ways to present it to others. *CW*



SEQUOIA is one of several new projects that will utilize an IBM Q System One quantum computer recently installed in nearby Ehningen. Image: IBM, used with permission.

SEQUOIA Project to Bring Quantum Computing to Industry

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

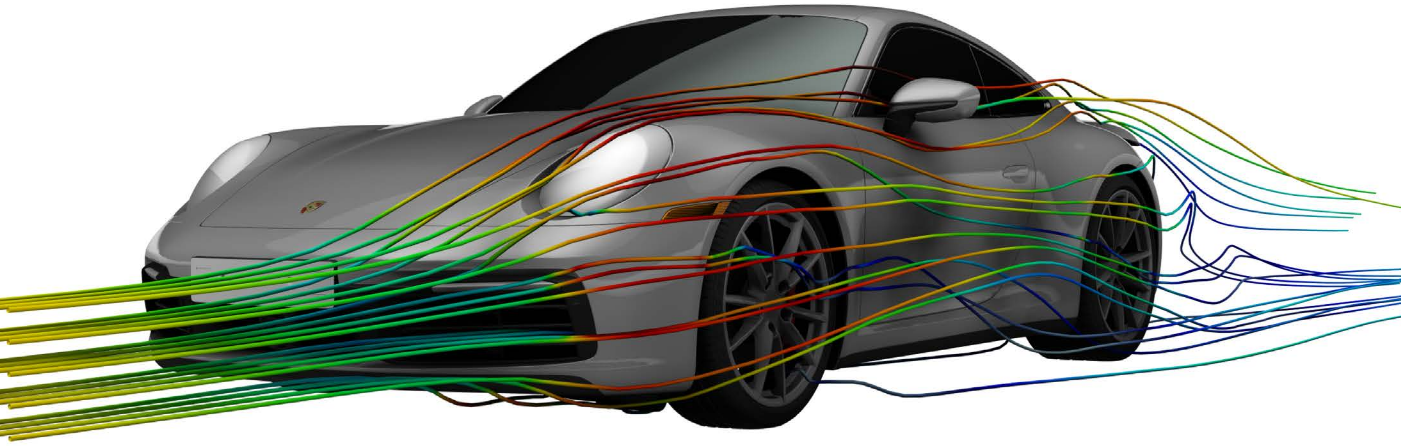
Quantum computing promises advantages over even the fastest supercomputers. Because the technology is so new, however, there is an urgent need to identify what applications would benefit most from its use. At the same time, research must develop the software, algorithms, and IT infrastructure that will be necessary to take full advantage of the power that quantum computing could offer.

HLRS aims to help fulfill these ambitious goals in a project called SEQUOIA. Working with the Fraunhofer Institute for Industrial Engineering and five additional partners, HLRS has begun research to improve the performance of algorithms for quantum computing. Additionally, HLRS is focusing on developing hybrid approaches that integrate quantum computing with existing high-performance computing (HPC) and artificial intelligence (AI) methods. By pursuing this research alongside industry partners, the results should lead to quantum computing applications that both resolve current challenges facing HPC and AI, and demonstrate the potential benefits of quantum computing for the private sector.

SEQUOIA is one of six projects funded through grants totaling €19 million from the Baden-Württemberg Ministry of Economic Affairs, Labor, and Housing, and is part of a competence center that is managing the testing of an IBM Q System One quantum computer recently installed in Ehningen, a small town just south of Stuttgart.

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

Engineers at Porsche use simulation in many ways during the development and testing of new designs, including for the optimization of automobile aerodynamics. Image: Porsche



Supercomputing that Breathes: An Interview with Monika Wierse

Even before the founding of the High-Performance Computing Center Stuttgart (HLRS) in 1996, computer simulation was an important tool for automobile development at Porsche. Since then the company has been a close partner of HLRS, and continues to use its supercomputing resources to this day.

Mathematician Dr. Monika Wierse joined Porsche in 2006 after working onsite at HLRS for 10 years as an industrial application engineer and manager for supercomputer manufacturer Cray. Currently, she is the automaker's Manager of Methods and Model Based Systems Engineering. In this role she oversees the development of new techniques that use simulation for product testing across the entire company, including numerical, hybrid, and experimental methods.

These experiences have given Wierse a unique perspective on HLRS's evolution, particularly with respect to its support of industrial applications of high-performance computing (HPC). In this interview she explains how Porsche uses HPC and artificial intelligence (AI) for automobile development, and reflects on the opportunities that access to HLRS's computing resources makes possible.

Photo courtesy of Dr. Monika Wierse

Why is simulation so important for automobile development at Porsche?

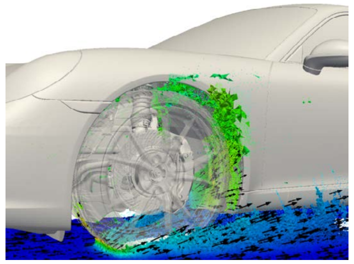
At Porsche, simulation has become more and more the foundation for vehicle development. For example, new functions (e. g. assisted driving, connectivity) are being added in cars and it's important that all of the possible constellations are tested. This challenge becomes even more complicated when you consider that we don't only build cars for Europe, but also for other countries where humidity, temperature, and street conditions can vary widely. The amount of testing that is necessary is really crazy and because of that we use state-of-the-art simulation methods. Using simulation enables us to deliver a comprehensive "verified" vehicle; that is, a vehicle that has been fully tested virtually. Furthermore, simulation makes it possible to make decisions early (e. g. release of components), saving development time and costs, and can replace the need for hardware in the form of vehicles, test benches, and real components.

Years ago Porsche had fewer product lines than it does today. Nowadays we don't only have the 911, but also the Cayenne, Panamera, Taycan, and others. In the past this meant that we would have peaks where we needed a great deal of computing power, and then there would be more relaxed periods when less computation took place. Today we are in the situation where we need a lot of computing time on a continual basis, to the point that we are often at the limits of what our software licenses allow.

Porsche and HLRS have cooperated together closely for many years. What are the advantages of the partnership for Porsche?

Although Porsche has its own computers, we have nothing even close to the size of what HLRS makes available. When doing aerodynamics simulations, we use several thousand cores on Hawk. For virtual crash tests in which we need to model joining technologies, however, scaling to such a large number of cores can be very difficult. Therefore, what is often more important to us than scalability is the throughput; that is, computing resources at HLRS give us the possibility to run a large number of smaller simulations in parallel.

From this perspective it has always been to our advantage that HLRS's resources can breathe, so to speak. On the one hand, HLRS has a large-scale supercomputer, on the other it also operates systems with a variety of architectures, including systems with GPUs (graphic processing units) for artificial intelligence.



Porsche uses simulation, for example, to study water management (left) and to carry out virtual crash tests (right).
Image: Porsche

There is a lot of talk today about the idea of cloud computing, where you just access resources when you need them. Although no one ever described it in these terms, this is something that we have always done with HLRS. We have a direct and secure connection, and the data transfer is for the most part automated. We have solved all of the key problems and because of this I would say that our HPC cloud lives at HLRS.

Are there other dimensions of your collaboration with HLRS aside from the provision of computing resources?

Although there are a lot of things that we can simulate, there are always gaps. The effects of weather conditions or dirt, for example, can be very important to how successful a car is but are also difficult to model. This is why I think it is a good thing that so many academic research projects are running at HLRS, as we will eventually be able to use the results once they are incorporated into commercial codes.

We have also always worked with HLRS in the context of industry-supported doctoral research projects in which we focus on topics in simulation with relevance to high-performance computing and automobile development. Six years ago, for example, we wanted to understand water management better. Where does water go when you drive through a deep puddle? Or if it rains, will it leak into the trunk when you lift the rear hatch? A colleague here at Porsche did research on this topic with support from Prof. Michael Resch, using the computing resources at HLRS. Since then we have implemented the results in ways that enable us to identify problems early in product development. The cooperation enabled us to take some significant steps forward.

Recently HLRS added graphic processors to its systems to support AI. How is Porsche using these new approaches?

Artificial intelligence has become a huge theme in method development at Porsche. At HLRS we compute tens of thousands of crash simulations of a complete automobile. This is incredible, but it also creates a big problem: the effort needed to look at thousands of small components in order to determine whether some panel was bent is getting larger and larger. We'd like to use AI to make this easier.

And there are other applications. Using AI, for example, we have been developing what we call metamodels that let us make calculations faster. We are also using AI on test benches to identify inconsistency early in tests. In addition, we can also use AI to avoid situations in which we need to take a car apart simply to mount another sensor at a certain position in the car.

Such applications are not just a question of data analysis methods — we also need a lot of IT support. HLRS can also help us to meet these new challenges.

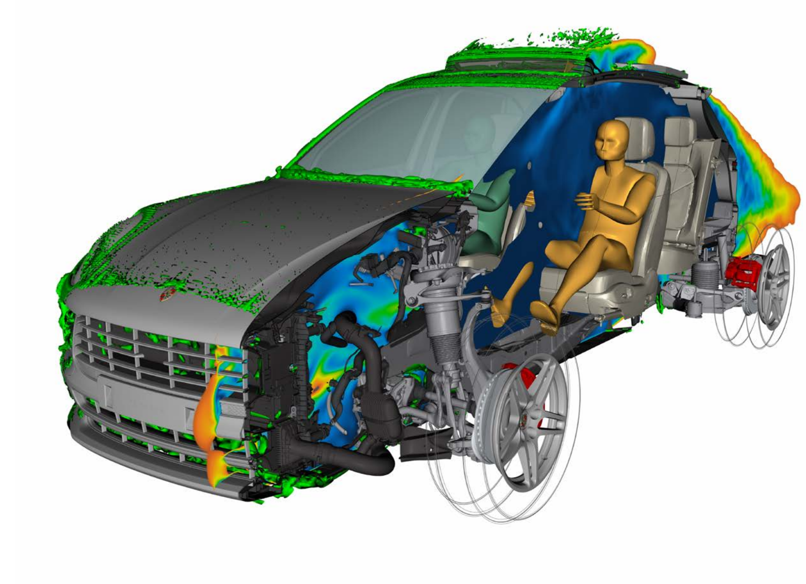
In 2021 HLRS celebrated the 25th anniversary of its founding. From your perspective, how has HLRS changed over the years?

