HLRS

HIGH-PERFORMANCE COMPUTING CENTER
STUTTGART

2017

ANNUAL REPORT

ENERGY HEALTH CLIMATE MOBILITY PHILOSOPHY

Editorial

Grußwort

Looking back on 2017, I am struck by two significant events representing several years of hard work that came to a successful conclusion.

In a press conference at HLRS in August 2017, Baden-Württemberg Minister of Science, Research and the Arts Theresia Bauer introduced the state's future high-performance computing (HPC) strategy. During her presentation, she acknowledged HLRS's importance as a German federal supercomputing center and for the entire European research community. As part of Baden-Württemberg's strategy, HLRS looks forward to introducing new, more powerful HPC systems in 2019 and 2023, ensuring that it will continue to stay at the forefront of supercomputing through the middle of the next decade and beyond.

In April, HLRS also reached an important milestone in its effort to increase the number of scientists and engineers with HPC knowledge and skills. In July, State Secretary of Finance Giesla Splett and other honored guests from the federal and state governments joined us to celebrate the opening of a new HLRS building

Im Jahresrückblick zeichneten sich zwei besonders wichtige Ereignisse ab, die lange vorbereitet wurden und 2017 zu einem erfolgreichen Abschluss kamen.

Anlässlich eines Pressegespräches am HLRS stellte die baden-württembergische Wissenschaftsministerin Theresia Bauer im August 2017 die zukünftige HPC-Strategie des Landes Baden-Württemberg vor und unterstrich dabei die besondere Rolle des HLRS sowohl als Bundeszentrum als auch als europäisches Zentrum. Im Rahmen der Landesstrategie wird das HLRS in den Jahren 2019 und 2023 jeweils einen neuen Höchstleistungsrechner beschaffen und damit die technische Entwicklung bis in die Mitte des nächsten Jahrzehnts und darüberhinaus sichern können.

Bereits im März konnte das HLRS mit der Eröffnung seines neuen HPC Training Centers einen wesentlichen Meilenstein in seiner Weiterbildungsstrategie erreichen. Im Juli wurde das Gebäude dann offiziell von Staatsekretärin Splett im Beisein von Ehrengästen aus Land, Stadt und Wissenschaft an das HLRS dedicated to HPC training. This spectacular new facility will enable HLRS to expand its efforts to address the large, unmet need for continuing education in supercomputing—an important part of our mission.

In a project supported by the European Social Fund and the State of Baden-Württemberg, we are also now working to foster new synergies with HPC users from industry. Using new educational technologies and methods, a new program called the Supercomputing-Akademie will offer continuing education that is tailored to the needs of scientists and engineers working at high-tech companies, as well as academic researchers, and enable them to stay up-to-date with the latest HPC methods.

In many ways HLRS can proudly look back on a very successful year. Our third-party funding saw additional increases over previous years, showing that HLRS's in-house research projects on topics relevant to the future of supercomputing are seen positively in our federal and state governments, as well as the European Union.

Users of our HPC systems also had a very productive year. This annual report showcases some examples of our users' research, including the millionth compute job run on Hazel Hen. You can also read about contributions that HLRS is making in research related to wind power generation, regional climate change prediction, and cosmology. We are also particularly grateful that Claus-Peter Hutter, leader of the Baden-Württemberg Academy for Nature Preservation and Environmental Protection, met with us to discuss our cooperation on issues related to sustainability. His external perspective provides insights into ways that HLRS and its expertise in simulation are contributing to sustainability.

With this annual report we thank all of our supporters and funders who have made our successes in 2017 possible. At the same time we look forward to tackling new challenges in 2018.

With best regards,

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

übergeben. Mit dem neuen Gebäude kann das HLRS nun seine Schulungsmaßnahmen ausbauen und insbesondere dem steigenden Bedürfnis nach Weiterbildung im Bereich der Digitalisierung Rechnung tragen.

Im Zusammenspiel mit dem vom europäischen Sozialfonds und dem Land Baden-Württemberg geförderten Projekt sollen Synergieeffekte mit Nutzern aus der Wirtschaft erzielt werden. Als Projekt wird die Supercomputing-Akademie, ein Weiterbildungsprogramm, entwickelt, das neue didaktische Technologien und Methoden nutzt und sich gleichermaßen an Kunden aus der Industrie und Wissenschaft wendet, um ihnen die Möglichkeit zu bieten, kontinuierlich mit den Entwicklungen im HPC vertraut zu bleiben.

Auch über diese beiden Ereignisse hinaus blickt das HLRS auf ein sehr erfolgreiches Jahr 2017 zurück. So konnten die Einnahmen aus Drittmitteln weiter gesteigert werden, was zeigt, dass die eigene Forschung des HLRS auf den Ebenen des Landes, des Bundes sowie der europäischen Union verstärkt und positiv wahrgenommen und unterstützt wird.

Indem das HLRS den millionsten Job auf seinem HPC System feierte konnten auch seine Benutzer ein sehr erfolgreiches Jahr verzeichnen. Darüber hinaus wurden in Bereichen wie dem Design von Windturbinen, der Simulation des regionalen Klimas sowie der Astrophysik herausragende Ergebnisse erzielt, die wir in diesem Jahresbericht vorstellen.

Besonders freuen wir uns, dass Claus-Peter Hutter, Leiter der Akademie für Natur- und Umweltschutz Baden-Württemberg, sich zu einem Interview bereit erklärte und mit uns über unsere Kooperation in Bezug auf Nachhaltigkeit diskutierte. Damit können wir Ihnen einen externen Blick auf das HLRS und dessen Beitrag zur Nachhaltigkeit präsentieren.

Mit diesem Jahresbericht danken wir allen Unterstützern und Förderern des HLRS, die unsere Erfolge im Jahr 2017 erst möglich gemacht haben. Gleichzeitig freuen wir uns auf das Jahr 2018 mit seinen neuen Herausforderungen.

High-Performance Computing Center Stuttgart (HLRS)

University of Stuttgart
Nobelstrasse 19 | 70550 Stuttgart | Germany

phone ++49 (0)711 685-87269
fax ++49 (0)711 685-87209

email info@hlrs.de
web www.hlrs.de

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

Leader: Dr. Jutta Oexle

Editor: Christopher M. Williams

Lector: F. Rainer Klank

Contributing Writers: Lena Bühler *(LB)*, Eric Gedenk *(EG)*, Christopher M. Williams *(CW)*

Translations: Anna-Carina Kemper, Amelie Liebgott

Photography and Images: Unless otherwise indicated, all images property of HLRS.

Printing: www.dcc-kaestl.de

Design: Zimmermann Visuelle Kommunikation

Hazel Hen's Millionth Compute Job

In a milestone for the HLRS supercomputer, researchers simulated how non-Newtonian fluids disperse when injected through a nozzle.

Across nature are many cases in which materials in different states or phases (gases, liquids, and solids) physically interact. These phenomena are called multiphase flows.

In meteorology, for instance, raindrops, dew, and fog constitute multiphase flows, as does the exchange of gases between the oceans and the atmosphere. Multiphase flows also occur in our daily lives when water bounces off our skin in the shower or when we inhale nasal sprays to control the symptoms of a cold.

In engineering, multiphase flows can also be extremely important. Perhaps their most familiar application is in the design of fuel injection systems in automobiles, gas turbines, and rockets. Other examples include the spreading of fertilizers for farming or the use of spray drying in the production of pharmaceuticals and foods. In all of these cases, understanding how multiphase flows behave in detail could both enhance our ability to study the natural world and improve the design of more effective and more efficient products. But because of the enormous numbers of droplets that are involved in multiphase flows and the extremely small scale at which they interact, our ability to gain precise knowledge about them purely through observation has been limited.

For this reason, researchers in the laboratory of Professor Bernhard Weigand, Director of the Institute of Aerospace Thermodynamics at the University of Stuttgart, turned to HLRS and its Hazel Hen high-performance computer to simulate multiphase flows computationally. Their work has led to a variety of insights with wide-ranging practical relevance.

Supercomputing simulates droplet dynamics

Professor Weigand and his group are primarily interested in basic multiphase flows involving droplets and in the past have investigated topics related to water dynamics and ice crystal formation in clouds. Such problems are important for precipitation forecasting as well as for air travel, as ice formation on airplane wings can negatively affect flight stability and decrease fuel efficiency.

To study such phenomena, Weigand and his group use a mathematical approach called direct numerical simulation (DNS). Over many years they have been building DNS methods into an in-house software program called FS3D (Free Surface 3D), which they use to model droplet dynamics. FS3D can, for example, precisely simulate what happens when a water droplet falls onto a liquid film and forms a "crown," taking a new shape and breaking apart into smaller droplets.

High-performance computing (HPC) is essential to the success of FS3D because the software requires an extremely high "gate resolution." Like the frame rate in a video or movie camera, the program must represent the complex collisions, adhesions, and breaking apart of droplets and molecules at extremely small scales of space and time. FS3D can simulate such interactions in 2 billion "cells" at once, each of which represents a volume of less than 7 cubic micrometers, tracking how the composition of every cell changes over time. Achieving such a high resolution generates massively large datasets, and it is only by using a supercomputer as powerful as HLRS's Hazel Hen that such simulations become practical.

Having so much power at your disposal presents some unique challenges, though. In order to take full advantage of the opportunities that supercomputers offer, software behind algorithms like FS3D must be written specifically for the parallel computing architecture of high-performance computing systems. Programming in this way requires special expertise, and as FS3D has developed, staff members at HLRS and at Cray, the company that built Hazel Hen, have helped the Weigand Lab to optimize it for HPC. "It's not really practical for us to have HPC experts in our lab, and so staff at HLRS and Cray have been very supportive in helping us to run FS3D effectively on Hazel Hen," says Dr. Weigand. "Their knowledge and advice have been very important to the success of our recent studies."

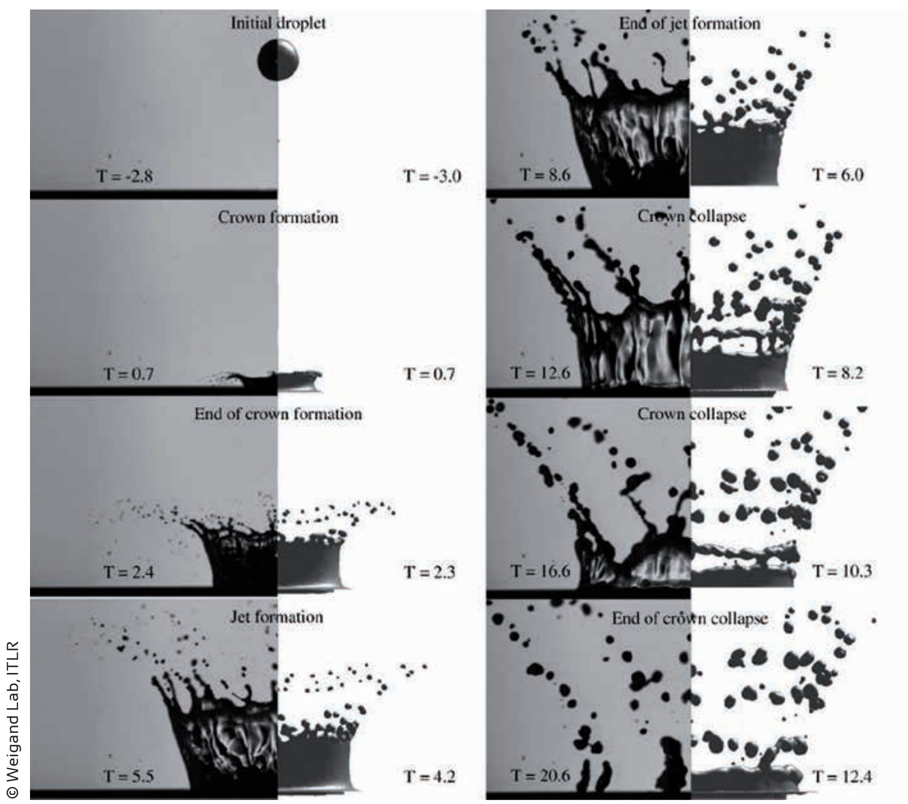
The millionth job: visualizing how non-Newtonian fluids break apart in jets

The millionth job on Hazel Hen was not focused on atmospheric water, but instead on multiphase flows in non-Newtonian fluids. Such fluids—which include materials like paint, toothpaste, or blood—do not behave in ways that Newton's laws of viscosity would predict; instead, their fluid dynamic properties follow other rules that scientists do not understand as thoroughly.

Weigand's team wanted to gain a better understanding of how non-Newtonian jets break up when injected into a gaseous atmosphere. This question is important because droplet sizes and the increase in a fluid's surface area as it becomes atomized can be important factors in optimizing the efficiency of a process—such as in the application of aerosolized paint to a car body. The researchers simulated the injection of aqueous solutions of the polymers Praestol2500® and Praestol2540® through different pressure nozzles into air. When used in water treatment, the viscosity of these polymers decreases due to shear strain. The fluid properties for this case were approximated by flow curves obtained from experiments by colleagues at the University of Graz.

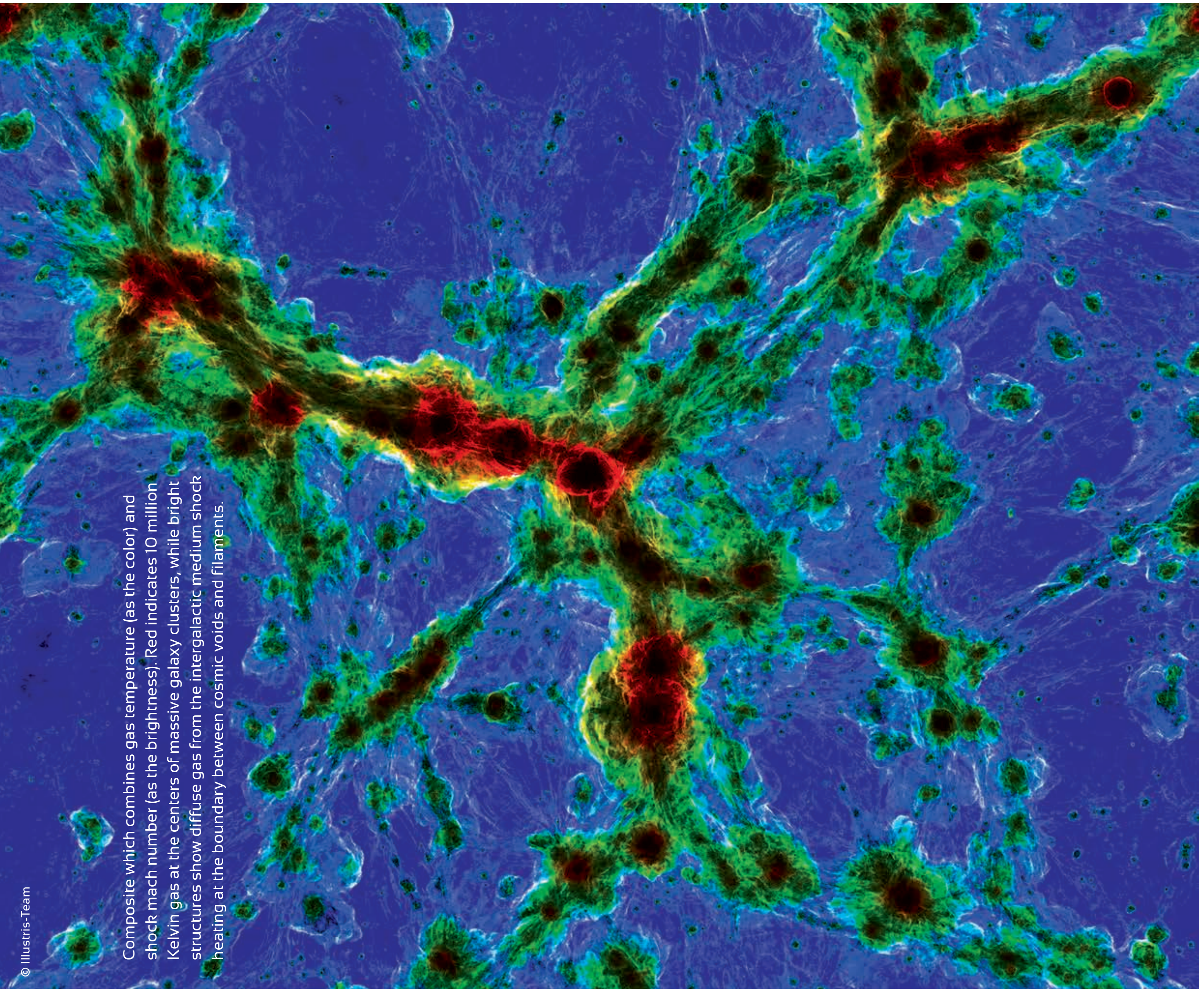
Running FS3D on Hazel Hen, the Weigand team performed a variety of "virtual" experiments on the supercomputer to investigate specific features of these flows, gaining a much more precise picture of how the solutions disperse. For example, they modeled jet breakup after injection and how factors such as flow velocity and the shape of the nozzle changed the fluids' viscous properties. The millionth job run on Hazel Hen was one of several post-processing visualizations the team undertook in cooperation with VISUS (University of Stuttgart Visualisation Research Centre) to investigate the development of a liquid mass over time. In this series of studies, they generated extremely fine-grained visualizations of changes in the shape of the flow passing through the jet, identified differences in the loss of flow cohesion under different conditions, and discovered changes in surface area as the flow becomes atomized, among other characteristics. This led to insights about similarities and differences between Newtonian and non-Newtonian flows, and about how nozzle shape affects flow properties.

In the future, such information could enable engineers to improve the efficiency of their nozzle designs. *(CW)*



© Weigand Lab, ITLR

A comparison of high-speed photographs of droplet crown formation (left side of each column) with FS3D simulations.



Composite which combines gas temperature (as the color) and shock mach number (as the brightness). Red indicates 10 million Kelvin gas at the centers of massive galaxy clusters, while bright structures show diffuse gas from the intergalactic medium shock heating at the boundary between cosmic voids and filaments.

Cosmologists Create Largest Simulation of Galaxy Formation, Breaking Their Own Record

A multi-institutional team gives the cosmology community a world-class simulation to study how the universe formed.

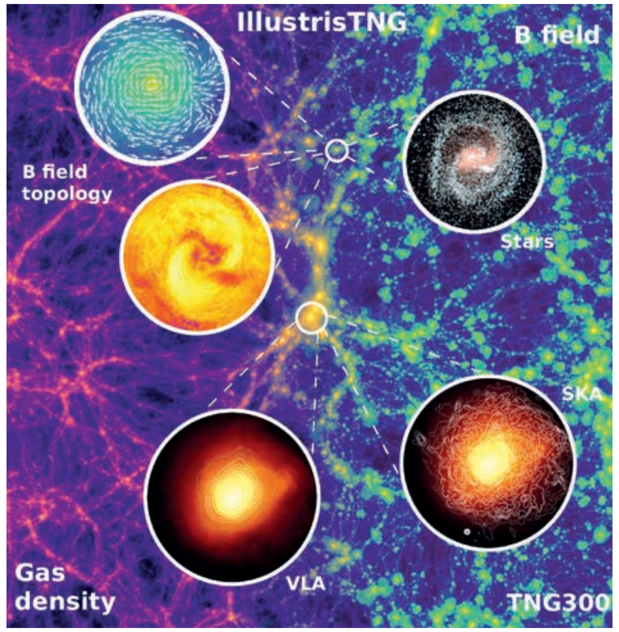
Humans have long tried to explain how stars came to light up the night sky. The wide array of theories throughout history have one common (and correct) governing principle that astrophysicists still use to this day: by understanding the stars and their origins, we learn more about where we come from.

However, the vastness of our galaxy—let alone our entire universe—means experiments to understand our origins are expensive, difficult, and time consuming. In fact, experiments are impossible for studying certain aspects of astrophysics, meaning that in order to gain greater insight into how galaxies formed, researchers rely on supercomputing.

In an attempt to develop a more complete picture of galaxy formation, researchers from the Heidelberg Institute for Theoretical Studies, the Max-Planck Institutes for Astrophysics and for Astronomy, the Massachusetts Institute of Technology, Harvard University, and the Center for Computational Astrophysics in New York have turned to supercomputing resources at the High-Performance Computing Center Stuttgart (HLRS). The resulting simulation will help to verify and expand on existing experimental knowledge about the universe's early stages.

Recently, the team expanded on its 2015 record-breaking "Illustris" simulation—the largest-ever hydrological simulation of galaxy formation. Hydrodynamic simulations allow researchers to accurately simulate the movement of gas. Stars form from cosmic gas, and stars' light provides astrophysicists and cosmologists with important information for understanding how the universe works.

The researchers improved on the scope and accuracy of their simulation, naming this phase of the project, "Illustris, The Next Generation," or "IllustrisTNG." The team released its first round of findings across three journal



Gas density (left) and magnetic field strength (right) across the TNG300 box, centered on the most massive galaxy cluster. Zoomed panels show the magnetic field orientation and stellar light (top) and xray and radio emission from massive cluster (bottom).

© Illustris team

articles appearing in the *Monthly Notices of the Royal Astronomical Society* and are preparing several more for publication.

Magnetic modelling

Just as humanity cannot envision exactly how the universe came to be, a computer simulation cannot recreate the birth of the universe in a literal sense. Instead, researchers feed equations and other starting conditions—observations coming from satellite arrays and other sources—into a gigantic computational cube representing a large swath of the universe and then use numerical methods to set this "universe in a box" in motion.

For many aspects of the simulation, researchers can start their calculations at a fundamental, or ab initio, level with no need for preconceived input data, but processes that are less understood—such as star formation and the growth of supermassive black holes—need to be informed by observation and by making assumptions that can simplify the deluge of calculations.

As computational power and know-how have increased, so too has the ability to simulate larger areas of space and increasingly intricate and complex phenomena related to galaxy formation. With IllustrisTNG, the team simulated 3 different universe "slices" at different resolutions. The largest was 300 megaparsecs across, or roughly 1 billion light years. The team used 24,000 cores on Hazel Hen over the span of 35 million core hours.

In one of IllustrisTNG 's major advances, the researchers reworked the simulation to include a more precise accounting for magnetic fields, improving the simulation's accuracy. "Magnetic fields are interesting for a variety of reasons," said Prof. Dr. Volker Springel, professor and researcher at the Heidelberg Institute for Theoretical Studies and principal investigator on the project. "The magnetic pressure exerted on cosmic gas can occasionally be equal to thermal (temperature) pressure, meaning that if you neglect this, you will miss these effects and ultimately compromise your results."

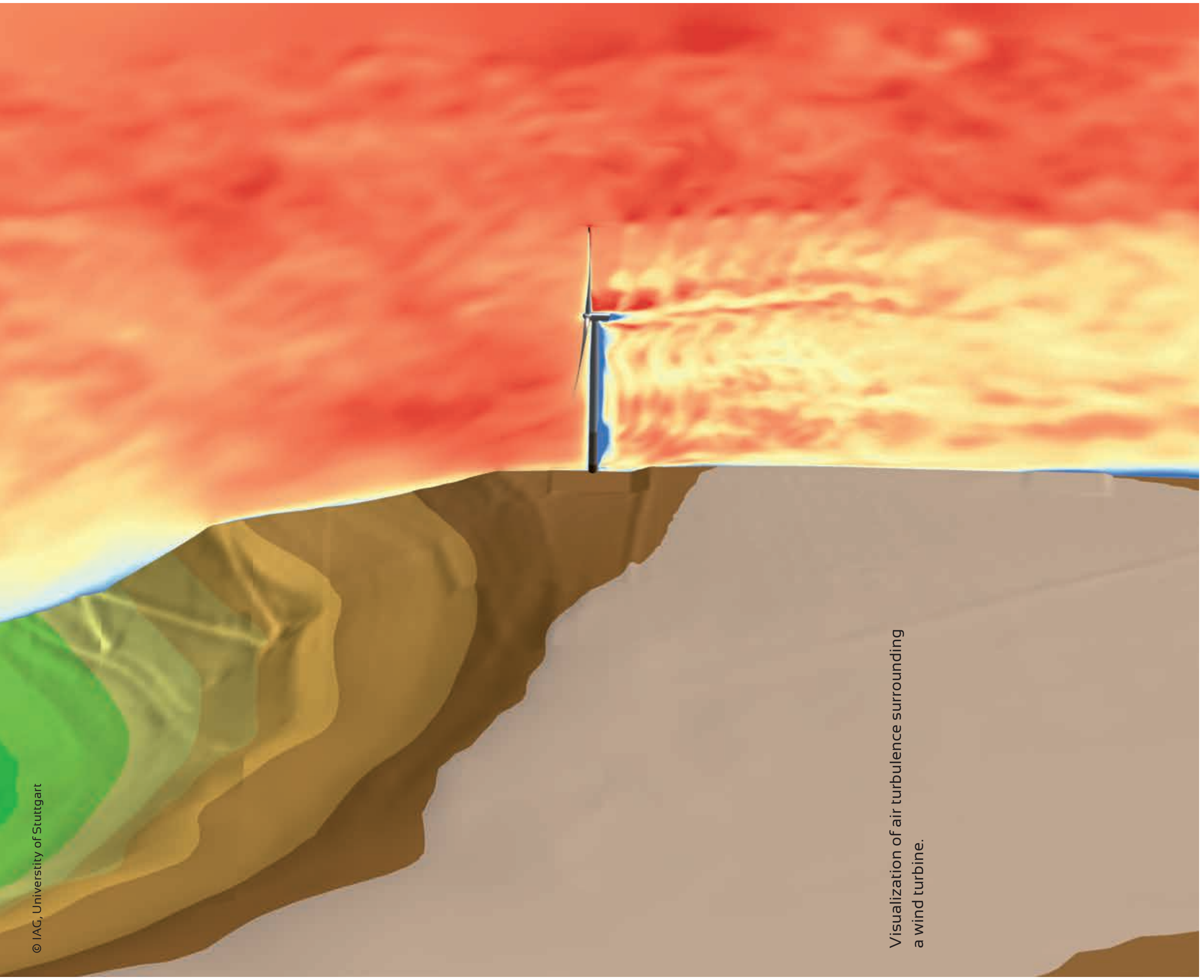
While developing IllustrisTNG the team also made a surprising advance in understanding black hole physics. Based on observational knowledge, the researchers knew that supermassive black holes propel cosmic gases with a lot of energy while also "blowing" this gas away from galaxy clusters. This helps to "shut off" star formation in the biggest galaxies and thus imposes a limit on the maximum size they can reach.

In the previous Illustris simulation, researchers noticed that while black holes go through this energy transfer process, they would not shut off the star formation completely. By revising the black holes' physics in the simulation, the team saw much better agreement between the data and observation, giving researchers greater confidence that their simulation corresponds to reality.

A long-standing alliance

The team has been using GCS resources since 2015 and been running the IllustrisTNG simulation on HLRS resources since March 2016. Considering that the IllustrisTNG dataset is both larger and more accurate than the original, the researchers are confident their data will be used far and wide while they apply for more time to continue refining the simulation. The original Illustris data release garnered 2,000 registered users and resulted in more than 130 publications. The team's long-standing collaboration with HLRS also resulted in winning 2016 and 2017 Golden Spike awards, which are given to outstanding user projects during HLRS's annual Results and Review Workshop.

IllustrisTNG team member Dr. Dylan Nelson pointed out that while current-generation supercomputers have enabled simulations that have largely overcome most fundamental issues related to massive-scale cosmological modelling, there are still opportunities for improvement. "Increased memory and processing resources in next-generation systems will allow us to simulate large volumes of the universe with higher resolution," Nelson said. "Large volumes are important for cosmology, understanding the large-scale structure of the universe, and making predictions for the next generation of large observational projects. High resolution is important for improving our physical models of the processes going on inside of individual galaxies in our simulation." *(EG)*



© IAG, Universtity of Stuttgart

Visualization of air turbulence surrounding a wind turbine.