Together, HLRS and Porsche have gone through what seems like a huge technology shift. Before I started at Cray, the focus in high-performance computers was without a doubt on vector architectures. When the Cray T3E came along, we suddenly had a significantly larger number of microprocessors and it became important to have a network that was capable of high performance with respect to latency and bandwidth. This also meant that simulation codes needed to be rewritten for the new system. Even today, things like scalability and performance optimization continue to be important with Hawk.

Availability of commercial codes has also always been an issue. Because the supercomputer is not always optimized for the relevant simulation codes that Porsche uses, HLRS has also steadily built up a standard cluster that we can access. This means that in addition to the large-scale computer there is also a sufficient number of normal clusters available. This was another way in which HLRS was able to react to help us address our needs.

Since my time with Cray, HLRS has seen a substantial growth in its computing resources. The connectivitiy, firewalls, and network bandwidth all had to grow alongside these developments at the same time. Even the smaller clusters have been expanded in parallel with the flagship supercomputer. I am very pleased about the excellent cooperation that Porsche and HLRS have built over the last 25 years and every day remain excited to see what new kinds of simulation opportunities HPC and AI can offer. *CW*

A complete vehicle model of the Porsche Macan not only includes the flow around and through the vehicle but also calculates flow inside the car when the sunroof is open. This makes it possible to virtually evaluate aeroacoustic features of the sunroof and how occupants experience wind while driving. Image: Porsche



HLRS Completes Data Security Assessment

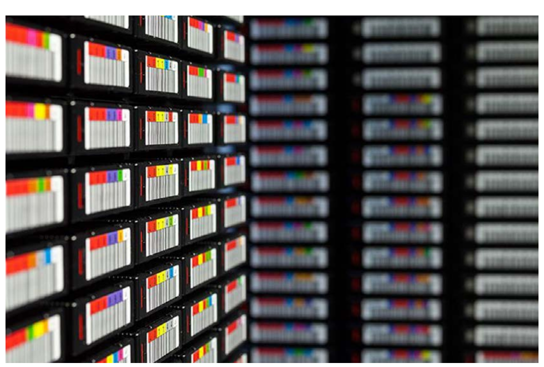
In accord with the TISAX framework, the center formalized its systems for information security management.

In 2021 the University of Stuttgart registered on behalf of HLRS as a participant in the Trusted Information Security Assessment Exchange (TISAX). By following this international standard for data security HLRS will ensure the protection of the data belonging to users of its computing systems.

Governed by the ENX Association on behalf of the German Association of the Automotive Industry (VDA), the TISAX framework covers a range of best practices for data security, including protecting physical access to computing facilities, defining security responsibilities for technology providers and vendor staff, and implementing formal processes for managing security risks and information breaches. In addition, it details responsibilities of data center employees for data security, outlines relevant considerations in the procurement of new systems, and provides for formal review processes to guarantee that the center is meeting all relevant legal requirements.

Following registration with TISAX, HLRS's data security practices were assessed by an independent, accredited audit provider. HLRS's TISAX assessment result is available on the ENX Portal under the Scope-ID S55W0V and the Assessment-ID AC6GXZ.

"Making sure that our users' data is secure has always been of the highest priority," said HLRS Director Prof. Michael Resch." Although TISAX was principally formulated for the automotive industry, completion of this assessment means that all academic and industrial users of HLRS's computing systems can feel confident that we are protecting their proprietary information from being accessed, changed, or manipulated, and that redundancies are in place to prevent data loss." *CW*



HLRS's high-performance storage system keeps HLRS system users' data safe.

Building Trust in Science

Two Science and Art of Simulation events brought together scholars to discuss issues that affect public confidence in trustworthy computational science.

Organized by HLRS's Department of Philosophy of Computational Sciences, a workshop series called "The Science and Art of Simulation" (SAS) has been exploring how and why people trust information. Its goal is to build a theoretical framework for improving trust in science and, more specifically, for helping to ensure that people across society can recognize trustworthy science and act based on appropriate assessments of its truthfulness.

In February, the Sixth SAS Workshop looked at this issue from a broad perspective, focusing on concepts such as imitation, adaptation, and deception that affect our perception of trustworthiness. Talks considered these themes from a historical perspective, connecting the history of technology to its applications in a parallel history of deception. The wide-ranging workshop brought examples of illusion and deception from the past — such as the design of church altars, Renaissance-era gardens, and theater sets — into dialogue with contemporary phenomena like the spread of disinformation over the Internet, deepfakes, and the AI language model GPT-3. By reflecting on the ways in which changing social and cultural assumptions have also shaped the practice and experience of deception over time, participants developed perspectives for better understanding how it functions today.

An SAS conference held in late October focused more specifically on the question of how and on what basis an appropriate trust in science can be built. Trust in trustworthy science is crucial in policy making but can be undermined by many factors, from disinformation to the inscrutability of "black box" models that use machine learning. In addition, while debate and even controversy among scientists is a healthy part of the scientific enterprise, it can complicate public conversation about science and be used to sow doubt about basic scientific facts. At the conference, scholars discussed strategies for improving trust in trustworthy science at a time when the scientific landscape is both complex and embedded in fast-moving communication systems. *CW*

Theatrical illusion in Pierre Corneille's *Andromède*, first performed in 1650 in Paris. Image: Wikimedia Commons

HLRS by Numbers

153 Staff

2 Visiting Researchers

108 Scientists

37 Nonscientists

5 Student Assistants

3 Research Assistants

60
Talks by HLRS Staff

System Usage

4.339 billion
Core Hours Produced

130
User Projects

61
Industrial Customers

139
User Publications

Staff Publications

43 Papers in Journals, Books an Conference Proceedings

4 Books

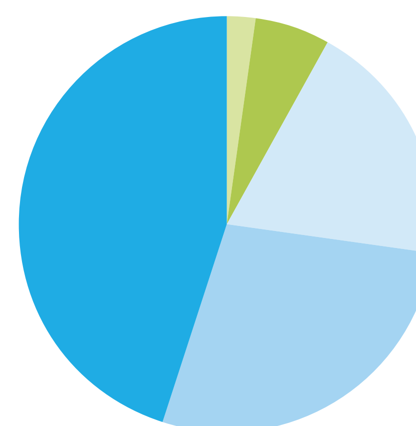
Education and Training

36 Continuing Education Courses	7 Scientific Workshops	16 University Lectures
1,191 Participants	375 Participants	2,206 Participants
121 Course-Days	16 Days	36 SWS