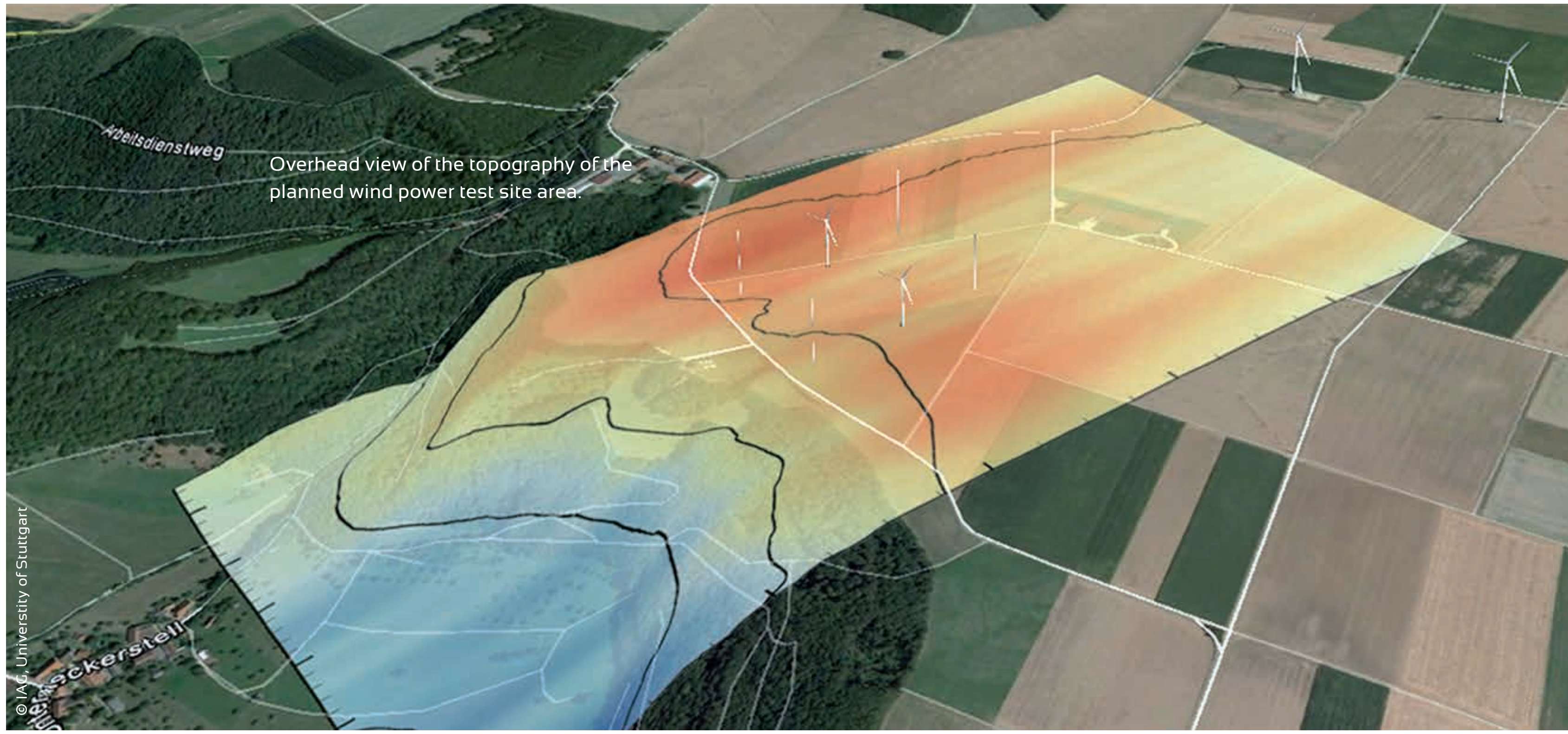
Investigating Wind Energy Generation on Complex Terrain

Using HLRS computing resources, scientists at the University of Stuttgart have been partners in designing and realizing an experimental facility that could help make wind power generation feasible in new areas.

As part of its ongoing Energiewende—a turn away from fossil fuels to renewable energy sources—Germany has invested heavily in wind power. In some parts of the country such as the low-lying, flat region near the North Sea coast, large wind farms have become a common feature of the landscape.

Despite this progress, Germany's largest energy needs are in the West and South of the country, where the population is larger and industry is more intensive. Although power companies have in recent years installed transmission wires to bring wind power from the North to these areas, many argue that generating wind power locally will be necessary to meet clean energy demands. Doing so will be challenging, however, as the terrain in the South and West tends to be much more uneven than in the North. When the land is flat or a wind farm is mounted on the sea, engineers have good models for predicting how turbines will operate. However, if a planner wants to install a facility in complex topography, like that present in Southern Germany, he or she must contend with wind patterns that are irregular and non-uniform. Existing models for such locations are not as reliable as those for simpler landscapes, while the rougher atmospheric conditions can be tough on existing wind turbine designs. These factors make it harder for planners to identify locations that could be effectively used for wind generation and to quantify energy yield and turbine loads.

To address this issue, the wind energy research cluster WindForS (www.windfors.de) launched a project in 2016 aimed at establishing a research site in the Swabian Jura, a chain of large hills located southeast of Stuttgart. The research facility will be the first in the world set in complex terrain where scientists will have full access to the turbine control and settings. Among the team members are researchers in the University of



Overhead view of the topography of the planned wind power test site area.

Stuttgart's Institute for Aerodynamics and Gas Dynamics (IAG). Using HLRS's Hazel Hen supercomputer, the investigators performed detailed simulations that were important in choosing and planning the location for the test site and the specific locations of the turbines. And by providing computing power needed to model such complex systems, HLRS will play an ongoing role in supporting the project's future research.

A wind energy laboratory

The IAG team, led by Dr. Thorsten Lutz, uses numerical methods from computational fluid dynamics (CFD) to develop comprehensive models of the complex interactions between wind turbines and their surroundings. During planning of the forthcoming wind power test site, the WindForS cluster's scientists integrated data including topographical maps, wind speed measurements, vegetation surveys, and geometrical and structural data of the wind turbines to develop an extremely detailed model of how it would function. Once built, the test site will include two wind turbines as well as measurement towers, Lidar devices, and drones for documenting wind flow and turbulence. The wind turbines will also be embedded with extremely sensitive sensors to track mechanical loading and changes in shape that occur during operation. The data that the test site produces will enable the computational researchers from Stuttgart to validate and refine their models in ways that will improve understanding of the physics underlying wind power generation.

Improving durability and reducing noise

In practical terms, this unique research facility will address several key problems facing wind power generation in complex terrain. One important focus will be on studying and reducing physical stress on wind turbines. The disturbed inflow of wind on hills can cause larger, more irregular vibrations that affect aerodynamic efficiency, while also raising loads and therefore the risk of damage to the turbine. Preventing this and ensuring that turbines have a longer lifespan is thus an important concern. "Using simulation," Lutz says, "we are helping to develop concepts for managing loads on the rotors and reducing vibrations." This knowledge could not only improve durability but also increase efficiency in power generation.

In the future, the investigators also hope to improve understanding of aeroacoustic noise mechanisms and reducing the noise that can result from wind turbine operation. Noise occurs as a result of interactions between wind and the rotor blades, when fluctuations in air pressure produce sound that is audible to the human ear. This disturbance can make it difficult to identify acceptable locations for wind turbines in densely populated areas. Lutz anticipates that the new test site will enable researchers to better understand how noise arises and to develop experiments with modified blades and rotor geometries capable of reducing it.

A proving ground for new wind energy technologies

"In the future," Lutz explains, "WindForS wants to create opportunities to test new technologies." This could include, for example, trying out prototypes of new blade designs or investigating the effects of subtle changes in rotor shape.

WindForS also aims to be a partner for industrial and academic researchers. Once built, Lutz imagines that companies would be able to rent time at the facility to take measurements necessary for their development of new wind generation concepts. For the simulation scientists involved in the project, the test site also offers the opportunity to test and refine their own CFD models. As new data accumulates and computing power increases at HLRS, it will be possible to develop increasingly precise simulations that will provide the foundational knowledge necessary for future technological improvements.

Most of the preparations have been completed for the test site and, pending a final environmental review, the scientists anticipate that construction will begin in 2019. Once operational, they hope that it will provide new insights that will expand opportunities for wind power generation not just in Germany, but across the world.

(CW)

Building More Precise Models of Weather and Climate

Researchers at the University of Hohenheim have been increasing the resolution of available models, providing improved methods for predicting local and regional effects of climate change, including in specific regions in Germany.

For years a team of climate scientists at the University of Hohenheim has been using computer models capable of providing increasingly precise models to study the Earth's climate and predict future climate changes and major adverse weather events. Computer modelling using Hazel Hen, the HLRS supercomputer, has been an indispensable tool in supporting the team's research.

Understanding an area's climate is not just predicting the weather. In fact, weather and climate are often used interchangeably, but have significantly different meanings—weather is the temperature, precipitation, and wind speed (among other factors) occurring at a specific place and time. Climate refers to general weather patterns and trends over a longer time period (most researchers consider anything longer than 30-year statistics representative of an area's climate).

As part of studying both weather and climate computationally, the University of Hohenheim researchers are part of an international consortium of research teams developing and improving the Weather Research and Forecasting Model (WRF), one of the most well-regarded and well-developed numerical atmospheric circulation models in the world.

Seasonal simulations, improved insights

Even with leading HPC resources, many computational climate researchers run simulations at relatively low—or coarse—resolution in order to perform simulations over a large area and an extended period of time. Due to computational constraints, many large-scale international climate consortiums' simulations apply a computational grid of 12 by 12 kilometer boxes or coarser over a limited area.

The finer the grid that researchers use, the more details they see in their simulations. Further, the more input details they include, such as sophisticated cloud microphysics, proper representation of the land surface, aerosols in the atmosphere, and more precise sea surface temperatures, the more accurate a simulation becomes. This higher resolution and increased amount of detail makes computation much more time-consuming, though. To address this problem, researchers use regional atmospheric models such as WRF to focus more on a region of interest, such as a specific continent, while also including data representing the entire planet's atmosphere.

Hohenheim researchers including Dr. Thomas Schwitalla are working to improve seasonal weather forecasting by comparing a high-resolution WRF model simulation to global meteorological analysis data and other high-resolution observations from the same period of time. Schwitalla indicated that by focusing on one season, he can verify a model's ability to forecast weather in a region during this period in statistical terms. In turn, this can help improve its predictive skills for future adverse weather events like droughts or heat waves.

In his most recent work, Schwitalla performed a simulation across the entire globe (minus the ice caps) during a single spring season, from February to June 2015, at ultra-high resolution—3 kilometer by 3 kilometer squares (so-called "convection-permitting" resolution). This is extremely computationally expensive, but allows researchers to observe their model's ability to model weather and climate at a level that more closely corresponds to the actual needs of communities and researchers.

In the future Schwitalla hopes that he can gain access to the entire Hazel Hen machine and its successor system in order to attempt another major leap forward in the team's climate research. He and his group hope to run an ensemble of seasonal simulations, gradually increasing resolution to 1 kilometer as they gain more computational power. This would allow the team to assess forecast uncertainty and create a better representation of physical processes.

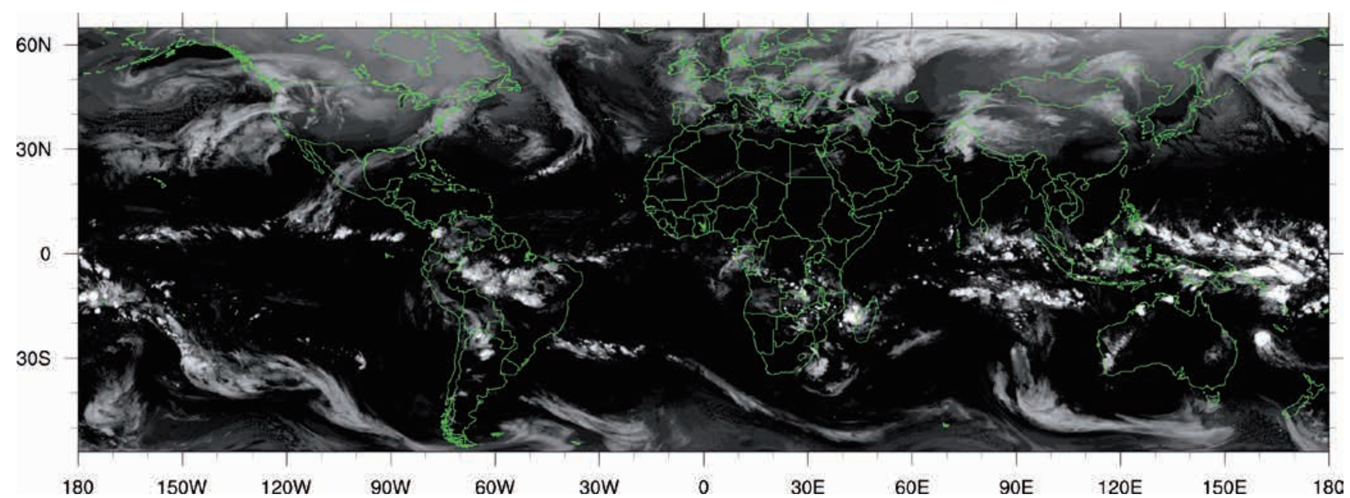
Modeling the future of Germany's climate

In addition to relatively small spans of time at ultra-high resolution, Hohenheim researchers also use HLRS resources to anticipate larger-scale climate trends far into the future. In one of these projects, ReKliEs-De, Drs. Kirsten Warrach-Sagi and Viktoria Mohr spent much of the last three years working with a consortium of other climate scientists to model the Earth's climate past, present, and future over the span of 140 years. This German Federal Ministry of Education and Research (BMBF)-funded national effort—an initiative contributing to a large set of European simulation promoted by the Intergovernmental Panel on Climate Change (IPCC)—focused on refining global climate models to be more accurate on a continental level.

To this end, Warrach-Sagi and collaborators used 97 million core hours on Hazel Hen, generating 2 petabytes—more than 2 million gigabytes—of data during their simulation. The team used 5,400 cores per run, and ran 4 runs in parallel. The team modeled climate patterns from 1958 to the year 2100, simulating climate in 1-minute timesteps, and exporting data for every three hours of simulated time.

The team found that if the Earth were to warm by an average temperature of 4°C over the next century—a number many models point to as plausible if greenhouse gas emissions are not reduced following standards such as those in the Paris Agreement of 2015—Southwestern Germany's summers would become hotter and drier, and the winters warmer and wetter (a potentially terrible result for German winter crop production), while Northeastern Germany would be more humid than it is today.

The team has the important task of providing datasets that are hosted on the Earth System Grid Federation (ESGF) website, meaning its massive volume of data has to be stored somewhere. Warrach-Sagi indicated that the team spends much of its time moving data on and off resources for analysis, transferring data to store longer term, and sifting through information to see what is most valuable for other researchers (the team's datasets are hosted on the ESGF website so that other researchers involved in climate science can apply this data for impact studies related agriculture, forestry or hydrology, among other areas. As computing power grows, Warrach-Sagi feels confident that climate scientists can not only model climate changes in higher resolution, but also focus on a broader, multidisciplinary approach to modelling, in turn helping to make better predictions about the effect of climate change on other aspects of human activity. She indicated that she is beginning to increasingly study land use effects in WRF, and would like to begin running crop models with these simulations in the near future. *(EG)*



© Universität Hohenheim

Visualization of clouds taken from a high-resolution Weather Research and Forecasting (WRF) simulation. University of Hohenheim researchers have been contributing to the development of WRF, one of the most highly regarded climate models in the world.

© Simon Sommer for HLRS

SPOTLIGHT

Do Good and Teach about It: HPC Training at HLRS

The opening of a new building dedicated to HPC training is just one of many ways in which HLRS is expanding efforts to share its expertise with academic and industrial researchers.

The year 2017 witnessed an important milestone in the history of the High-Performance Computing Center Stuttgart (HLRS). During an inauguration ceremony on July 14, high-ranking representatives of the state of Baden-Württemberg, the city of Stuttgart, the University of Stuttgart, and other invited guests gathered to celebrate the opening of a new HLRS building dedicated to training professionals in high-performance computing (HPC).

The approximately 1,000 square-meter, €6.8 million facility offers a state-of-the-art lecture hall, smaller seminar rooms, and space to expand HLRS staff. It is already having a major impact on the quality of the training activities, conferences, and symposia that HLRS can offer. Speaking at the inaugural celebration, Baden-Württemberg State Secretary for Finance Gisela Splett called HLRS a "lighthouse" for advanced science and research and hailed the opening of the new HLRS training facility as an event that will enhance the center's global reach. "This will be a meeting point for a network that will play an important role in future generations for the scientific and industrial competitiveness of Baden-Württemberg and Europe," she said.