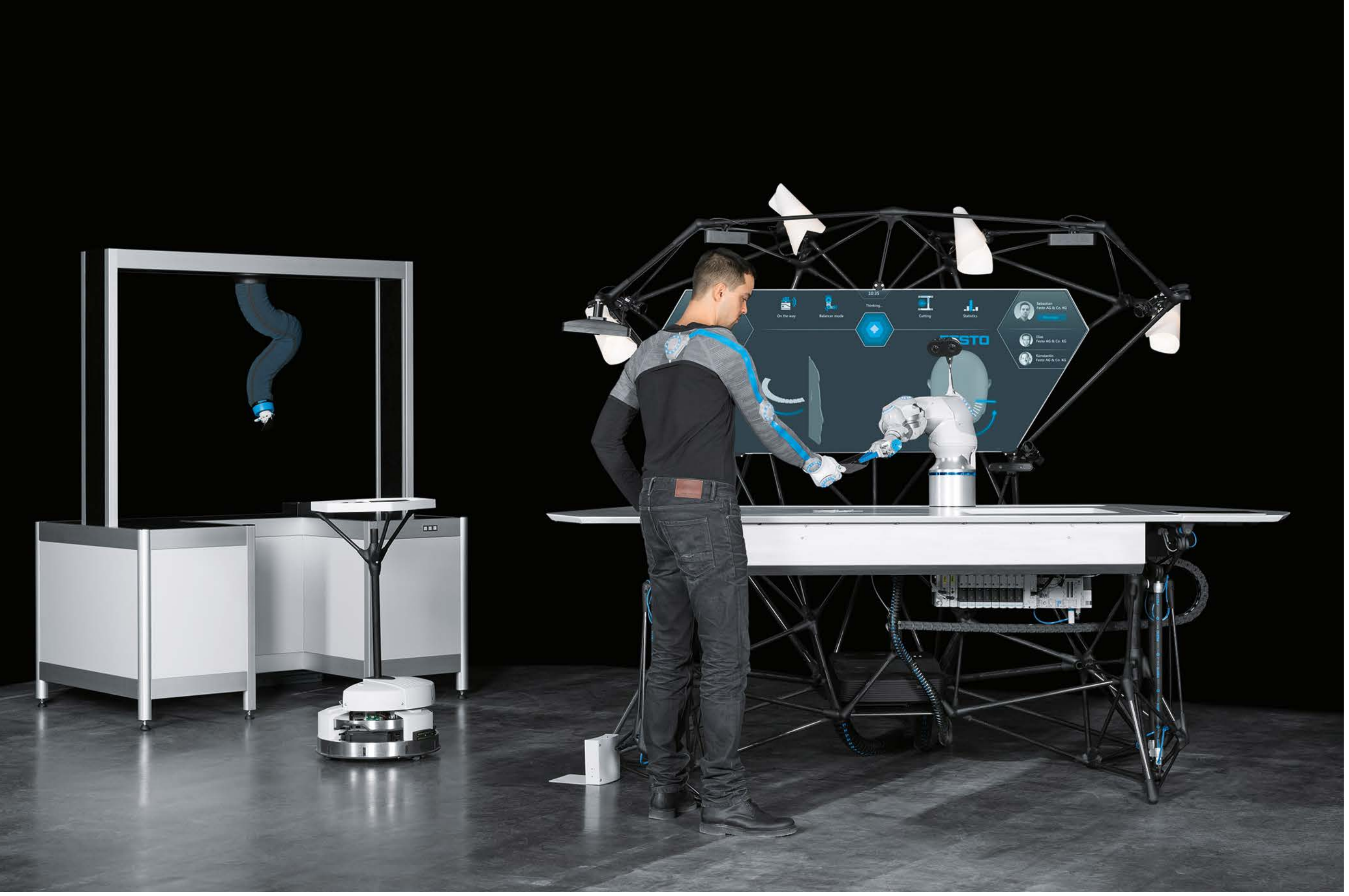
223
Vistors at HLRS

Third-Party Funds

7,333,300 €



- EU 45 %
- State Gov. 28 %
- Federal Gov. 19 %
- DFG 6 %
- Industry 2 %



In the Festo R&D lab, experiment and reinforcement learning come together to train robots to work safely alongside humans. Photo: Festo

Artificial Intelligence for Safer Automation

Researchers at Festo are working with HLRS staff to “teach” robots to collaborate with humans more efficiently.

Industrial controls manufacturer Festo has helped businesses large and small to improve their efficiency by delivering technologies that automate difficult tasks. As manufacturing processes become increasingly complex, though, Festo has turned to the power of high-performance computing (HPC) to better tailor solutions to customers’ individual needs.

“With artificial intelligence (AI) and other new tech, people are starting to ask for more custom-made solutions in their factories,” said Festo researcher Dr. Shahram Eivazi. “These systems must be adaptive so they can change, while also being safe and interactive with humans that are involved in the manufacturing process.”

Working with HLRS through the CATALYST project, Festo is using the center’s HPC resources and partnering with HLRS staff to develop an AI workflow for training robots based on biological learning principles.

Build on your best behavior

When training a machine to “learn” a new behavior, researchers primarily use three different methods. The first two, supervised and unsupervised learning, involve using large amounts of data to train an algorithm to pick out patterns effectively.

Robots being designed to automate complex tasks need to be trained in a more detailed manner, however. For this reason, the Festo team uses reinforcement learning, a method for artificial intelligence that draws heavily from methods used in early childhood development. Simply put, researchers train the algorithm by using a mixture of input data from the Festo R&D lab as well as video and sensor data from real-world manufacturing environments to give the algorithm feedback, forcing it to learn through trial and error.

By tailoring this method to specific scenarios, Festo can help clients develop complex automation workflows that involve interactions between humans and robots. “We want to make these kinds of interactions safer, so we don’t have to put barriers between robots and workers,” Eivazi said.

Data-driven training methods need world-class HPC infrastructure

The Festo team requires about 70 to 100 terabytes of data to train its algorithm, an amount that was too large for its in-house computing resources. By partnering with HLRS, however, they have taken advantage of the center’s GPU-based Cray CS-Storm system. “Working with HLRS lets us answer the question, ‘What if we have access to thousands of CPUs instead?’” Eivazi said.

To take advantage of that performance, though, the researchers need to build their software with a larger system in mind. The team has collaborated with HLRS’s Dennis Hoppe and Oleksandr Shcherbakov, who helped them to port their application to run effectively on HLRS’s systems.

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

Future plans for a fruitful collaboration

As the collaboration grows, Festo indicated three main challenges the team will have to overcome.

First, they need to effectively train their algorithm to get “smarter” as it goes. This could be done by reusing datasets for later training opportunities.

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

Finally, the team must optimize the movement of data from HLRS in order to apply the resulting insights quickly in real-world manufacturing scenarios. Here, HLRS will rely on its experience in building out its data transfer capabilities in the Gauss Centre for Supercomputing’s InHPC-DE initiative, which has supported development of its high-speed data transfer infrastructure. *EG*

Researchers in the Vlasiator project used HLRS's Hawk supercomputer to complete the first 6-dimensional simulation of ion-scale dynamics within near-Earth space. In this visualization, the solar wind encounters the Earth's magnetic field, resulting in a bullet-shaped magnetosphere. Image: University of Helsinki, used with permission.

User Research

Supercomputing Enables Analysis of Massive Atmospheric Datasets

HLRS supported researchers at the Karlsruhe Institute of Technology and the Instituto de Astrofísica de Andalucía of the Spanish Research Council (CSIC) in processing and analyzing a decade's worth of data gathered during an expansive, space-based project.

On March 1, 2002, European researchers looked to the sky as the Envisat satellite mission began. Envisat hosted nine instruments designed to gather information about the Earth's atmosphere in unprecedented detail. The satellite continued to send data back to Earth until 2012, when European Space Agency (ESA) staff lost contact and declared an official end to the mission.

One of the instruments aboard Envisat was the Michelson Interferometer for Passive Atmospheric Sounding (MIPAS), which measured the infrared radiation emitted by the Earth's atmosphere. These measurements help scientists better understand the role greenhouse gases play in our atmosphere.

Since many gases found in the atmosphere exhibit characteristic "fingerprints" in these high-resolution spectra, each set of spectra, recorded at a given location, allows researchers to obtain the vertical profiles of more than 30 key gases.

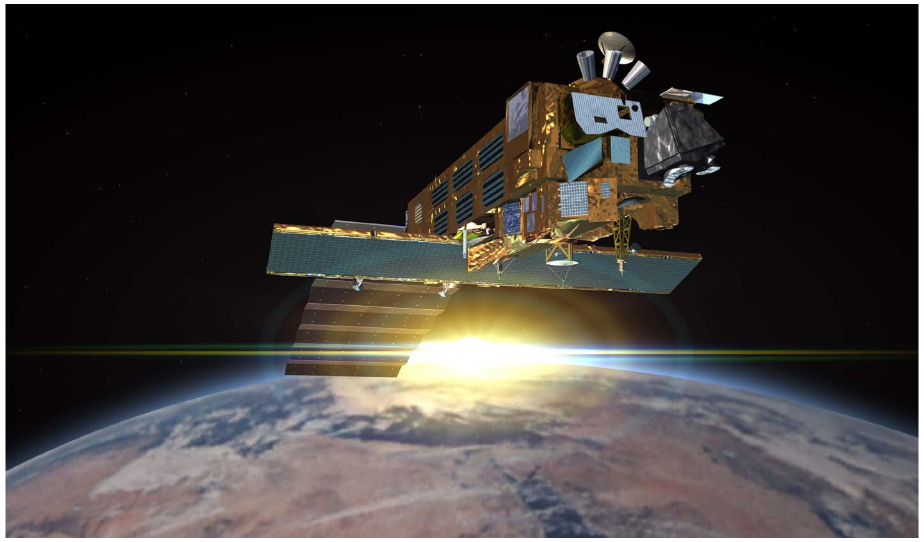
During each of the satellite's 14 daily orbits, the instrument took measurements at up to 95 different locations, each of them consisting of 17 to 35 different spectra corresponding to altitudes from 5 to 70 km, but sometimes reaching up to 170 km.

Taken together, a decade of compressed MIPAS spectral data fills roughly 10 terabytes. In order to analyze such a massive amount of data in a timely manner, researchers at the Karlsruhe Institute of Technology (KIT) and the Instituto de Astrofísica de Andalucía (IAA-CSIC) turned to the power of high-performance computing (HPC). The team partnered with the High-Performance Computing Center Stuttgart (HLRS) to securely store their large dataset and used the center's supercomputing resources to model and analyze MIPAS's infrared spectra.

"Using HLRS's supercomputer we were able to assemble a complete dataset for our 10-year time series quickly and thoroughly," said Dr. Michael Kiefer, researcher at KIT and principal investigator for the project. "We could attempt to do this work on cluster computers, but the processing would take years to get the result. With HPC we can quickly look at our results and extract a wider variety of chemical species from the measured spectra. This isn't just a quantitative improvement, but also a qualitative one."

Combing through the ever-expanding data deluge

In recent years, scientific computing has entered a new phase of development. For decades, computing advancements were rooted in the idea of Moore's Law — a prediction by Gordon Moore that the shrinking size of transistors would make it possible to double the number of transistors on a computer chip every two years. This, he proposed in 1965, would lead to a nearly exponential increase in computing power over the decades to come. While Moore was correct for several decades, the last 10 years brought this trend to an end.



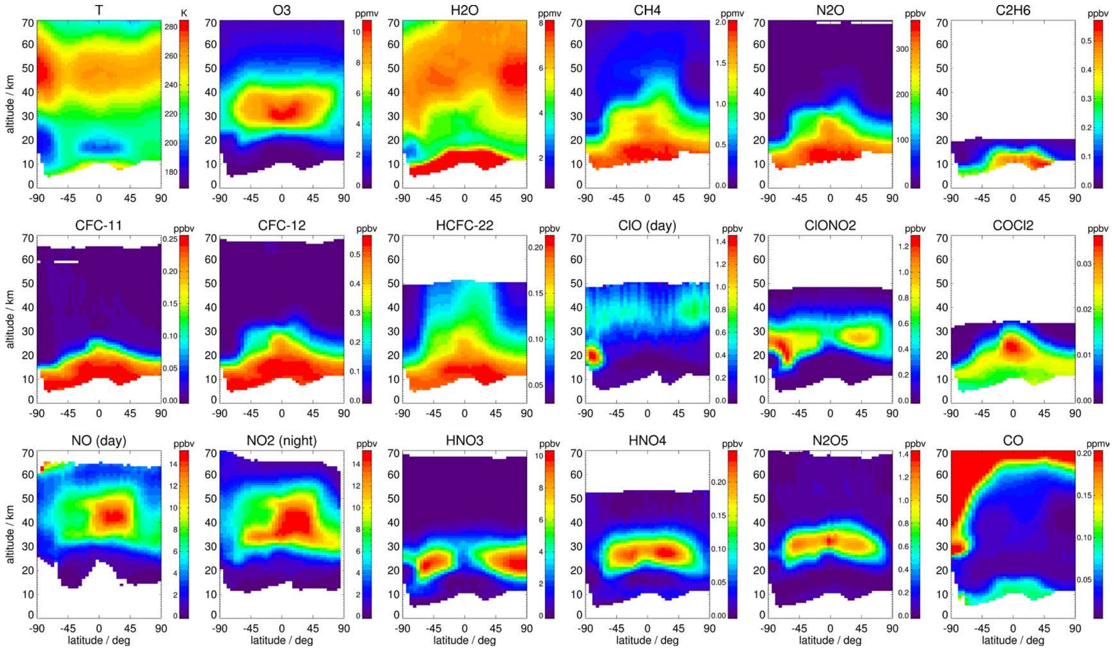
Artist's rendering of the Envisat satellite that carried the MIPAS sensing system. Image: European Space Agency

As luck would have it, however, raw computing power was also no longer what many researchers needed most. Today, solving scientific challenges is often no longer limited by processing speed, but rather by the need to efficiently transfer, analyze, and store large datasets.

This holds true for the MIPAS researchers, who must process and analyze a decade of data tracking 36 different chemical species and temperature. The team's work is made even more complex by the complex relationship trace gases have with one another at higher altitudes — researchers must chart the interplay of temperature, radiation, concentrations of other chemicals, and how all these characteristics influence one another. As a result, the team has to do computationally expensive non-local thermodynamic equilibrium (NLTE) calculations for these species. Water vapor alone required roughly one million core hours for these calculations, and the team had to model nine species using NLTE methods.

While these calculations could individually be performed on more modest computing resources, they would collectively take far too long without access to HPC resources. "Earlier in the project we were just working on a local cluster to run a month of data from the upper atmosphere, where this complex NLTE is required," said Dr. Bernd Funke, a senior researcher at IAA and collaborator on the project. "Getting results for one month of data could take almost one month of computation. Now we can run these things in two or three nights. From a scientific point of view, this quick access to the data is extremely valuable."

Both Kiefer and Funke indicated that HLRS computing resources — as well as the ability to store their data on HLRS's fast and secure High-Performance Storage System — enabled the team to rapidly analyze its data.



Monthly zonal means of temperature and volume mixing ratios (vmr) of several chemical species calculated from the spectra measured by the MIPAS instrument during September 2009. The abscissa gives the latitude from -90 degree (South Pole) to 90 degree (North Pole) and the ordinate is the geometric altitude. The vmr values are given as part per million (ppmv) or part per billion (ppbv), while temperatures are given in Kelvin. Image: Michael Kiefer/KIT

Next-generation experimental techniques drive need for next-generation computing

As the researchers finish their analysis of the MIPAS dataset, they anticipate that the near future will see new mid-infrared space missions. Considering the massive datasets they expect these missions to produce, HPC centers like HLRS will continue to play a major role in hosting, processing, and analyzing the data.

Future missions such as the Earth Explorer candidate mission CAIRT, recently selected by ESA for pre-feasibility studies, will use imaging methods, which increase the number of measurements per orbit and add two additional dimensions to the data. This will not only give researchers an even more detailed view of atmospheric composition and processes, but also greatly increase the complexity and volume of data analysis that will be required. The researchers estimate that one of the projected instruments could result in up to a 1,000-fold increase in datapoints gathered.

The team also indicated that HLRS was quick to embrace their relatively "non-traditional" need for supercomputing resources. The current pivot across the sciences to even more data-centric HPC applications underscored the need for HPC centers to provide a suite of tools in the realms of data storage and management. *EG*

HPC Helps Scientists in Quest to Advance Hydrogen-Based Energy Storage

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

Although advances in renewable energy technologies continue to move humanity closer to being able to power our lives using cleaner, safer methods, one major issue remains: humans have no influence over when the wind blows or the sun shines. This means that in order to use renewable energy on a global scale, methods are needed for efficiently storing excess energy generated during "boom" times so there is ample power for moments when renewables can not keep up with demand.

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

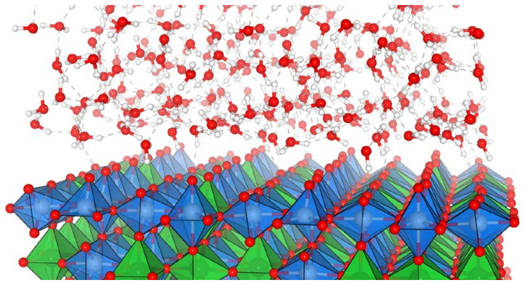
While researchers have made some progress identifying ways to do electrolysis at an industrial scale, there is still one major hurdle to clear: currently, iridium is the only catalyst proven to remain both active and stable enough to facilitate water oxidation, a key step in water electrolysis. Unfortunately, natural sources of iridium are vanishingly rare on the Earth's surface. This means that researchers must search for either an entirely new material or develop metal alloys — mixes of two or more metals that retain certain characteristics from their constituent materials — in order to scale up water electrolysis.

Researchers from the Fritz Haber Institute in Berlin have been using HLRS's Hawk supercomputer to model the complex chemical reactions that take place during electrolysis at a molecular level. The team hopes to gain a greater insight into what makes iridium so effective in order to develop an efficient method for using hydrogen to store energy on a global scale.

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

Viewing fine-grained interactions through two different lenses

To gain a more fundamental view into how molecules behave during electrolysis, scientists need to observe these chemical reactions at the atomic level, charting the paths of electrons for individual atoms while watching several hundred atoms interacting with one another. Moreover, they would like to study these phenomena under a variety of conditions, an approach that would be impossible experimentally but can be done using computational modelling. Computational scientists then share these models with experimentalists, providing further insights into experiments using spectroscopy.



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

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

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

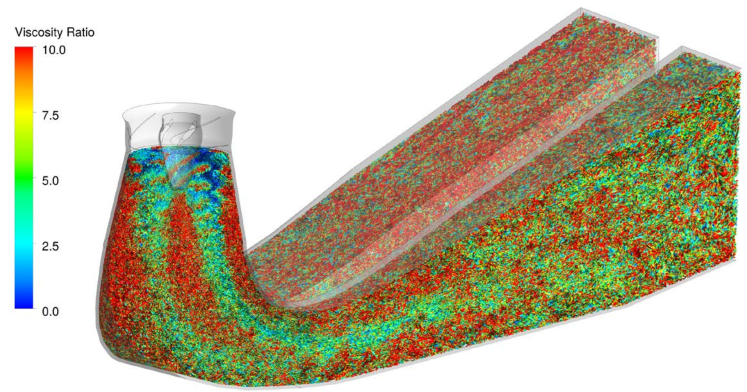
Through its work, the team identified a particular alloy, iridium oxide mixed with niobium ($Ir_{60}Nb_{40}O_x$) that behaves nearly as stably as pure iridium, but requires 40 percent less of the precious metal. While the team knows that much more work needs to be done to identify other materials that might be suitable as an electrocatalyst, it feels confident that the two-pronged approach of spectroscopic experiments and large-scale simulations is the ideal method for moving the research forward.

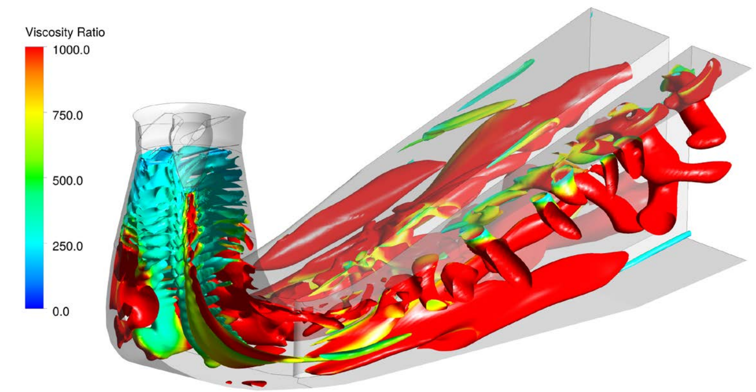
Today's supercomputers focused on tomorrow's reimagined energy grid

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

While Jones indicated that faster, larger computers make it possible for the team to study larger molecular systems or more permutations of a given system, the investigators are still limited in the number of atoms they can simulate during each run. Next-generation systems will help address some of these computational hurdles. At the same time, however, simulating ever larger systems will introduce a new problem: limits on system memory availability, an increasingly common challenge for computational researchers in many research domains. Despite such technical challenges, the team expects that using HPC to accelerate experimentation will be indispensable.