The opening of the new HLRS training center has not been the only improvement in the center's training activities in recent years, however. By cultivating collaborations within its extensive network and integrating new pedagogical approaches and education technologies, HLRS is pursuing a multifaceted strategy aimed at disseminating the technical knowledge necessary to use high-performance computing.

"You all know the saying 'Do good and talk about it,'" said Simone Rehm, Chief Information Officer at the University of Stuttgart, at the inauguration ceremony. "I'd like to modify the saying and suggest we should


Gisela Splett (Baden-Württemberg State Secretary for Finance)

'Do good and teach about it.'" Indeed, by making training a core component of its mission, HLRS is amplifying the impact of simulation technologies in research and development.

Filling important gaps in education and training

Numerical simulation has long provided powerful tools for R&D. However, running simulations on supercomputers requires specialized knowledge that many scientists and engineers do not gain during their academic training. According to Dr. Rolf Rabenseifner, who oversees the HLRS training program, "Our goal is to address this niche, providing continuing professional education that delivers the essential practical skills that researchers need when using simulation to solve complex problems."

Because HLRS is a German national supercomputing center located at the University of Stuttgart, the overwhelming majority of its trainees are academic scientists working on publicly funded research. When young investigators join a lab that works on problems in aerodynamics, climate modeling, or molecular dynamics, for example, the lab will often send them to HLRS to gain the HPC skills necessary for that lab's research. For this reason—for more than 20 years—the core HLRS training program has focused on the most important basic skills that HPC users need: parallel programming interfaces such as MPI and OpenMP, as well as Fortran and advanced C++ for high-performance computing and HPC architectures. Over the years its portfolio has grown to include other related topics such as cluster file systems and performance optimization, as well as specialized HPC domains such as visualization and computational fluid dynamics. (See page 52 for a complete list of courses offered in 2017.)

The curriculum that HLRS offers continually adapts to the latest HPC trends, tools, and challenges. In 2017, for example, it hosted a two-day workshop organized by Cray (the builder of HLRS's supercomputer, Hazel Hen) and hardware manufacturer NVIDIA that was designed to demystify the up-and-coming fields of artificial intelligence and deep learning. In the Stuttgart region—home to a large high-tech community surrounding auto manufacturers Daimler and Porsche—these fields have attracted interest because of their relevance for future self-driving vehicles. The course was the most highly attended of the year, covering topics including object detection, image segmentation, and neural networks.

"Supercomputing and its applications are constantly evolving and we need to stay current with these trends," says Rabenseifner. "In the near future, for example, we anticipate a convergence between data analytics and high-performance computing that will present new kinds of challenges. Staff at HLRS will be on the front lines of navigating this convergence and our training program will enable us to share the knowledge we gain with people in both academia and industry whose work will benefit from it."

Building networks, crossing borders

HLRS's training activities are not aimed only at local researchers, but constitute an ambitious effort to build HPC know-how in Germany, across Europe, and internationally. As one of three members of the Gauss Centre for Supercomputing (GCS)—an alliance that forms the backbone of Germany's national HPC infrastructure—HLRS coordinates HPC training with GCS partners the Jülich Supercomputing Centre and the Leibniz Supercomputing Centre, as well as other German supercomputing centers at the Technical University Dresden, University of Siegen, and University of Frankfurt. Some training courses are held in Stuttgart, while others are hosted offsite to make HLRS knowledge more easily accessible to investigators in other cities.

In addition, as a member of the Partnership for Advanced Computing in Europe (PRACE), HLRS is a PRACE Advanced Training Center, providing state-of-the-art courses for scientists across the continent. In addition to offering traditional classroom learning HLRS is also helping to develop a massive open online course (MOOC) covering parallel computing.

To increase the reach of technical expertise hosted at HLRS, the center also offers a "train the trainer" program focusing on parallel computing. Designed with HPC instructors located at other institutions in mind, the program not only covers the latest standards for MPI and OpenMP, but also provides trainers with pedagogical strategies for conveying this knowledge more effectively to their own students. Thus far, HLRS's train the trainer program has enabled the development of new courses at supercomputing centers in Belgium and Austria, and in 2018 plans to expand this effort in the Netherlands and Ireland.

HLRS's international training collaborations also include a biannual, 10-day German-Russian Young Scientists' School and Conference on Parallel Programming and High-Performance Computing, held in Novosibirsk, as well as tutorials at major annual supercomputing conferences such as ISC High Performance in Frankfurt and the International Conference for High Performance Computing Networking, Storage, and Analysis (SC) in the United States.

Maintaining this network has an important online component, as HLRS distributes updated course materials through the center's website. "By making electronic recordings and slide sets of previous courses available," Rabenseifner explains, "we give researchers anywhere, regardless of geography, access to useful training information when they need it." This "just-in-time" delivery approach also allows course participants to review material they might have been exposed to but didn't completely master in the classroom. Maximizing flexibility in this way helps scientists to navigate the significant challenges that come with HPC.

The Supercomputing-Akademie: continuing education for HPC users in industry

Although the traditional HLRS trainee works in academic research, simulation is also extremely important for the ecosystem of small and mid-sized precision engineering companies that make Baden-Württemberg an economic powerhouse. Many of these companies, however, are not large enough to support full-time, in-house HPC experts able to keep up with best practices in programming and data management.

In 2016 HLRS set out to address this critical knowledge gap. With grants totalling €2.5 million from the European Social Fund, Baden-Württemberg Ministry of Science, Research and the Arts, and the University of Stuttgart, HLRS launched a project to develop a specialized training program targeting industry's unique needs. The initiative is being developed in collaboration with partners at the University of Freiburg, the University of Ulm, and Sicos BW, and will open to trainees in 2018 as the Supercomputing-Akademie.

"The Supercomputing-Akademie is the next generation of continuing education at HLRS," says Dr. Andreas Wierse, CEO of Sicos BW, an independent organization based at HLRS that facilitates access to HPC for small and mid-sized companies. "Just as the new training building at HLRS is physically connected to the building that houses Hazel Hen, the Supercomputing-Akademie will be an integral, core part of HLRS's training operations."

During curriculum planning for the Supercomputing-Akademie, HLRS set out to address several limitations that have made it difficult for industrial HPC users to take advantage of its existing training program. "From the beginning," says Sicos BW's Markus Klietmann, "we engaged in a dialog with industry representatives to find out what their needs are and how the expertise that exists at HLRS could best help them."

One important practical consideration was that industrial HPC users typically don't have the time to dedicate days or weeks away from their job to spend in a traditional classroom. For this reason, the Supercomputing-Akademie will use an educational approach called blended learning, which combines the best qualities of classroom learning and online learning. Trainees will meet the instructor and students onsite at HLRS, though the majority of instruction will happen online. In addition to independent study that participants can do at their convenience, there will be virtual classrooms where they can meet over the Internet each week, exchanging ideas and asking questions of the instructor.

Considering that the typical industrial user works 8 to 10 hours a day, has family commitments, and then needs to sit down and learn HPC, the flexible approach that blended learning offers is meant to make this as easy as possible. The interactive dimension will also give participants valuable cross-industry perspectives that they wouldn't gain otherwise.

The Supercomputing-Akademie will launch in April 2018 with a module focused on parallel programming, and the HLRS team is in the early stages of developing additional modules that will appear in the coming years. Future module topics are likely to include other topics including cloud computing in HPC environments, performance optimization, economic and ecological aspects of HPC, simulation, visualization, and data management.

An additional interesting dimension of the Supercomputing-Akademie's curriculum is its modular nature. This was also done intentionally based on interviews with industry representatives that revealed several different kinds of HPC users—engineers for whom HPC is an important component of product development, programmers whose code must be optimized to run on HPC systems, and computing resource managers who must ensure that staff at their company has the computing resources it needs. Each type of user has different interests and so the Supercomputing-Akademie aims to be like a chameleon, changing appearance based on an individual trainee's needs.

"Knowledge and experience with HPC can provide a company with a number of advantages," says Hanna Skubski, project coordinator for the Supercomputing-Akademie at HLRS. "Through the activities of the Supercomputing-Akademie we aim to transfer the knowledge that HLRS experts have developed over the years to industry in ways that will ultimately benefit their ability to innovate."

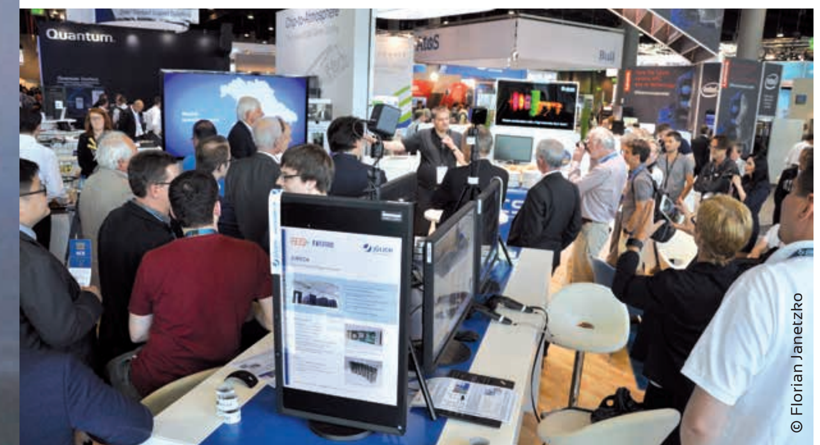
More than a building

Data analytics, simulation, and visualization will grow in importance for basic research, precision engineering applications, and other fields in the coming years. Taking advantage of these tools will mean that HLRS needs not only to maintain a first-class supercomputing infrastructure but also to empower people to use it efficiently and effectively.

The new HLRS training center has been a major step for us," says HLRS director Michael Resch. "But at the end of the day, a building and a supercomputer are only as valuable as what people do with them. In this sense, continuing to develop our training offerings—especially for industry—has to be an absolutely essential part of HLRS's activities. They will continue to ensure HLRS's place as a leading scientific center for simulation technology in Germany and in Europe, and will ultimately enable the scientists and businesses that work and train here to be as globally competitive as possible."

(CW)

NEWS



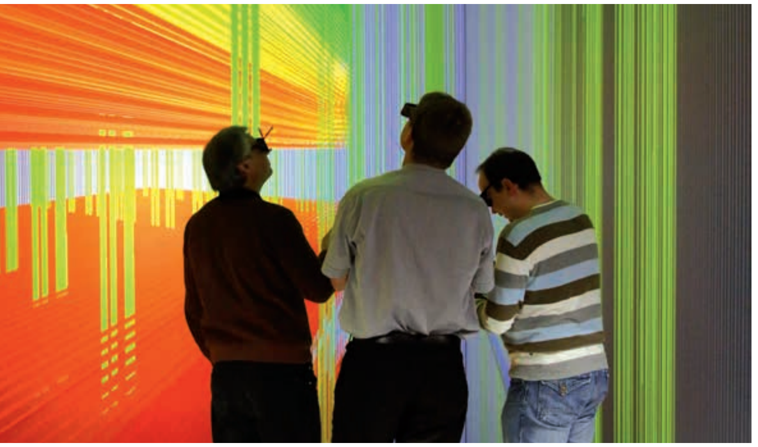
© Florian Janetzko

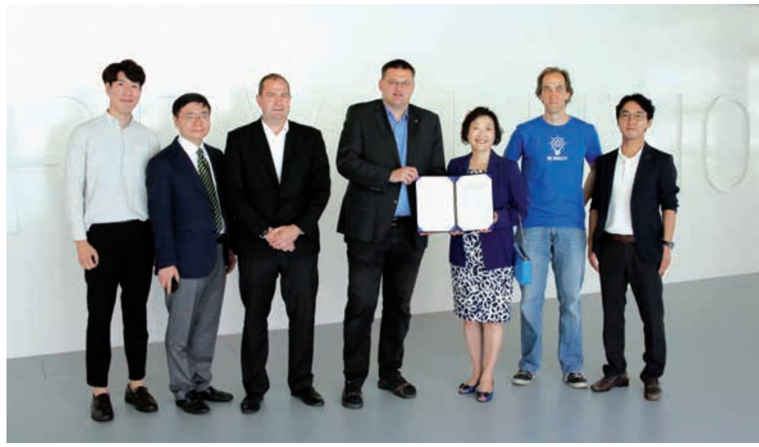
HLRS Joins Gauss Centre for Supercomputing in Celebrating 10th Anniversary

At the ISC 2017 convention in Frankfurt, HLRS joined its partner German national supercomputing centers—Jülich Supercomputing Centre and Leibniz Supercomputing Centre—in celebrating 10 years of cooperation. HLRS Director Prof. Michael Resch, also currently GCS Chairman, presented GCS's vision for the future of HPC at Germany's tier 1 supercomputing centers. During ISC 2017, Prof. Wolf-Dieter Lukas, Head of the Key Technologies Unit at the German Federal Ministry of Research and Education (BMBF) praised GCS as one of Germany's great scientific success stories, and indicated that the federal government plans to invest deeper in high-performance computing, focusing on a "smart scale" strategy on the path toward exascale computing. *(EG)*

State Minister Announces New HPC Strategy at HLRS

During an August 24 visit to HLRS, Theresia Bauer, Baden-Württemberg Minister for Science, Research, and the Arts, pledged € 500 million toward advancing the state's high-performance computing (HPC) capabilities, pointing to HLRS as a key component in the state's digitalization strategy. The success of this strategy, Bauer said, not only depends on infrastructure—building bigger, faster machines—but also on cooperation between academia and industry and the ability to train next-generation HPC experts. In this regard, HLRS's partnerships with industrial users are good examples of the benefits of training researchers in science and engineering to use these tools. *(EG)*





Mid-Sized Businesses Get to Know HLRS

An event organized by the IHK Region Stuttgart and Sicos BW offered a rare opportunity for technology directors from the local business community to get a behind-the-scenes look at HLRS and to learn more about the services it provides. Visitors received a tour of the HLRS computer room and of the CAVE virtual reality facility. "Our goal is to accelerate access to high-performance computing and simulation," says Sicos BW Director Dr. Andreas Wierse. "For smaller companies, there is always an initial sense of inhibition that needs to be overcome. We try to help them jump over barriers that might seem insurmountable and to gain the knowledge and resources they need to integrate high-performance computing into their practices." The May event was one instance of this ongoing outreach. *(CW)*

Golden Spike Awards Given at 20th Annual Results and Review Workshop

At this two-day workshop, researchers who use HLRS's Hazel Hen supercomputer presented progress reports on their recent work. The projects addressed topics across a wide range of scientific and engineering disciplines, including computational fluid dynamics, climate research, life sciences, materials science, and basic research in physics and astrophysics. At the end of the event, a jury recognized leaders of three outstanding projects with the Golden Spike Award: Johannes Letzgus (Institute of Aerodynamics and Gas Dynamics, University of Stuttgart), Prof. Volker Springel (Heidelberg Institute for Theoretical Studies, Heidelberg University), and Thorsten Zirwes (Engler-Bunte-Institute, Karlsruhe Institute of Technology). *(CW)*

Reallabor Presented at Spring Fair Stuttgart

Taking place each April, the Spring Fair Stuttgart is one of Germany's largest sustainability events, drawing over 100,000 visitors. This year HLRS presented its work as part of the project Reallabor Stadt:quartiere 4.0, one of 14 urban labs in Baden-Württemberg funded by the state Ministry of Science, Research, and Art that are exploring new methods and technologies for participatory urban planning. HLRS's contribution has involved developing virtual reality models of Stuttgart and the nearby city of Herrenberg that enable users to imagine and explore new planning strategies before they are built. Among the booth's visitors were Baden-Württemberg Minister of Transportation Winfried Hermann and Environment Minister Franz Untersteller. *(CW)*

Asian Collaboration Agreements Renewed

In 2017 HLRS renewed collaboration agreements with the Shanghai Supercomputing Center and the Korea Institute of Science and Technology Information. The memoranda of understanding identify opportunities for collaborative activities between HLRS and each center, including applications for numerical algorithms, parallel and network computer technologies, immersive visualization technologies, and cross-institutional educational and exchange programs. *(CW)*

Federal Minister for Education and Research Prof. Dr. Johanna Wanka (center) visited the HLRS booth at CEBIT 2017.