While water electrolysis may not immediately become the dominant method for changing the world's energy grid, Jones feels confident that hydrogen will prove to be a game-changer in electrical energy storage and conversion. "Electrolytic water splitting links the electrical and chemical sectors, and when we think about going climate-neutral by 2050, that link becomes critical," Jones said. "It is not just energy storage that we have to worry about; it is also sustainable chemical production. Green hydrogen could help solve both of these issues." *EG*





Joβberger's LES simulation (left) of a water turbine calculates the energy transfer due to turbulence at a much finer scale than is possible in a conventional RANS simulation (right). Image: University of Stuttgart Institute of Fluid Mechanics and Hydraulic Machinery

Simulation Could Improve Durability of Hydroelectric Turbines

Kaplan turbines are among the most widely used turbines for water power generation. University of Stuttgart researchers are using HLRS's supercomputer to understand in fine detail how to deploy them more reliably in a wider range of operating conditions.

Since James Francis patented his Francis turbine in the mid-nineteenth century, hydroelectric power has been one of world's most reliable, safest, and cleanest sources of electricity. As technology advanced, new turbine designs allowed engineers to adapt hydroelectric dams to a wider range of landscapes, climates, and waterways.

The Kaplan turbine, developed in 1913 by Viktor Kaplan, was more complex than Francis' turbine, but offered engineers more flexibility due to its ability to generate power efficiently over a wide range of flow rates. This is especially important in rivers where the intake water pressure can fluctuate, or under circumstances where large vertical drops for water at dams are not possible, such as on rivers with little elevation change.

The Francis and Kaplan turbines, along with the Pelton wheel, represent the overwhelming majority of turbines used in hydroelectric dams today. While these devices can be remarkably resilient—well-maintained Kaplan turbines can be used for more than 50 years in some cases – the demands being put on them in humanity's changing energy landscape are causing more frequent breakdowns and higher turnover for the turbines. Specifically, as countries scale up other renewable sources of energy such as wind or solar power, the need to more frequently start, stop, and change the flow rate on these turbines is wearing them down.

In an effort to better understand how flow conditions impact turbine reliability, researchers at the University of Stuttgart's Institute of Fluid Mechanics and Hydraulic Machinery (IHS) have been using supercomputing resources at the High-Performance Computing Center Stuttgart (HLRS) to study these machines at a fundamental level.

"Kaplan turbines have a big operating range, which also means you have to account for different kinds of fluid conditions and what can happen in the turbine," said Simon Joβberger, a PhD student at the University of Stuttgart and researcher on the project. "The simulation results are normally fine when you simulate at the design operating point, but it is difficult to know if your simulations are right or wrong for a specific turbine when you simulate other operation points, for example at higher and lower flow rates and / or higher and lower hydraulic heads. We need reliable results for Kaplan turbines across the whole operating map, and we need these results during the design process so that we can adapt the turbine to the specific conditions at the operational site."

Go with the flow

In order to accurately model the conditions in a turbine using simulations, researchers have to account for the chaotic, turbulent motions of fluid passing through the turbine. When simulating fluid flows on a supercomputer, researchers often divide the area of study into a grid, then calculate the fluid behavior within individual grid boxes for each "time step." When the size of the grid becomes finer, the interval between time steps is reduced, or the fluid flows faster (or any combination of these factors), the simulation becomes more computationally demanding.

Generally speaking, researchers want to calculate fluid behavior based on fundamental physical principles, with the fewest assumptions possible. However, even the most powerful computers are often incapable of completely calculating fluid behavior across all necessary length and time scales. As a result, certain simulation methods include assumptions about how flows behave at the finest scales.

In perhaps the most fundamental class of turbulence simulations, Reynolds-Averaged Navier-Stokes (RANS) equations, researchers reduce computational complexity by using averages that approximate behavior in turbulent flows. This enables researchers to focus on specific calculations while using reliable assumptions about how other aspects of the fluid might behave.

Another class of simulation provides an unvarnished understanding of larger swirling turbulent motions, or eddies, in the fluid. These aptly named large-eddy simulations (LES) enable researchers to focus computational resources on aspects of the fluid that have the largest role in determining turbine efficiency, stress points, or wear and tear during turbine operation.

Using HLRS's Hawk supercomputer, Joßberger is focused on making the most detailed Kaplan turbine simulation possible by running high-resolution large-eddy simulations whenever possible, supplementing the results with RANS in regions where LES simulation would be computationally too expensive.

Hawk's computing power enables Joßberger to study flow through the turbine at much higher resolution than is usually done. "For what I would call a 'normal' unsteady state simulation of a Kaplan turbine, you would normally use 50 to 100 time steps for a single rotation of the turbine," he said. "Currently, we are running about 1,600 time steps for one rotation. In combination with the much finer computational grid this means that our level of detail is 4 to 5 orders of magnitude greater than what would normally be done."

Individualized insights for industry

In addition to RANS and LES, engineering researchers use supercomputers to do much more complex direct numerical simulations (DNS) that use virtually no assumptions to model fluid behavior. Meaningful DNS that approaches the complexity of real-world conditions or geometries can only be done using the world's fastest computers, however, and only when focusing on small areas or simple designs. Joßberger sees his work as helping inform and improve modelling and simulation being done at the commercial level.

"The ultimate goal is to understand what is happening in the turbine and then take this information so we can compare it with less complex simulations to see what effects are really important in modelling," he said. "With this approach, we learn what we need to account for, and what we can actually achieve with smaller or less complex simulations that could be used in industry. The results of this work can serve as a benchmark for assessing the quality of less complex models."

After having completed simulations for 25 rotations of the turbine, Joßberger feels confident that he can accurately model real-world conditions for the Kaplan turbine under a variety of conditions. Ultimately, his work could help to guarantee that hydroelectric dams remain a reliable, cost-effective source of green energy that support power grids around the world. *EG*

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About Us

Inside Our Computing Room

Hewlett Packard Enterprise Apollo (Hawk)

HLRS's flagship supercomputer, called Hawk, was ranked #16 in its November 2020 debut on the Top500 List of the world's fastest supercomputers. Based on second-generation EPYC processors from AMD, the system is optimized for the sustained application performance and high scalability required for large-scale simulation, particularly for engineering and the applied sciences. In September 2021, HLRS announced the beginning of production of an expansion of Hawk that includes HPE Apollo systems with NVIDIA graphic processing units (GPUs). The upgrade has enhanced the center's capacity for deep learning and artificial intelligence applications, and enables new kinds of hybrid computing workflows that integrate HPC with Big Data methods.

System Type: Hewlett Packard Enterprise Apollo
CPU Type: AMD EPYC Rome 7742, 64 core, 2.25 GHz
Number of compute nodes: 5,632
Number of compute cores: 720,896
System peak performance: 26 petaflops
Total system memory: ~ 1.44 PB
Total disk storage capacity: ~ 25 PB

System Type: Apollo 6500 Gen10 Plus
GPU Type: NVIDIA A100
Number of GPUs: 192
Performance: 120 petaflops AI performance

Funding for Hawk was provided by the Baden-Württemberg Ministry of Science, Research and Arts, and by the German Federal Ministry for Education and Research through the Gauss Centre for Supercomputing (GCS). Hawk is part of the GCS national supercomputing infrastructure.

Baden-Württemberg
MINISTRY OF SCIENCE, RESEARCH AND ARTS

Federal Ministry
of Education
and Research

Cray CS-Storm

The Cray CS-Storm is optimized for artificial intelligence (AI) workloads, including processing-intensive applications for deep learning. Based on a GPU architecture, the CS-Storm provides a high-performance platform for deep learning frameworks such as TensorFlow and PyTorch, while also supporting use of classical machine learning tools such as Apache Spark and scikit-learn. The system is installed with the Cray Urika-CS AI and analytics suite, enabling HLRS users to address complex problems and process data with higher accuracy.

Deep learning partition: 64 NVIDIA Tesla V100 GPUs
Cray CS500 Spark partition: 8 CPU nodes
Software compiler: Urika-CS AI Suite
Interconnect: HDR100 Infiniband

AMD GPU System

Installed in 2021, this GPU-based system was donated to HLRS by hardware manufacturer AMD as a part of AMD's COVID-19 High-Performance Computing Fund. The system is dedicated to providing computing resources for medical research related to the COVID-19 pandemic and other diseases, and provides data analytics capacity for addressing sudden demands for simulation and data analytics that can occur in crisis situations. This system is integrated into HLRS's Vulcan cluster.

Processors: 10 × AMD EPYC
Accelerators: 80 × AMD Instinct
Performance: 530 TFlops, 64-bit

NEC Cluster (Vulcan)

This standard PC cluster was installed in 2009. Its configuration has been continually adapted to meet increasing demands and provide requirement-optimized solutions, including CPU, GPU, and vector computing components. The current configuration is as follows.