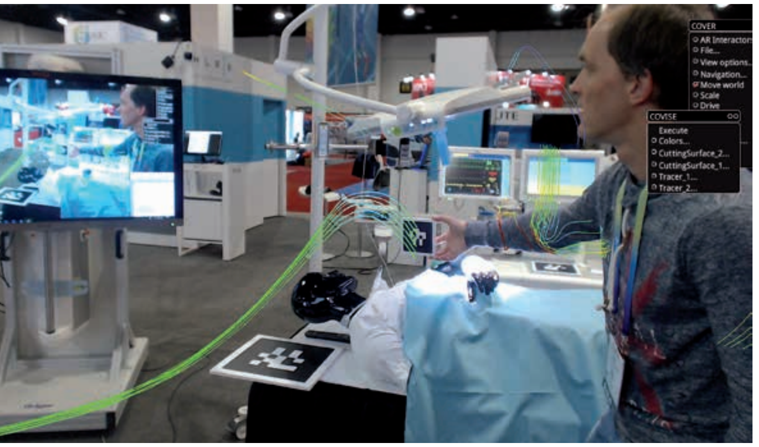
Government Officials Visit HLRS

In 2017 HLRS welcomed representatives from German federal, state, and city governments to improve understanding of the powerful technologies the center maintains and the innovative research it makes possible.

Prof. Dr. Johanna Wanka, Federal Minister for Education and Research, visited the HLRS booth at CEBIT 2017 in Hannover. She spoke at length with Dr. Uwe Wössner, head of the HLRS Visualization Department, and enjoyed a demonstration of a simulation illustrating airflow around a moving motorcycle. Wanka expressed interest in the ways in which high-performance computing and data visualization can be used to address societal and engineering challenges.

Members of the Baden-Württemberg state parliament Sabine Kurtz (CDU) and Christine Neumann (CDU) together with Tim Stephan, parliamentary advisor to the CDU state parliament faction, visited HLRS in April. They engaged in a lively discussion about the role of high-performance computing in science and industry, and how simulation can assist in the political decision making process. Kurtz and Neumann also learned about the wide variety of activities at HLRS, including among its young researchers.

Stuttgart Mayor Fritz Kuhn, together with Minister of General Operation, Culture, and Law Fabian Mayer and Director of Economic Development Ines Aufrecht visited HLRS in February. After receiving a brief overview of HLRS, the visitors toured Hazel Hen and received a demonstration of the CAVE virtual reality environment. Discussions also focused on HLRS's role within Stuttgart's cultural scene. *(CW)*



Virtual Operating Room Displayed at SC17

At the SC17 conference in Denver, Colorado, USA, HLRS demonstrated a visualization approach developed in collaboration with medical technology company Dräger that combines augmented reality and airflow simulations running on a supercomputer. The visualizations are enabling Dräger to design medical instruments in ways that reduce return airflows from unclean areas of an operating room, decreasing the risk of bacterial infections in patients' wounds. At SC17 HLRS Managing Director Dr. Bastian Koller also engaged in public presentations focusing on high-performance data analytics. *(CW)*

HPC-Europa 3 Project Launched to Foster Pan-European Collaborative Research

HPC-Europa 3 offers grants to young researchers to support international research exchange at one of the eight participating HPC centers. HLRS plans to provide up to 150 young scientists with access to its computing systems to the tune of 4.2 million compute hours. Altogether, the participating centers plan to host 1,220 junior researchers and provide 100 million compute hours. In addition, HLRS will invite representatives from small- and medium-sized enterprises (SMEs) to Stuttgart to share information on how HPC can benefit their competitiveness in the global marketplace. As a center with strong technical-engineering expertise, HLRS aims to build up long-term technology transfer actions with participating SMEs and thus enable them to effectively use HPC technologies and services. *(LB)*

Japanese SMEs Visit HLRS

Representatives from Japanese small- and medium-sized enterprises (SMEs) and from the NEC Corporation visited HLRS to learn how it supports industrial R&D. Dr. Andreas Wierse, director of Sicos BW, introduced the industrial HPC concept of the state of Baden-Württemberg. Sicos BW, an independent organization located at HLRS, is an important part of this effort, supporting SMEs interested in integrating high-performance computing into their work. The event was marked by a lively discussion of how HLRS and Sicos BW help SMEs to overcome problems that they face in using advanced computing technologies like HPC, data analytics, and machine learning. *(CW)*

Accident Analysis Technology Demonstrated at CEBIT

In March digital innovators converged on Hannover for CEBIT 2017, the world's largest trade show for information technology. HLRS presented several recent applications of its powerful 3D laser scanning and HPC visualization technologies, including VISDRAL. The approach uses 3D scanners to scan vehicles that were involved in an accident in great detail, capturing the shape of the damaged vehicles after the collision, as well as other important factors such as the condition of the road surface and the locations of objects in the surrounding environment. These data are then imported into the computer and superimposed on one another, making it possible to simulate models of the crash and gain a precise understanding of what happened. *(CW)*

COLLABORATIONS

HLRS Researchers Support Design of New thyssenKrupp Elevator System

Using virtual reality and numerical simulation, visualization experts at the High-Performance Computing Center Stuttgart (HLRS) make important contributions to the development of a groundbreaking technology.

In June 2017 the engineering company thyssenkrupp Elevator AG began operating the world's first elevator capable of moving horizontally as well as vertically. Called the MULTI, the new concept mounts elevator cabins on rails instead of suspending them on cables, offering increased flexibility of movement and exciting opportunities for architects to begin rethinking how large buildings and building complexes are designed. The first fully operational prototype is now running in a specially built tower located in Rottweil, Germany.

Working behind the scenes since 2014, HLRS played an important role in the MULTI's development. Researchers in the HLRS Visualization Department collaborated with thyssenkrupp Elevator engineers and construction managers at Ed. Züblin AG to conduct simulations that tested key features of the new system before it was built. Using data from thyssenkrupp Elevator, the HLRS team created a virtual reality simulation of the elevator system and tower. Once displayed in the CAVE, an immersive three-dimensional virtual reality facility located at HLRS, engineers and architects could interact with the model, moving through it to gain a sense of how a user might experience the actual elevator and observing its highly complex mechanics in action. The simulation helped the developers identify features in the design that either caused usability problems or that could be improved upon, such as collisions between machine parts in motion that would have been much harder to detect in computer-aided design (CAD) software alone.

Working with Züblin, HLRS also integrated its virtual reality simulation into the firm's building information modeling (BIM) strategy. This made it possible to simulate how efficiently the elevator would move through the structure. The BIM model also enabled the construction managers to plan the build itself—for example, determining how large components such as motor blocks should be brought into the building and how they should be rotated into position.

HLRS researchers also used simulation to model important features of airflow both inside and around the tower. This effort addressed questions related to turbulence that arises as elevator cars pass one another in an elevator shaft and to how the tower would respond to stresses caused by wind.

The model HLRS developed for optimizing airshaft design was particularly innovative. "Normally every time you lay out a new elevator geometry you need to start again at the beginning and redo a lot of calculations," says Dr. Uwe Wössner, head of the HLRS Visualization Department. "With the simulation approach we used, it's just a matter of importing the new geometry digitally and running a couple of scripts. It makes it much quicker and thus less expensive than other methods to test new ideas."

"In the future it's going to be a huge advantage to be able to virtually install a MULTI system in a specific building during the development phase," Wössner points out. "This will make it possible for the client to see, long before construction begins, how it operates and to try out different combinations to see what options best meet his or her needs. Does a new building need two shafts, for example, or would three make more sense? You wouldn't be able to answer questions like this by looking at one specific building because the needs will be different every time."

When building physical prototypes becomes prohibitively time-consuming and expensive, simulation and visualization offer powerful tools that can save time and costs, and prevent construction delays. As the MULTI system becomes more widely adopted, HLRS's contributions to its development will continue to be important for its future success. *(CW)*

Maya the Bee Recognized with HPC Innovation Excellence Award

During the ISC High-Performance 2017 conference in Frankfurt, Hyperion Research presented its annual High-Performance Computing Innovation Excellence Award to M.A.R.K. 13 and Studio 100 Media for their animation work on the animated film *Die Biene Maja* (*Maya the Bee*). During production, they used supercomputing resources at HLRS to calculate approximately 115,000 computer-generated stereo images. Each frame was calculated from the perspective of both left and right eye, a prohibitively large computation using traditional computers. The success of the project encouraged HLRS to join the Media Solution Center BW, which provides HPC solutions for the media industry. HLRS will continue partnering with M.A.R.K. 13 for production of the forthcoming *Maya the Bee 2: The Honey Games*.

Supercomputing Supports Sustainability: An Interview with Claus-Peter Hutter

Since 2010, HLRS has partnered with the Baden-Württemberg Academy for Nature Preservation and Environmental Protection on a state-funded project titled Sustainability in Supercomputing. With support from the State Ministry for Science, Research, and Culture, the effort is not only focused on making HLRS more environmentally, economically, and socially responsible, but also aims to generate guidelines that high-performance computing centers anywhere can use to achieve these goals.

As Academy Director Claus-Peter Hutter explains, the collaboration with HLRS has exceeded expectations, revealing additional opportunities for partnerships between HLRS and local companies and municipalities.

Why is the Academy for Nature Preservation and Environmental Protection working with HLRS?

Because the Academy is an office of the State of Baden-Württemberg's environmental ministry, an important part of our mission is to help anchor the theme of sustainability in society. Because no single person, company, or municipality can make sustainability a reality alone, we network extensively and try to bring together partners who can together help to promote our sustainability goals.

In 2009 partners from the business world brought HLRS to our attention and over the course of conversations with HLRS Director Michael Resch we quickly realized that we shared certain approaches that would make it possible to promote themes like sustainability and environmental responsibility in a high-performance computing center and among others in its network.

At the beginning we developed a kind of itinerary that would enable HLRS to begin engaging with the theme of sustainabilty, and held various workshops to define what sustainability could mean for the center and its daily operation. Building on this, and with our support, HLRS developed a sustainability strategy and is now working hard to live and develop this strategy further. In 2018 the center will also apply for EMAS certification—EMAS (Eco-Management and Audit Scheme) is the most demanding program for sustainability for organizations in the EU. HLRS will also introduce an energy management system meeting ISO 50001 requirements in 2019.

During this process it was also very interesting to learn about additional opportunities that HLRS offers for improving sustainability in Baden-Württemberg.

What are some things that HLRS can contribute to sustainability in Baden-Württemberg?

As an environmental provider, HLRS offers incredible opportunities for city planning and in the development of infrastructure projects for commercial planning. Together with HLRS, for example, we have organized symposia with the Verband Region Stutgart—an organization that is responsible for regional planning of towns and open space in the greater Stuttgart area. The symposia showed very quickly that HLRS, using simulation and visualization, can help make planning processes, including the challenges and opportunities that they bring, easier to understand. Simulation is also extremely relevant for studying aspects of climate in cities and in climate protection. Since then the Academy has referred several town councils to HLRS; many were not previously aware of the capabilities that HLRS offers for making the most of data they had gathered.

Simulation is also important for sustainability in industry in Baden-Württemberg. It's an unavoidable fact that high-performance computing requires high energy usage, but when one thinks about the importance of wind resistance and technologies for optimizing fluid dynamics in automobile design, one quickly recognizes how simulation helps to save enormous amounts of energy. Today these kinds of approaches can be found everywhere in the engineering sciences.

How does society profit from the research taking place at HLRS?

People often accuse scientists of forgetting to point out how humanity, including the taxpayer, benefits from basic research. HLRS is, of course, a scientific institute but because of the research it supports from industry and society, it also has a great deal of practical experience. This offers the opportunity to facilitate the diffusion of work taking place at the University of Stuttgart into society.

From my perspective, the collaboration between the Academy and HLRS has been a very successful project that has far exceeded our initial goals, and will continue to do so. Working together with HLRS, we have been able to expand our existing network and even create new networks from which all participants are now benefiting. At a basic level, what's happening here is no different than what occurs in nature. Ecological systems are fundamentally networks in which all of the parts depend on one another. The more open we are to working with others—and not just working in isolation—the better we can work for the benefit of the environment and society. *(CW)*

Virtual Reality Artwork Debuts on Tag der Wissenschaft

As part of the University of Stuttgart's annual public outreach event, HLRS presented a virtual reality installation by Brazilian artist Regina Silveira. Ms. Silveira recently visited HLRS to work with the CAVE, a virtual reality facility used to visualize large datasets. The project—called *Infinities*—was undertaken in cooperation with the Instituto Itaú Cultural, São Paulo, in an initiative conceived by MATTconcept, an international art projects platform. Silveira donated the artwork for exclusive display at HLRS.

WORKSHOPS AND SYMPOSIA

Improving Sustained Simulation Performance on Supercomputers

Participants in a two-day international meeting at HLRS discussed new strategies for improving HPC systems.

Taking full advantage of parallel computing systems requires that hardware be properly configured and that software be written to distribute components of a calculation across many processors. In addition, different types of operations running within a calculation can require varying amounts of computing resources. To make HPC systems run most efficiently, these operations need to be managed to maintain a consistent usage of resources for the duration of the calculation. Within the HPC field this is known as sustained simulation performance.

On October 10–11, HPC system users and builders met at HLRS to discuss challenges in sustained simulation performance and innovations that are making this goal more achievable. Organized by HLRS in cooperation with Tohoku University and technology company NEC, the conference began with talks focusing on next-generation supercomputers currently being developed in Germany and Japan, focusing particularly on hardware improvements meant to address challenges in sustained simulation performance.

The remainder of the workshop featured presentations describing new approaches for programming HPC systems. Speakers discussed strategies for optimizing algorithms for parallel computing structures, reducing memory requirements, accelerating input/output rates for application data, and improving sustained simulation performance on cloud computing platforms, in agent based systems, and in visualization environments.

Presentations also discussed applications of these computer science methods in the context of computational fluid dynamics, structural mechanics, aerodynamics, multiphysics, physics of the human body, and the social sciences, all disciplines that are benefiting from new insights that HPC systems enable. *(CW)*

Designing for Energy Efficiency in HPC Centers

High-performance computing has become an essential tool for investigating many kinds of problems in research and technology development. But the opportunities that it offers come at a cost. Operating a supercomputer can burn through the energy needed to power a small city, requires large cooling systems to prevent electronic equipment from overheating, and relies on literally tons of electronic hardware whose creation and disposal have sizable environmental impacts.

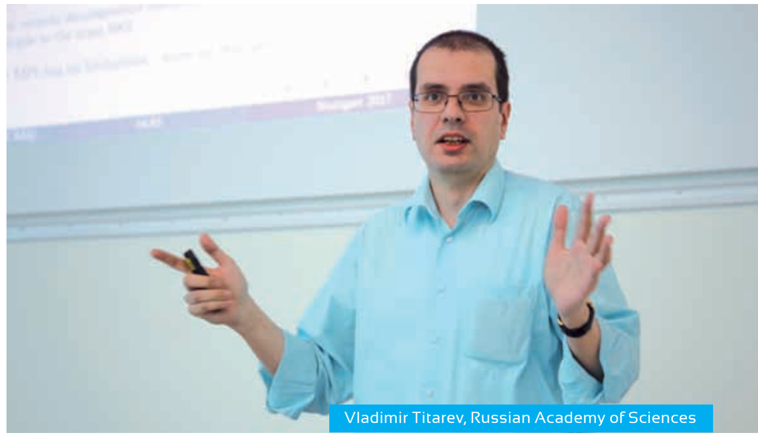
All of these facts also make HPC systems expensive to run, meaning their operators have a vested interest in designing them to be as efficient as possible. Currently, however, each computing center must individually find its own way to make its supercomputing more sustainable, not just in terms of its economic costs, but also with respect to its environmental and social implications.

Marina Köhn, Umweltbundesamt

In an effort to promote discussion connecting these issues within this broader context of sustainability, HLRS organized and hosted its first Energy Efficiency Workshop for Sustainable High-Performance Computing on October 25–26. The event brought together representatives from supercomputing facilities in the Gauss Allianz, the Gauss Centre for Supercomputing (GCS)—HLRS, the Jülich Supercomputing Centre (JSC) and the Leibniz Supercomputing Centre (LRZ), Germany's three largest HPC centers—and other academic institutions in Baden-Württemberg. Many of the presentations focused on recent innovations in cooling systems and heat reuse, which currently offer some of the greatest opportunities for increasing efficiency in computing centers. *(CW)*

Summer School: Simulation and the Social Sciences

Recent advances in simulation technologies have led some to begin exploring how computational methods could support social and political research. Meanwhile, academics with backgrounds in the humanities and social sciences have been critically reflecting on how simulation influences the practice of science and political decision-making. In an effort to increase cross-disciplinary understanding among these different disciplines, HLRS hosted a five-day workshop that brought these communities together. In addition to providing social scientists an introduction to the foundations of high-performance computing, talks investigated questions concerning the reliability of mathematical simulation, the challenges facing the use of simulation in the social sciences, and how virtual reality is being used in research and technology development. The event was the first in what the organizers anticipate will be an ongoing interdisciplinary collaboration among HLRS, Middlesex University London, and Politecnico Milano. *(CW)*



Vladimir Titarev, Russian Academy of Sciences

Conference Brings Together German and Russian HPC Experts

Organized in partnership with the Keldysh Institute of Applied Mathematics of the Russian Academy of Sciences, the conference provided a friendly venue for international idea exchange and envisioning potential collaborations. Approximately 70 scientists gathered, including key members of the mathematics and high-performance computing communities in Moscow, Novosibirsk, St. Petersburg, Rostov am Don, and Pokrowsk, Ukraine. In addition to local presenters based at HLRS and the University of Stuttgart, the German research community was also represented by scientists from Ludwig-Maximilians-University Munich, the Albert-Ludwig University Freiburg, and the Technical University Dresden. Talks focused on optimizing numerical methods for HPC systems, the future of HPC system architecture, and industrial and academic use cases of high-performance computing. Said HLRS Director Michael Resch: "The exchange of scientific ideas in workshops like this helps to keep communication channels open in Europe and beyond." *(CW)*

Roundtable Meeting Discusses Unique Challenges for Industry in Using HPC

Although HLRS dedicates the majority of its computing resources to large-scale academic research projects, clients from industry also form an important segment of its users. Working with private technology companies from many fields, HLRS is a partner for industrial R&D, particularly for the dynamic community of small and medium-sized enterprises (SMEs) in the German state of Baden-Württemberg.

It's clear that high-performance computing (HPC) offers valuable opportunities that can make companies more efficient and competitive in the global marketplace. At the same time, however, it's also evident that even when using comparatively modest computing resources, industrial HPC users have unique needs and face different challenges than their counterparts in academia. The first Industrial HPC User Roundtable, hosted at HLRS on December 8, 2017, set out to identify exactly what those special challenges are, as well as how HPC centers like HLRS could help businesses to overcome them.

The full-day event brought together representatives of companies of different sizes and in different industries to discuss problems they share when using HPC. Organized by Sicos BW, an independent organization physically based at HLRS that helps SMEs to access HPC resources, presentations and open discussion indicated that the HPC industry is not necessarily evolving in ways that best meet its industrial users' needs. Attendees discussed unique challenges that industry faces related to hardware, software, and workflow integration as well as the need for continuing education opportunities to keep them up-to-date on new developments in computing technology and methods. *(CW)*

Workshops and Conferences 2017

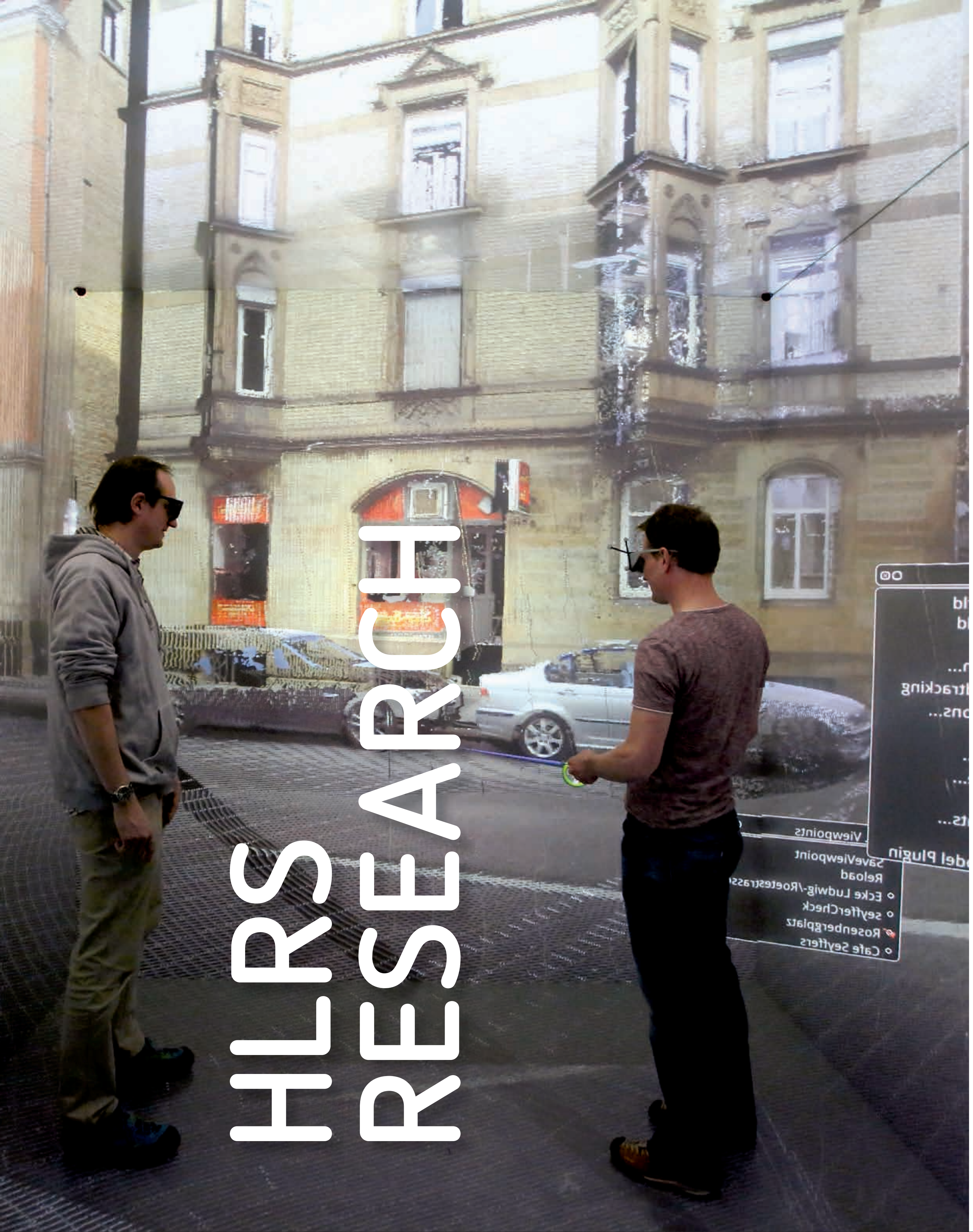
Date	Location	Partners	Topic
Feb 17	Stuttgart		Computer Simulation: Prediction, Risk, Uncertainty
Mar 27-29	Stuttgart		German-Russian Conference: Supercomputing in Scientific and Industrial Problems
Apr 3-5	Stuttgart	Russian Academy of Sciences Keldysh Institute	16th HLRS/hww Workshop on Scalable Global Parallel File Systems
Jun 1-2	Stuttgart		Workshop on Epistemic Opacity
Sep 11-13	Dresden		11th Parallel Tools Workshop
Sep 25-29	Stuttgart	Middlesex University London Politecnico Milano	Summer School: On Computer Simulation Methods
Oct 5-6	Stuttgart		High-Performance Computing in Science & Engineering: 20th Results and Review Workshop
Oct 10-11	Stuttgart	Tohoku University	26th Workshop for Sustained Simulation Performance
Oct 25-26	Stuttgart		Energy Efficiency Workshop for Sustainable High-Performance Computing 2017
Nov 2-3	Bad Boll		Science and Art of Simulation Workshop 2017
Dec 4-5	Stuttgart		7th German HPC Status Conference

HPC Training Courses in 2017

HLRS offered 39 courses in 2017, providing continuing professional education on a wide range of topics relevant for high-performance computing. The courses took place over 126 course-days in Stuttgart and at other locations in Germany and internationally. More than 1,000 trainees participated in these activities.
For a current listing of upcoming courses, please visit **www.hlrs.de/training/**.

Date	Location	Topic
Jan 12	Garching	Introduction to Hybrid Programming in HPC *
Feb 13-17	Siegen	Introdution to Computational Fluid Dynamics
Feb 20-24	Dresden	Parallel Programming with MPI, OpenMP, and Tools
Mar 7-8	Stuttgart	OpenMP GPU Directives for Parallel Accelerated Supercomputers *
Mar 9-10	Stuttgart	Introduction to Parallel Programming with HPX NEW
Mar 13-15	Frankfurt	Parallelization with MPI and OpenMP
Mar 14-17	Stuttgart	Advanced C++ with Focus on Software Engineering
Mar 20-24	Stuttgart	Fortran for Scientific Computing *
Mar 27-31	Stuttgart	Iterative Linear Solvers and Parallelization
Apr 3-7	Stuttgart	CFD with openFOAM®
Apr 4-7	Stuttgart	Cray XC40-Workshop on Scaling and Node-Level Performance
Apr 27-28	Stuttgart	Node-Level Performance Engineering *
May 4-5	Stuttgart	Cray & NVIDIA DLI — Deep Learning Workshop NEW
May 9-11	Vienna	Parallelization with MPI
May 29-30	Stuttgart	Cluster Workshop
May 31 - Jun 1	Stuttgart	Scientific Visualization
Jun 8-9	Vienna	Shared Memory Parallelization with OpenMP
Jun 12	Stuttgart	Introduction to Hybrid Programming in HPC (MPI+X)
Jun 29-30	Stuttgart	Introduction to Unified Parallel C (UPC) and Co-Array Fortran (CAF) *
Jul 3-4	Stuttgart	Efficient Parallel Programming with GASPI *
Jul 10-21	Novosibirsk	9th German-Russian Young Scientists' School and Conference on Parallel Programming and High-Performance Computing
Aug 21-24	Zurich	Parallel Programming with MPI/OpenMP
Aug 28 - Sep 1	Stuttgart	CFD with openFOAM®
Sep 4-8	Garching	Interative Linear Solvers and Parallelization
Sep 11-15	Stuttgart	Introduction to Computational Fluid Dynamics
Sep 14-15	Stuttgart	Workshop on ZFS (Zonal Flow Server)
Sep 19	Stuttgart	Introduction to the Cray XC40 HPC System at HLRS
Sep 20-22	Stuttgart	Cray XC40-Workshop on Scaling and Node-Level Performance
Sep 26	Stuttgart	Introduction to Cluster File Systems
Oct 16-20	Stuttgart	Parallel Programming Workshop (MPI, OpenMP, and Advanced Topics) * Including Parallel Programming Train the Trainer Program*
Nov 6-7	Stuttgart	Scientific Visualization
Nov 13-17	Stuttgart	StarCCM+ Training
Nov 20-22	Vienna	Parallelization with MPI
Nov 20-23	Stuttgart	Advanced C++ with Focus on Software Engineering
Nov 23-24	Vienna	Shared Memory Parallelization with OpenMP
Nov 27-29	Jülich	Advanced Parallel Programming with MPI and OpenMP
Nov 27 - Dec 1	Stuttgart	Fortran for Scientific Computing
Dec 1 + 4	Heverlee	Parallel Programming with MPI
Dec 14	Heverlee	Parallel Programming with OpenMP

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



Reallabor 4.0: Digital Models for Participatory Urban Planning

Cities are complex systems that can be difficult to understand. Virtual reality and other methods being developed at HLRS can simplify the challenge, facilitating informed, multidisciplinary discussion among all stakeholders.

As a participant in "Reallabor Stadt:quartiere 4.0," a research project funded by the Baden-Württemberg Ministry of Science, Research, and Art, HLRS researchers have been developing digital visualization tools that make it easier to demonstrate and discuss complex, technical details of city planning. Such innovations could improve the general public's ability to understand and participate in planning their cities' futures.

Focusing on the cities of Stuttgart and Herrenberg, the researchers developed detailed models that integrated data representing many layers of the built environment. Three-dimensional topographical survey data provided basic geographic information, to which the scientists added 3D laser scans of streets, buildings, and other physical features. In addition, they integrated other kinds of data from citizen groups, including air quality measurements from the OK Lab Stuttgart and a map of hazards on bicycle paths from the ADFC Herrenberg.