Intel Xeon Gold 6248 @2.5GHz (CascadeLake)
Number of nodes: 96
Memory per node: 128 GB

Intel Xeon Gold 6138 @2.0GHz (SkyLake)
Number of nodes: 100
Memory per node: 192 GB

Intel Xeon E5-2660 v3@ 2.6 GHz (Haswell)
Number of nodes: 88
Memory per node: 256 GB

Intel Xeon E5-2680 v3 @ 2.5 GHz (Haswell)
Number of nodes: 168
Memory per node: 384 GB

AMD Radeon
CPU: Intel Xeon Silver 4112 @ 2.6 GHz (Skylake)
Number of nodes: 6
Memory per node: 96 GB
CPU: 1 × AMD Radeon Pro WX8200
CPU memory: 8 GB

Intel Xeon E5-2667 v4 @ 3.2 GHz (Broadwell) mit P100
Number of nodes: 10
Memory per node: 256 GB
CPU: 1 × Nvidia P100
CPU memory: 12 GB

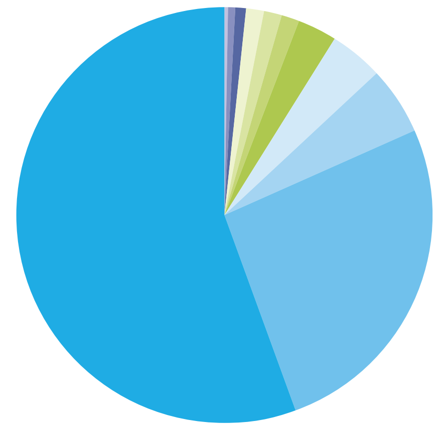
NEC SX-Aurora TSUBASA A300-8 @ 2.6 GHz
Number of nodes: 8
Memory per node: 192 GB
Vector engines: 8 × NEC Type 10B @ 1.4 GHz
Vector engine memory: 48 GB @ 1.2 TB/second

Interconnects
Infiniband EDR/FDR/HDR/QDR

User Profile

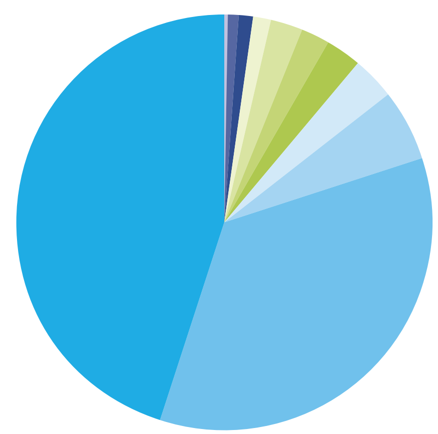
In 2021 the Gauss Centre for Supercomputing approved 8 new large-scale projects (each project requiring more than 35 million core hours) for HLRS's flagship supercomputer, Hawk, for a total of 1.946 billion core-hours. The Partnership for Advanced Computing in Europe (PRACE) also approved 6 international simulation projects for HLRS, for a total of 526 million core-hours. In total, 130 projects, including test projects, were active on Hawk in 2021, for a total of 4.339 billion core hours.

System Usage by Scientific Discipline



- CFD **55.77 %**
- Physics **26.02 %**
- Chemistry **5.25 %**
- Other **4.10 %**
- Solid State Physics **3.06 %**
- Reacting Flows **1.53 %**
- Bioinformatics **1.41 %**
- Transportation and Climate **1.21 %**
- Computer Science **0.87 %**
- Astrophysics **0.66 %**
- Materials Science **0.11 %**

System Usage by State



- Baden-Wurttemberg **45.16 %**
- North Rhine-Westphalia **34.91 %**
- Rheinland-Palatinate **5.55 %**
- Hesse **3.37 %**
- Berlin **2.77 %**
- Saxony **2.33 %**
- Brandenburg **2.32 %**
- Federal Research Center **1.41 %**
- Hamburg **1.27 %**
- Thuringia **0.76 %**
- Bavaria **0.12 %**
- Saxony-Anhalt **0.02 %**
- Lower Saxony **0.01 %**

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 (HPC), artificial intelligence, visualization, and high-performance data analytics. These activities, many of which are conducted in collaboration with investigators at other institutes and in industry, address key problems facing supercomputing and are opening up new opportunities for addressing key German, European, and global challenges. The following is a list of funded projects that operated in 2021.

For more information about our current projects, visit *www.hlrs.de*.

aqua3S
September 2019 – August 2022
EU
Developing a new system for detecting threats in drinking water safety and security, combining data from state-of-the-art sensors and other detection mechanisms.

bwHPC-S5
July 2018 – June 2023
MWK
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.

Cape Reviso
July 2020 – June 2023
BMVI
By combining machine learning, sensor technology, network analysis and VR in digital twins, HLRS is developing planning and decision support tools for conflict analysis and reduction between cyclists and pedestrians.

CASTIEL
September 2020 – August 2022
EU
This coordination and support action will enhance the activities of the EuroCC project by promoting collaboration and the exchange of knowledge and skills among HPC national competence centers across Europe.

CATALYST
October 2016 – December 2021
MWK
Researched methods for analyzing large datasets produced by modelling and simulation, with the goal of implementing a framework that combines HPC and data analytics.

ChEESE
November 2018 – March 2022
EU
Prepared European flagship codes for upcoming pre-exascale and exascale supercomputing systems focusing on fields such as computational seismology, magnetohydrodynamics, physical volcanology, tsunamis, and the monitoring of earthquake activity.

Funding Agency Abbreviations:
BMBF – Federal Ministry of Education and Research | BMVI – Federal Ministry of Transport and Digital Infrastructure | BMWi – Federal Ministry for Economic Affairs and Energy | DBU – German Federal Environmental Foundation | DFG – German Research Foundation | ESF – European Social Fund | EU – European Union | MWK – Baden-Württemberg Ministry for Science, Research, and Art | UM – Baden-Württemberg Ministry of the Environment, Climate Protection and the Energy Sector | WAT – Baden-Württemberg Ministry of Economic Affairs, Labor and Tourism

CIRCE
New in 2021
November 2021 – October 2024
BMBF, MWK
A study to assess potential applications of high-performance computing (HPC) in crisis situations, and what organizational procedures are needed to ensure that HPC resources are immediately available.

CYBELE
January 2019 – March 2022
EU
Integrates tools from high-performance computing, high-performance data analytics, and cloud computing to support the development of more productive, data driven methods for increasing agricultural productivity and reducing food scarcity.

DEGREE
New in 2021
June 2021 – June 2023
DBU
Investigating a method for increasing energy efficiency in data centers by dynamically controlling cooling circuit temperatures, and developing guidelines for implementing the resulting concepts.

ENRICH
New in 2021
April 2021 – March 2023
UM
Analyzing current developments in IT and the operation of high-performance computing (HPC) centers regarding their resource efficiency and sustainability potential.

EuroCC
September 2020 – August 2022
EU
HLRS is the coordinating center of this Europe-wide project to establish national HPC competence centers and develop a shared, high level of expertise in high-performance computing, high-performance data analytics, and artificial intelligence.

exaFOAM
New in 2021
April 2021 – March 2024
EU
Working to reduce bottlenecks in performance scaling for computational fluid dynamics applications on massively parallel high-performance computing systems.

EXCELLERAT
December 2018 – May 2022
EU
Facilitates 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 in industry.

FF4EuroHPC
September 2020 – August 2023
EU
Conducts outreach and provides support to Europe's small and medium-sized enterprises (SMEs) to enable them to profit from the advantages offered by high-performance computing (HPC) technologies and services.

FocusCoE
December 2018 – March 2022
EU
Coordinates strategic collaboration and outreach among EU-funded Centres of Excellence to more effectively exploit the benefits of extreme scale applications for addressing scientific, industrial, or societal challenges.

HiDALGO
December 2018 – February 2022
EU
Develops novel methods, algorithms, and software for HPC and high-performance data analytics to accurately model and simulate the complex processes that arise in connection with major global challenges such as forced migration, air pollution, and the spread of disinformation through social media.

HPC-Europa 3
May 2017 – April 2022
EU
Fosters transnational cooperation among EU scientists (especially junior researchers) who work on HPC-related topics such as applications, tools, and middleware.

HPCWE
June 2019 – November 2021
EU
A consortium of academic institutes, HPC centers, and industrial partners in Europe and Brazil developed novel algorithms and state-of-the-art codes to support the development of more efficient technologies for wind power.

HyForPV
September 2018 – October 2021
BMWi
Developed and operationalized new prediction products for the integration of photovoltaics (PV) into the energy market and smart grids by delivering simulations of PV power output at high resolution.

IKILeUS
New in 2021
December 2021 – November 2024
BMBF
HLRS is the coordinating center for this project to integrate artificial intelligence (AI) topics into curricula at the University of Stuttgart, and to implement AI technologies to improve instruction.

InHPC-DE
November 2017 – December 2021
BMBF
Coordinated integration among Germany's three Tier-1 supercomputing centers to create a standardized and distributed HPC ecosystem. It provides funding for 100 Gbit networking and opportunities for high-speed data management and visualization.

KoLab BW
New in 2021
March 2021 – December 2024
MWK
Developing tools for meeting and collaborating from remote locations in three-dimensional virtual reality environments.

MoeWe
July 2016 – March 2021
ESF, MWK
Developed a modular, flexible training program called the Supercomputing-Akademie address demand for supercomputing experts, particularly in industry.

NFDI4Cat
October 2020 – September 2025
DFG
As a participant in the German National Research Data Infrastructure initiative, this consortium is creating a national platform for data integration in catalysis and chemical engineering research.

OpenForecast
September 2019 – May 2021
EU
Developed approaches for combining freely available data and supercomputing resources to create a new generation of searchable data products for European citizens, public authorities, economic operators, and decision makers.

ORCHESTRA
December 2020 – November 2023
EU
By developing a networked platform for data sharing, this project is creating a new large-scale, pan-European cohort that will improve research and responses to the SARS-CoV-2 pandemic and provide a model for addressing future public health threats.

OSCCAR
June 2018 – November 2021
EU
Used a novel, simulation-based approach to develop new systems for protecting vehicle occupants in accidents.