Using such data HLRS developed two prototype models designed as immersive visualizations. In one they created a physical model of the Stuttgart West district and an accompanying virtual model. Users can test different planning scenarios by moving objects around and those changes are visualized in the CAVE—a 3D visualization room at HLRS—in real time. In the second prototype, an immersive visualization of the city of Herrenberg was used for traffic simulations, connecting SUMO (a free software package for road traffic simulation) to the visualization environment at HLRS. Using the CAVE the investigators could then track traffic streams and pinpoint traffic hubs in virtual reality. This prototype could support Herrenberg in its concept planning for future mobility development (IMEP 2030). Discussions between HLRS and the city are underway to determine how this approach could be implemented for planning and decision support. *(LB)*

MIKELANGELO: Bringing HPC into the Cloud

As partners in a multinational EU research project, HLRS investigators developed software that facilitates the integration of two powerful technologies.

Oftentimes researchers or companies need to solve problems that require high-performance computing but don't have access to the computing systems they need. One option is to calculate on physical HPC systems like the one at HLRS, although such systems are not always configured to accommodate all applications (for example, because they don't support specific programming languages or operating systems).

Another option that is becoming increasingly attractive is to be able to perform such calculations in the cloud. Cloud-based services offer the benefits of computing availability and cost efficiency, and have more options for customizing resources to an individual user's needs. However, they also show shortcomings in performance when doing the kinds of compute- and data-intensive tasks that HPC demands.

Funded with roughly €6 million under the auspices of the European Union's Horizon 2020 research program, an international collaborative project called MIKELANGELO developed a software stack that enables big data and HPC applications to be carried out efficiently in the cloud. As a partner in the MIKELANGELO team, HLRS contributed to the project's success by creating a job management system that makes this possible.

Improving resource allocation and I/O

Bringing together HPC and the cloud requires virtual machines (VMs). VMs enable users to reproduce their local computing tools and architectures remotely, while at the same time taking advantage of large CPU and memory amounts that they do not have on their own.

When users run computing jobs in virtual HPC environments, virtual resource administrators must define the memory, CPUs, software, operating system, and other resources and system requirements that they need. This enables users to utilize a virtual HPC environment—including all necessary application components or even operating systems—just as they might a traditional HPC environment.

As part of MIKELANGELO, HLRS developed a software tool for flexible resource allocation in the cloud that was essential to the project's success. The software, called vTorque, is designed not only to schedule traditional batch jobs but also to manage entire virtual infrastructures. With vTorque users can control an entire application remotely from their own computers, without being restricted to one specific operating system or software.

Another challenge that virtualization faces results from the process of data input and output (I/O). This challenge is even more problematic when using HPC applications. Because of the large amounts of data they need to process, they demand vast resources for data processing, management, and storage. HLRS's MIKELANGELO partners developed software components to address such I/O challenges—for example, by accelerating virtual I/O and establishing high-performance interconnect networks.

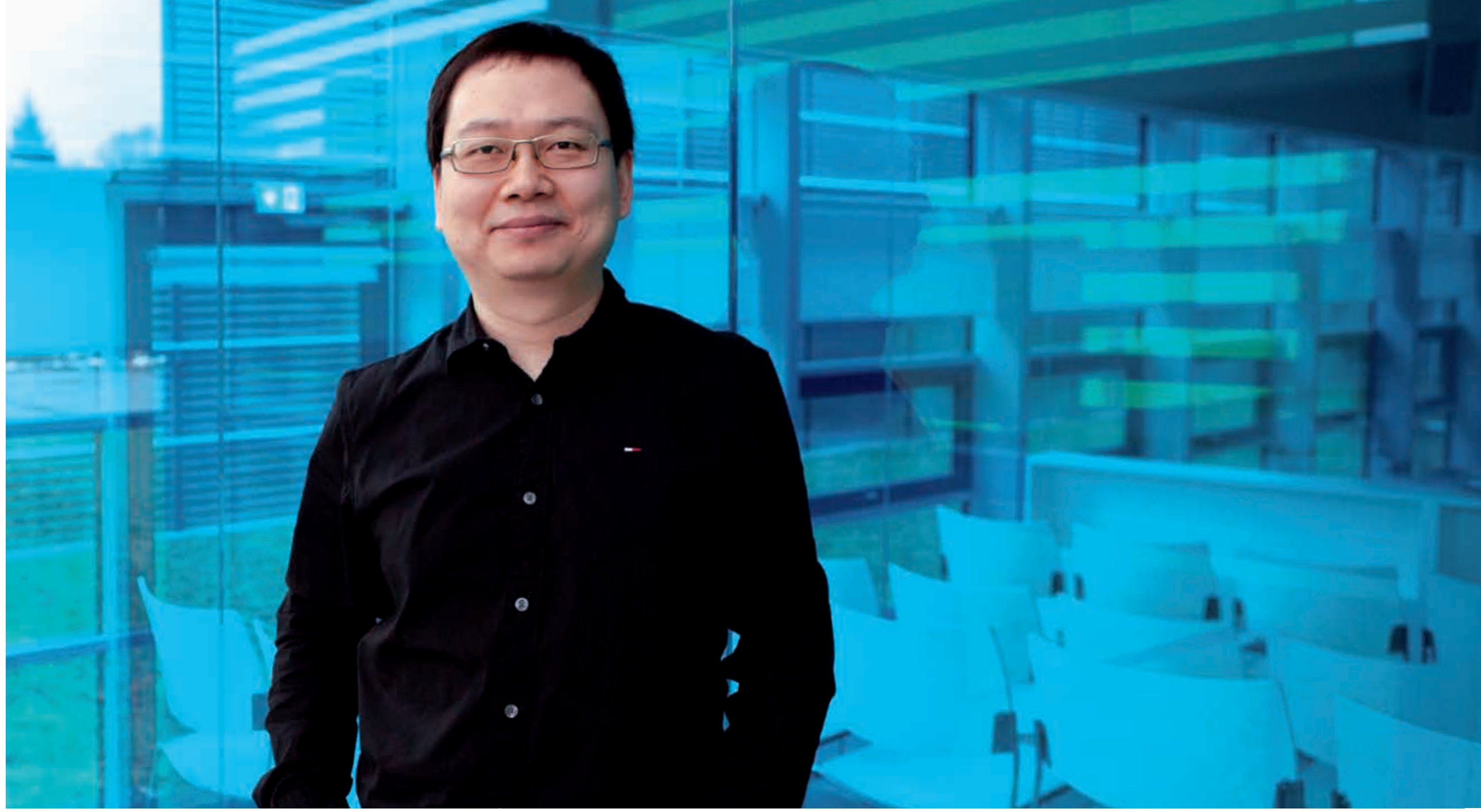
HLRS staff successfully integrated these software components into vTorque, demonstrating its functionality on both cloud-based and HPC-based system environments. When they compared an HPC application's performance in both environments HLRS investigators found that it only ran a maximum of 3% more slowly on a VM using vTorque than it did running on a physical HPC system, an impressive accomplishment.

A roadmap for the future

MIKELANGELO was recognized in an annual publication of the Horizon 2020 program as one of the top success stories in EU-funded German information and communication technologies research. The project also showed great impact on the ETP4HPC Strategic Research Agenda (SRA) of the European Commission. The SRA outlines a roadmap for achieving exascale capabilities within the European HPC ecosystem, serving as a foundation for future projects and for assessment of the entire Horizon 2020 program. The SRA's latest update in November 2017 showed great interest in conducting additional research on topics related to MIKELANGELO. Virtualization techniques in particular have been identified as technical research priorities for HPC system architecture and components and are on the list of trends to be monitored by the community.

MIKELANGELO was coordinated by Slovenian R&D company XLAB, with partners from Germany, Israel, Ireland, and Slovenia. *(LB)*

Combining Research and Practice: An Interview with Xuan Wang



Xuan Wang studied computer science at Tongji University in Shanghai before coming to Germany to pursue his master's studies at the University of Stuttgart. He later joined HLRS staff as a scientist while also pursuing his doctoral research, completing his PhD in December 2017. At the beginning of 2018 he began work at Daimler AG as a data and solution architect focusing on Big Data.

What was the topic of your doctoral research, Dr. Wang?

The efficiency of an HPC system is important for a computing center like HLRS. Before and after a calculation happens on a supercomputer enormous collections of data must be moved among various file systems. If we can optimize this process—which we call Input/Output or I/O—a job will run faster. And if we can make the runtimes for all of our computing jobs as short as possible, more jobs can run in the same amount of time, making the the system as a whole more productive.

At the same time, however, I/O issues do not have high priority for our users. They just want their results and sometimes have little understanding of I/O optimization in their programming. For my dissertation I developed a semi-automatic method for simplifying this problem. The software accelerates data reading and data writing without the user needing to know how the I/O functions. As a bonus, our systems administrators can review the users' programs and advise them on how they could better optimize their I/O. In the end this software enables HLRS to better support our users and use the valuable computing time of our high-performance computer more efficiently.

While working toward your PhD you also worked as a part of the HLRS scientific staff. What did that part of your work entail?

In addition to pursuing my research project I was a database administrator and was part a project to integrate the databases of the three members of the Gauss Centre for Supercomputing—HLRS, the Jülich Supercomputing Centre (JSC), and the Leibniz Supercomputing Centre (LRZ).

I used to think that focusing on cutting-edge topics during doctoral studies was the only important thing for finding a challenging job. But in several job interviews it became clear to me that my combination of operational and research experience made me very interesting for industry.

What are you looking forward to most at your new job with Daimler?

I'm going into industry because I want to work more closely with tangible, physical products. During my doctoral studies, for example, my code was used in a simulation to try to optimize a paint application process. I was happy to see that this led to a reduction in the number of core-hours that were needed, but I had no way to experience what the simulation results actually looked like. I'm expecting that it will be exciting to observe how my contributions influence the production of new products. As a computer scientist this will also provide valuable feedback and motivate me to always improve my software.

Although I'm leaving HLRS I'm sure that I will not be leaving high-performance computing behind. At the moment the automotive industry is very interested in autonomous driving and connectivity. These themes will demand many people with IT knowledge. This is another industry where companies are assembling gigantic data sets and they need HPC to analyze them. The combination of experiences that I am taking away from HLRS—my research as well as my operational activities—has prepared me well to make important contributions in this new world.

(CW)

Third-Party Funded Research Projects

In addition to providing supercomputing resources for scientists and engineers in academia and industry, HLRS conducts its own funded research on important topics relevant for high-performance computing. These activities, many of which are conducted in collaboration with investigators at other institutes, are designed to address key challenges and opportunities in the field. The following is a list of funded projects in 2017.

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

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

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

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

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

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

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

bwDataArchiv	**January 2015 - July 2017**	**MWK**

➜ bwDataArchiv is developing a technical infrastructure for long-term data storage, including a service for the safe preservation of scientific and culturally important data.

bwHPC-C5	**July 2013 - June 2018**	**MWK**

➜ BwHPC coordinates support for HPC users in Baden-Württemberg and the implementation of related measures and activities.

bwITsec	**October 2015 - December 2017**	**MWK**

➜ This project is developing cooperative strategies for maintaining IT security at Baden-Württemberg's nine state universities and is testing relevant services and processes.

bwVisu	**August 2014 - July 2017**	**MWK**

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

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

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

CoeGSS	**October 2015 - September 2017**	**EU**

➜ The Centre of Excellence for Global Systems Science provides advanced support for decision-making related to global challenges. By combining HPC and the latest perspectives on global systems, the project aims to improve decision-making in business, politics, and civil society.

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

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

EOPEN | November 2017 - October 2020 | EU

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

EuroLab-4-HPC | September 2015 - August 2017 | EU

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

EUXDAT | November 2017 - October 2020 | EU

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

ExaFLOW | October 2015 - September 2018 | EU

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

Exasolvers | May 2016 - April 2019 | DFG

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

EXPERTISE | March 2017 - February 2020 | EU

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

FORTISSIMO 2 | November 2015 - October 2018 | EU

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

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

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

InHPC-DE | November 2017 - September 2021 | BMBF

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

iWindow | September 2014 - August 2017 | BMBF

➔ Today's industrial machines integrate observation windows that enable operators to observe and control processes during operation. iWindow seeks to enhance the real machine window by integrating computer generated images and additional information.

Media Solution Center (MSC) | January 2015 - October 2017 | MWK

➔ The MSC is promoting better interconnectedness between the media industry and research in the fields of simulation and HPC by establishing a network and by doing research projects.

MIKELANGELO | January 2015 - December 2017 | EU

➔ MIKELANGELO is working to improve responsiveness, agility, and security of virtual infrastructures through packaged applications, using the lean guest operating system OSv and the newly developed superfast hypervisor sKVM.

MoeWe | July 2016 - December 2020 | ESF, MWK

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

MontBlanc 3 | October 2015 - September 2018 | EU

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

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

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

PetaGCS | January 2010 - December 2019 | BMBF / MWK

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

PHANTOM | December 2015 - November 2018 | EU

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

Pop-CoE | October 2015 - November 2018 | EU

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

PRACE | February 2015 - April 2017, May 2017 - April 2019 | EU

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

Reallabor Stadt:quartiere 4.0 | January 2016 - December 2018 | MWK

→ Reallabor is exploring new methods and technologies that support participatory town planning and sustainable development.

SIMTECH | June 2014 - October 2017 | DFG

→ SIMTECH develops reliable, easy-to-use methods such as simulation applets, error-controlle scientific tools, and intelligent simulation frameworks that are designed to scale to future hardware architectures.

Simulated Worlds | February 2011 - June 2018 | MWK

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

SiVeGCS | January 2017 - December 2025 | BMBF / MWK

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

Smart-DASH | May 2016 - April 2019 | DFG

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

TalPas | January 2017 - December 2019 | BMBF

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

TranSim | January 2016 - December 2018 | MWK

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

Visdral | May 2016 - August 2018 | BMWi

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

VRCITYPLAN | November 2016 - February 2017 | BMBF

→ This traveling conference focuses on how virtual reality and simulation can be used in participatory urban planning. It is connecting German research institutions and fostering cooperation with partners in China, South Korea, and Southeast Asia.

Funder Abbreviations

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

OUTREACH

HLRS Focuses on Sustainability in Supercomputing

As part of N!-Tage 2017, the High-Performance Computing Center Stuttgart (HLRS) organized an outreach event to present its sustainability efforts to the University of Stuttgart community.

Finding sustainable solutions has become an important concern in high-performance computing because of the enormous amounts of power and water that it requires. From this perspective, improving efficiency, using ecologically responsible products, and undertaking other efforts to manage environmental and social impacts will all be needed to ensure that HPC can continue being a feasible tool for research and technology development.

Beginning in 2014, HLRS received funding from Baden-Württemberg's Ministry of Science, Research and the Arts to launch a project called Sustainability in HPC Centers. In recognition of its success, the project was renewed in 2017. It has added an important dimension to the diverse research carried out at HLRS, contributing to environmentally responsible decision-making and improving working conditions at the center.