POP2
December 2018 – May 2022
EU
This Center of Excellence provides performance optimization and productivity services for academic and industrial users of HPC.

PRACE
May 2019 – June 2022
EU
Supports high-impact scientific discovery and engineering R&D to enhance European competitiveness for the benefit of society.

SDC4Lit
May 2019 – April 2023
MWK
An interdisciplinary research project to sustainably organize the data-life cycle in digital literature. The resulting infrastructure will offer a data repository and research platform for the digital humanities.

SEQUOIA
New in 2021
January 2021 – December 2022
WAT
Developing new software for quantum computers and investigating ways to integrate them with conventional systems for high-performance computing and artificial intelligence.

SERRANO
January 2020 – December 2022
EU
Aims to introduce a novel ecosystem of cloud-based technologies, from specialized hardware resources to software toolsets, to enable application-specific service instantiation and optimal customization.

SimTech
July 2019 – March 2023
DFG
An interdisciplinary Excellence Cluster at the University of Stuttgart that is developing simulation technologies to enable integrative systems science. HLRS supports the development of efficient methods for uncertainty quantification and management.

Simulated Worlds
January 2011 –August 2024
MWK
Offers students opportunities to develop and execute simulation projects in collaboration with HLRS 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.

SODALITE
February 2019 – January 2022
EU
Aims to provide an optimized, resilient, heterogeneous execution environment that enables operational transparency between cloud and HPC infrastructures.

Trust in Information
August 2020 – August 2023
MWK
Multidisciplinary research led by the HLRS Department of Philosophy that is developing perspectives for assessing the trustworthiness of computational science and limiting the spread of misinformation.

HPC Training Courses in 2021

HLRS offered 36 courses in 2021, providing continuing professional education on a wide range of topics relevant for high-performance computing. The courses took place over 122 course-days online and in Stuttgart and in cooperation with other institutes in Germany and internationally. A total of 1196 trainees participated in these activities.

For a current listing of upcoming courses, please visit *www.hlrs.de/training*.

Date	Location	Topic	Host
Jan 20	Online	Machine Learning with AMD GPUs and ROCm Software NEW	HLRS / AMD
Jan 21	Online	Machine Learning with AMD GPUs and ROCm Software NEW	HLRS / AMD
Feb 8–12	Online	Parallel Programming (MPI, OpenMP) and Tools	ZIH / HLRS
Feb 22–26	Online	Introduction to Computational Fluid Dynamics	HLRS / STS / IAG
Mar 2–5	Online	Modern C++ Software Design (Intermediate)	HLRS
Mar 8–10	Online	Iterative Linear Solvers	HLRS
Mar 23–26	Online	Parallelization with MPI and OpenMP	ZDV / HLRS
Apr 12–16	Online	Fortran for Scientific Computing *	HLRS
Apr 19–22	Online	Parallelization with MPI (TtT)	VSC / HLRS
May 4–7	Online	Modern C++ Software Design (Advanced)	HLRS
May 5–6	Online	Shared memory parallelization with OpenMP (with VSC Vienna) (TtT)	VSC / HLRS
May 25–27	Online	Introduction to MPI (TtT)	IT4I / VSC / HLRS
Jun 7–11	Online	Parallel Programming with MPI and OpenMP (TtT)	SURFsara / HLRS
Jun 11	Online	Introduction to NEC Sx-Aurora TSUBASA Vector Platform	HLRS
Jun 15–17	Online	Introduction to Hybrid Programming in HPC	VSC / LRZ / HLRS / NHR@FAU
Jun 21–22	Online	AMD GPU Training NEW	HLRS / AMD
Jun 24–25	Online	Efficient Parallel Programming with GASPI *	HLRS / F. ITWM
Jun 28–30	Online	From Machine Learning to Deep Learning: A Concise Introduction NEW	HLRS
Jul 6–9	Online	Modern C++ Software Design (Intermediate)	HLRS
Jul 12–15	Online	Node-Level Performance Engineering & Tools *	HLRS / NHR@FAU / ZIH
Jul 19–22	Online	Deep Learning and Acceleration with OpenACC on NVIDIA GPUs NEW	HLRS / NVIDIA
Jul 26–30	Online	Optimization of Scaling and Node-Level Performance on Hawk	HLRS
Aug 23–26	Online	Parallel Programming with MPI / OpenMP	ETH / HLRS
Sep 20–24	Stuttgart	CFD with OpenFOAM®	HLRS
Sep 30–Oct 1	Stuttgart	Scientific Visualization	HLRS

Date	Location	Topic	Host
Oct 11–15	Online	Parallel Programming Workshop (MPI, OpenMP & advanced topics) *	HLRS
Oct 19–21	Online	ChEESE Advanced Training on HPC for Computational Seismology *	HLRS / ChEESE
Oct 19–21	Online	Advanced MPI (TtT)	IT4I / VSC / HLRS
Oct 28–29	Online	Shared Memory Parallelization with OpenMP (TtT)	VSC / HLRS
Nov 8–12	Online	Optimization of Scaling and Node-Level Performance on Hawk	HLRS
Nov 15–Dec 10	Online	MOOC: One-Sided Communication and the MPI Shared Memory Interface NEW	HLRS / SURFsara / Astron
Nov 23–26	Stuttgart	Modern C++ Software Design (Advanced)	HLRS
Nov 23–26	Online	Parallelization with MPI (TtT)	VSC / HLRS
Nov 29–Dec 1	Online	Advanced Parallel Programming with MPI and OpenMP	JSC / HLRS
Dec 6–10	Stuttgart	Fortran for Scientific Computing	HLRS
Dec 13–14	Online	Data Analytics for Engineering Data Using Machine Learning NEW	HLRS / F. SCAI

- Parallel Programming
- Computational Fluid Dynamics (CFD)
- Performance Optimization and Debugging
- Data in HPC
- Programming Languages for Scientific Computing
- Scientific Visualization
- Compute Cluster – Usage and Administration
- Training for special communities

* PRACE courses: HLRS, a member of the Gauss Centre for Supercomputing, is an official PRACE Training Center of the European Union.

TtT: Train the Trainer Courses

Astron – Netherlands Institute of Radio Astronomy | ChEESE – Center of Excellence in Solid Earth | ETH – Scientific IT Services, ETH Zurich | F. ITWM – Fraunhofer Institute for Industrial Mathematics | F. SCAI – Fraunhofer Institute for Algorithms and Scientific Computing | HLRS – High-Performance Computing Center Stuttgart | IAG – Institute for Aerodynamics and Gas Dynamics (University of Stuttgart) | IT4I – IT4Innovations National Supercomputing Center (TU Ostrava) | JSC – Jülich Supercomputing Centre | LRZ – Leibniz Supercomputing Centre | NHR@FAU – Erlangen National High Performance Computing Center | STS – Simulation Techniques and Scientific Computing (University of Siegen) | SURFsara – SURFSara (Dutch National Supercomputing Center) | VSC – Vienna Scientific Cluster | ZDV – Data Center, University of Mainz | ZIH – Center for Information Services and High Performance Computing (TU Dresden)

Workshops and Conferences in 2021

February 16–17
SAS Workshop 2021: Nachahmung, Anpassung, Täuschung
Scholars examined the history and systematics of imitation, adaptation, and deception in an interdisciplinary way, as well as how the relevance and understanding of these concepts has been perceived across time and in different contexts.

March 16–19
31st Workshop on Sustained Simulation Performance
Organized in cooperation with NEC, this meeting brings scientists, application developers, and hardware designers from different continents together to discuss hardware architectures, programming styles, and strategies for achieving the highest possible sustained application performance.

May 10
19th HLRS/hww Workshop on Scalable Global Parallel File Systems
This year's workshop focused on major issues and developments associated with the evolution of global parallel file systems and high performance data storage, including new requirements related to research data management.

September 15–17
The Economic and Cultural Impacts of the Digital Age
This convention gathered experts from Europe and the Americas to discuss new developments in art, culture, and economy as a basis for future research and projects at the Media Solution Center Baden-Württemberg.

October 7–8
24th Results and Review Workshop
This event brings together scientists and engineers to present and discuss research results enabled by high-performance computing as well as challenges and best practices in using HPC systems.

October 27–29
SAS Conference 2021: Trust in Science
This interdisciplinary conference considered how and on what basis appropriate trust in science can be built and doubt alleviated, particularly considering the increasing complexity of science and challenges of communication.

December 1
5th Industrial HPC User Round Table (iHURT)
The annual iHURT meeting facilitates exchange between HLRS and its industrial user community, focusing on innovative applications of HPC for research and development as well as challenges that industry faces in using HPC.

HLRS Books

High Performance Computing in Science and Engineering '20
Editors: Wolfgang E. Nagel, Dietmar H. Kröner, Michael M. Resch

This book presents the state-of-the-art in supercomputer simulation. It includes the latest findings from leading researchers using systems from the High Performance Computing Center Stuttgart (HLRS) in 2020. The reports cover all fields of computational science and engineering ranging from CFD to computational physics and from chemistry to computer science with a special emphasis on industrially relevant applications. Presenting findings of one of Europe's leading systems, this volume covers a wide variety of applications that deliver a high level of sustained performance. The book covers the main methods in high-performance computing. Its outstanding results in achieving the best performance for production codes are of particular interest for both scientists and engineers. The book comes with a wealth of color illustrations and tables of results.

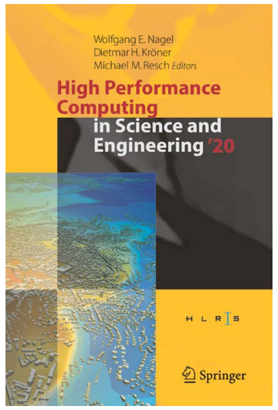


Image: Springer Verlag

Sustained Simulation Performance 2019 and 2020
Editors: Michael M. Resch, Manuela Wossough, Wolfgang Bez, Erich Focht, Hiroaki Kobayashi

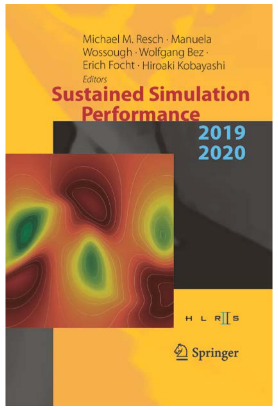


Image: Springer Verlag

This book presents the state of the art in High Performance Computing on modern supercomputer architectures. It addresses trends in hardware and software development in general. The contributions cover a broad range of topics, from performance evaluations in context with power efficiency to Computational Fluid Dynamics and High Performance Data Analytics. In addition, they explore new topics like the use of High Performance Computers in the field of Artificial Intelligence and Machine Learning. All contributions are based on selected papers presented at the 30th Workshop on Sustained Simulation Performance (WSSP) held at the High Performance Computing Center, University of Stuttgart, Germany in October 2019 and on the papers for the planned Workshop on Sustained Simulation Performance in March 2020, which could not take place due to the COVID-19 pandemic.

Tools for High Performance Computing 2018 / 2019

Editors: Hartmut Mix, Christoph Niethammer, Huan Zhou, Wolfgang E. Nagel, Michael M. Resch

This book presents the proceedings of the 12th International Parallel Tools Workshop, held in Stuttgart, Germany, during September 17–18, 2018, and of the 13th International Parallel Tools Workshop, held in Dresden, Germany, during September 2–3, 2019. The workshops are a forum to discuss the latest advances in parallel tools for high-performance computing. High-performance computing plays an increasingly important role for numerical simulation and modeling in academic and industrial research. At the same time, using large-scale parallel systems efficiently is becoming more difficult. A number of tools addressing parallel program development and analysis has emerged from the high-performance computing community over the last decade, and what may have started as a collection of a small helper scripts has now matured into production-grade frameworks. Powerful user interfaces and an extensive body of documentation together create a user-friendly environment for parallel tools.

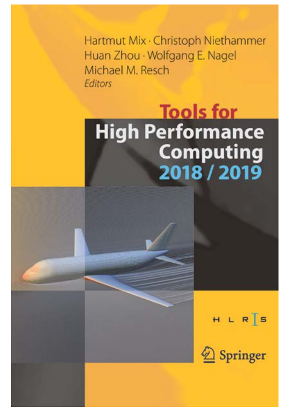
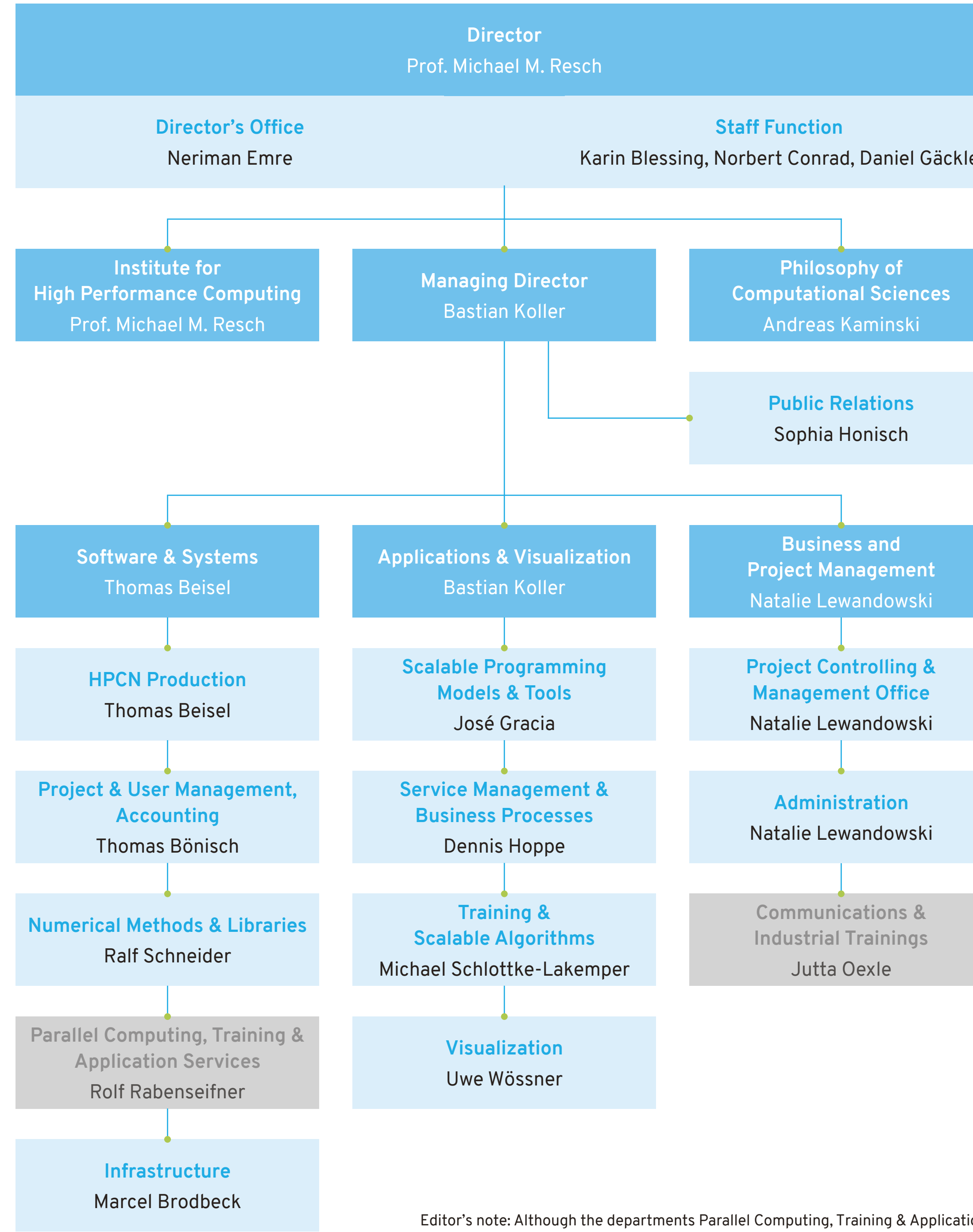


Image: Springer Verlag

Organization Chart



Editor's note: Although the departments Parallel Computing, Training & Application Services and Communications & Industrial Trainings were active in 2021, they were consolidated into the new Department of Training & Scalable Algorithms by the publication date of this Annual Report.

Departments

Administration

Leader: Dr. Natalie Lewandowski

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.

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.

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.

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.

Philosophy of Science and Technology of Computer Simulation

Leader: Dr. Andreas Kaminski

Examines both how computer simulation and machine learning are changing science and technology development, and how society and politics react to these changes: Does simulation and machine learning change our understanding of knowledge and how we justify scientific results? How can computer-based methods help to overcome uncertainties about the future? And how do we deal with the uncertainties of simulation and machine learning itself?

Project Controlling and Management Office

Leader: Dr. Natalie Lewandowski

The Project Controlling and Management Office (PCMO) is responsible for the controlling and quality assurance of current research projects at HLRS or with HLRS as a beneficiary, and the management of large-scale third-party funded projects, including coordination and business development tasks. The PCMO also assists coordination at the proposal planning and writing stage and acts as a supporting and coordinating entity between the HLRS management, department heads, and HLRS administration in project-related matters.

Project and User Management, Accounting

Leader: Dr. 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.

Public Relations

Leader: Sophia Honisch

Responsible for all areas of HLRS's external communications, from media relations to the management of HLRS's website and social media accounts: It is the main contact point for press and the broader public. The PR department communicates about HLRS's wide range of scientific and engineering disciplines, its research (projects) as well as its services, and disseminates results, new findings, and insights gained.

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: Dennis Hoppe

Advances the convergence of high-performance computing and artificial intelligence, in particular with the goal of supporting hybrid HPC/AI workflows on a single infrastructure. This includes developing AI solutions, specifically in a business context, using cutting-edge technologies for Big Data, machine learning, and deep learning. The group also conducts research on related virtualization technologies such as containers, orchestration, and job scheduling. Leveraging synergies between virtualization and HPC, it has gained expertise in the development and operation of dynamic and scalable cloud computing services. The department efficiently applies performance and availability monitoring, elastic workflow management, and energy-efficient operation for federated cloud environments.

Training and Scalable Algorithms

Leader: Dr. Michael Schlottke-Lakemper

Organizes and implements HLRS's training activities focusing on a variety of topics in high-performance computing, artificial intelligence, and modeling and simulation. These include compact, high-intensity courses, blended learning modules, and public outreach activities. In each area, our goal is to provide an outstanding learning experience by offering training on relevant topics, with up-to-date and audience-focused content, and given by highly-qualified instructors. Besides our teaching and outreach activities, we conduct research on the development of efficient algorithms for scientific computing applications.

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.

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Cover:
Scientists at the University of Hohenheim working on the MPAS (Model Prediction Across Scales) project are using HLRS's Hawk supercomputer for multiscale Earth systems simulations that are helping to predict the potential effects of climate change.

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High-Performance Computing Center Stuttgart
www.hlrs.de

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