These activities at HLRS constitute one effort among many underway at the University of Stuttgart to address challenges that industrial societies face in remaining sustainable. The University's first Nachhaltigkeitstag (Sustainability Day) aimed to bring together initiatives focusing on sustainability, raise interest among students, and inspire them to pursue new ideas that could help in such efforts.

In a series of four lectures, specialists from across the University focused on sustainability challenges and solutions. The event was capped by lectures by Brigitte-Maria Lorenz and Ursula Paul—both members of the HLRS sustainability project—who described the sustainability initiatives the supercomputing center has undertaken.

Outside the lecture hall, HLRS and several University-based sustainabilitiy initiatives exhibited their activities to engage with students and other passersby, offering an opportunity for representatives of the different programs to meet and exchange ideas. *(CW)*

Gymnasium Students Visit on Girls' Day

Girls' Day is an annual event that takes place across Germany to promote awareness of and interest in careers in science, engineering, and information technology among young women. On April 27, HLRS hosted girls from the Stuttgart area to explain basic concepts in supercomputing and to show some ways in which it is used in technology development. "Even if the girls who participated don't ultimately decide to work in high-performance computing," says HLRS Girls' Day organizer Jutta Sauer, "our hope is that they had fun and gained a new sense of possibilities as they think about what they might pursue in their future careers." *(CW)*

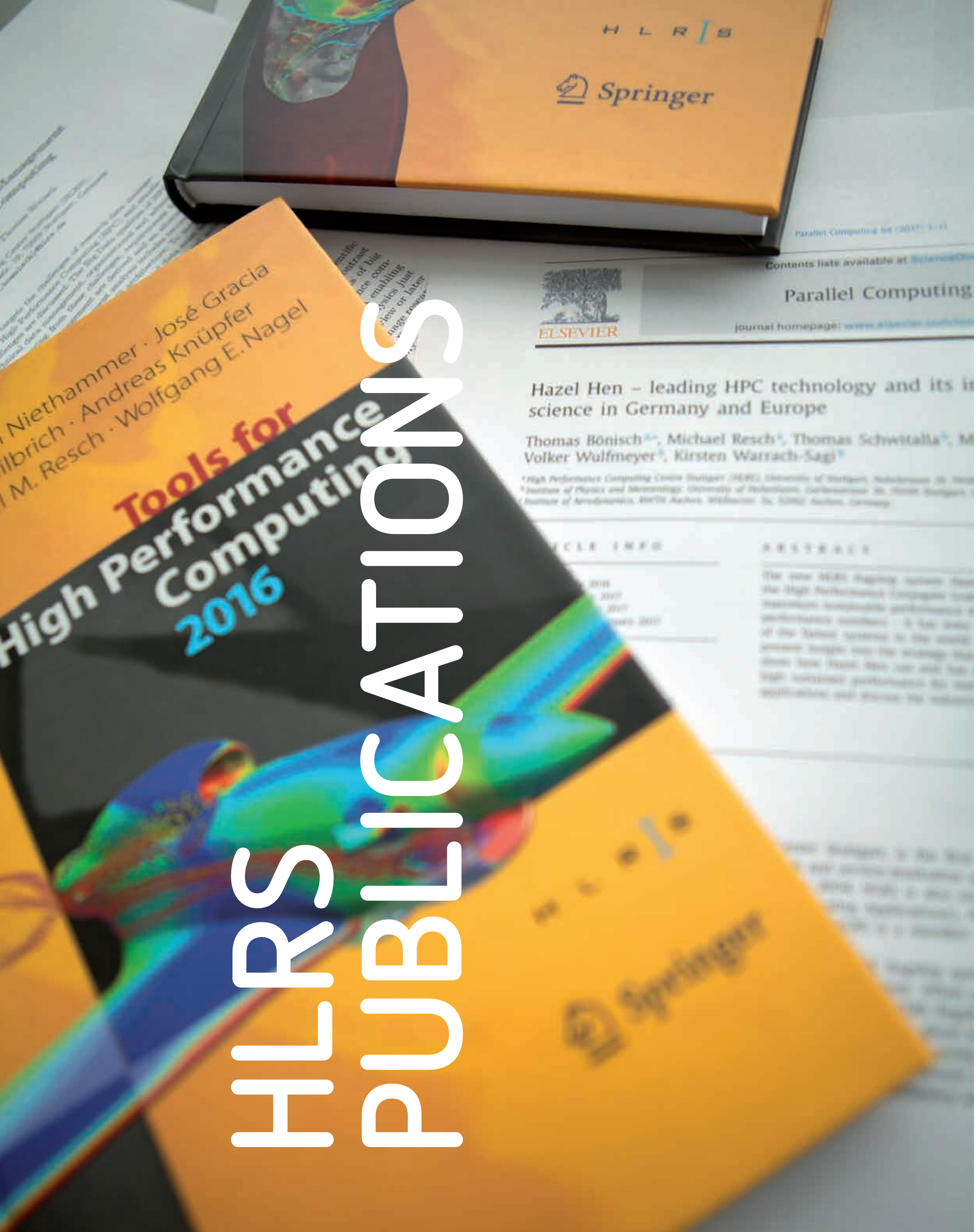
Students Awarded "Simulated Worlds" Scholarships

In July, six students accepted certificates for completing research involving simulation. The recipients received €1,000 from Simulated Worlds, a project led by HLRS that aims to raise pupils' and teachers' awareness of simulation and the technical skills it involves. The student projects focused on modeling blood flow through a human heart, traffic simulations, and a philosophical investigation of the veracity of results gained by computer simulation. *(CW)*

Public Lecture Explores Simulation and Its Limits

In a public lecture in front of a near-capacity audience at the Carl-Zeiss-Planetarium Stuttgart, HLRS Director Michael Resch explored some key theoretical issues underlying the nature and reliability of computer simulation. Although simulation offers powerful tools for analyzing complex problems, he cautioned that unavoidable human and technical flaws and biases mean that its users must always be careful to test models against reality. The lecture was the last in a series of scientific talks held for the general public in conjunction with the exhibit *Im digitalen Labor* (*Inside the Digital Laboratory*), organized by the University of Stuttgart. *(CW)*

HLRS PUBLICATIONS



Scientific Articles in Journals, Books, and Conference Proceedings

Bischof C, Formanek N*, Gehring P, Hermann M*, Hubig C, Kaminski A*, Wolf F (eds). 2017. **Computersimulationen verstehen. Ein Toolkit für interdisziplinär Forschende aus den Geistes- und Sozialwissenschaften.** TU Prints, Darmstadt.

Bonilla DR*, Glass CW*. 2017. **Exploiting functional directives to achieve MPI parallelization.** Proceedings of the Sixth International Conference on Parallel, Distributed and Cloud Computing for Engineering. Pécs, Hungary. June 4-5.

Bonilla DR*, Glass CW*. 2017. **Using functional directives to analyze code complexity and communication.** TMPA-2017: Tools and Methods of Program Analysis. Moscow, Russia. March 3-4.

Bönisch T*, Resch M*, Schwitalla T, Meinke M, Wulfmeyer V, Warrach-Sagi K. 2017. **Hazel Hen—leading HPC technology and its impact on science in Germany and Europe.** Parallel Comput 64:3-11.

Breuer T, Bussieck M, Cao KK, Cebulla F, Fiand F, Gils HC, Gleixner A, Khabi D*, Koch T, Rehfeldt D, Wetzel M. 2017. **Optimizing large-scale linear energy system problems with block diagonal structure by using parallel interior-point methods.** ZIB Report 17-75.

Cheptsov A*. 2017. **From static to dynamic: a new methodology for development of simulation applications.** In: Yurish SY (ed). Advances in Intelligent Systems: Reviews, Vol. 1: 69-88. IFSA Publishing.

Dimitriadis SI, Liparas D*, Tsolaki MN. 2017. **Random forest feature selection, fusion and ensemble strategy: combining multiple morphological MRI measures to discriminate among healthy elderly, MCI, cMCI and Alzheimer's disease patients.** J Neurosci Methods. Dec 18.

Duran JM*. 2017. **Computer simulations as a technological singularity in the empirical sciences.** In: Callaghan V, Miller J, Yampolskiy R, Armstrong S (eds). The Technological Singularity. The Frontiers Collection. Springer.

Duran JM*. 2017. **Varieties of simulations: from the analogue to the digital.** In: Resch M*, Kaminski A*, Gehring P (eds). The Science and Art of Simulation I. Springer.

Duran JM*. 2017. **Varying the explanatory span: scientific explanation for computer simulations.** Int Stud Phil Sci. 31(1):27-45.

Fan S, Chen F, Rauchfuss H, Har'El N, Schilling U*, Struckmann N*. 2017. **Towards a lightweight RDMA para-virtualization for HPC.** Proceedings of the Joint Workshops on Co-Scheduling of HPC Applications (COSH 2017) and Virtualization Solutions for High-Performance Computing (VisorHPC 2017). Stockholm, Sweden, January 24.

Friedrich A, Gehring P, Hubig C, Kaminski A*, Nordmann A (eds). 2017. **Technisches Nichtwissen. Jahrbuch Technikphilosophie 3.** Nomos.

Gehring P, Hubig C, Kaminski A*. 2017. **Was ist ein Hochleistungsrechner?** In: Bischof C, Formanek N*, Gehring P, Hermann M*, Hubig C, Kaminski A*, Wolf F (eds). Computersimulationen verstehen. Ein Toolkit für interdisziplinär Forschende aus den Geistes- und Sozialwissenschaften. TU Prints, Darmstadt.

Ham J, Kieferle JB, Wössner U*. 2017. **Exploring the three dimensional spatiality of polyrhythmic drum improvisation.** In: Fioravant A, Cursi S, Elahmar S, Gargaro S, Loffreda G, Novembri G, Trento A. (eds.) ShoCK! - Sharing Computational Knowledge! Proceedings of the 35th International Conference on Education and Research in Computer Aided Architectural Design. Rome, Italy, Sep 20-22. Volume 2.

Hoppe D*, Gienger M*, Bönisch T*, Shcherbakov O*, Moise D. 2017. **Towards seamless integration of data analytics into existing HPC infrastructures.** Proceedings of the Cray User Group (CUH '17). Redmond, WA, USA, May 2017.

Hoppe D*, Sandoval Y, Sulistio A, Malawski M, Balis B, Pawlik M, Figiela K, Krol D, Orzechowski M, Kitowski J, Bubak M. 2017. **Bridging the gap between HPC and cloud using HyperFlow and PaaSage.** Proceedings of the 12th International Conference on Parallel Processing and Applied Mathematics (PPAM 2017). September 10-13. Lublin, Poland. Springer

Hubig C, Kaminski A*. 2017. **Outlines of a pragmatic theory of truth and error in computer simulation.** In: Resch M*, Kaminski A*, Gehring P (eds). The Science and Art of Simulation I. Springer.

Kaminski A*. 2017. **Der Erfolg der Modellierung und das Ende der Modelle: Epistemische Opazität in der Computersimulation.** In: Brenneis A, Honer O, Keesser S, Vetter-Schultheiß S (eds). Technik—Macht—Raum: Das Topologische Manifest im Kontext interdisziplinärer Studien. Springer.

Kaminski A*. 2017. **Hat Vertrauen Gründe oder ist Vertrauen ein Grund? Eine dialektische Tugendtheorie von Vertrauen und Vertrauenswürdigkeit.** In: Kertscher J, Müller J (eds). Praxis und "zweite Natur": Begründungsfiguren normativer Wirklichkeit in der Diskussion. Mentis.

Kaminski A*. 2017. **Measuring intelligence effectively: psychometics from a philosophy of technology perspective.** In: Mößner N, Nordman A (eds). Reasoning in Measurement. Routledge.

Kaminski A*. 2017. **Technik und Weltbezug. Wie wissenschafliche Erfahrung möglich ist.** In: Friedrich A, Gehring P, Hubig C, Kaminski A*, Nordmann A (eds). Technisches Nichtwissen: Jahrbuch Technikphilosophie 3. Nomos.

Küster U*, Schneider R*, Ruopp A*. 2017. **The numerical approximation of Koopman modes of a nonlinear operator along a trajectory.** In: Resch M*, Bez W, Focht E, Gienger M*, Kobayashi H (eds). Sustained Simulation Performance 2017. Springer.

Montañana JM*, Hervás A, Soriano PP. 2017. **A procedure of generation of directed graphs for the comparative study of algorithms for the detection of communities.** Mathematical Modelling in Engineering & Human Behaviour 2017 Conference. Valencia, Spain.

Najmabadi SM, Offenhäuser P*, Hamann M, Jajnabalkya G, Hempert F, Glass CW*, Simon S. 2017. **Analyzing the effect and performance of lossy compression on aeroacoustic simulation of gas injector.** Computation 5(2):24.

Poke M*, Hoefler T, Glass CW*. 2017. **AllConcur: leaderless concurrent atomic broadcast.** In: Proceedings of HPDC '17. Washington, DC, USA, June 24-30.

Resch MM*. 2017. **On the missing coherent theory of simulation.** In: Resch M*, Kaminski A*, Gehring P (eds). The Science and Art of Simulation I. Springer.

Resch MM*, Bönisch T*. 2017. **High performance computing—trends, opportunities, and challenges.** In: Iyanyi P, Topping BHV, Varady G (eds). Advances in Parallel, Distributed, Grid and Cloud Computing for Engineering. Saxe-Coburg Publications.

Ruopp A*, Schneider R*. 2017. **MRI-based computational hemodynamics in patients.** In: Resch M*, Bez W, Focht E, Gienger M*, Kobayashi H (eds). Sustained Simulation Performance 2017. Springer.

Rutkai G, Köster A, Guevara-Carrion G, Janzen T, Schappals M, Glass CW*, Bernreuther M*, Wafai A*, Stephan S, Kohns M, Reiser S, Deublein S, Horsch M, Hasse H, Vrabec J. 2017. **ms2: A molecular simulation tool for thermodynamic properties, release 3.0.** Comput Phys Commun 221:343-351.

Schappals M, Mecklenfeld A, Kröger L, Botan V, Köster A, Stephan S, Garcia EJ, Rutkai G, Raabe G, Klein P, Leonhard K, Glass CW*, Lenhard J, Vrabec J, Hasse H. 2017. **Round robin study: molecular simulation of thermodynamic properties from models with internal degrees of freedom.** J Chem Theor Comput 13:4270-4280.

Schembera B*. 2017. **Myths of simulation.** In: Resch M*, Kaminski A*, Gehring P (eds). The Science and Art of Simulation I. Springer.

Schembera B*, Bönisch T*. 2017. **Challenges of research data management for high performance computing.** In: Kamps J, Tsakonas G, Manolopoulos Y, Iliadis L, Karydis I (eds). Research and Advanced Technology for Digital Libraries. Lecture Notes in Computer Science 10450. Springer.

Schöne R, Tschüter R, Ilsche T, Schuchart J*, Hackenberg D, Nagel WE. 2017. **Extending the functionality of Score-P through plugins: interfaces and use cases.** In: Niethammer C*, Gracia J*, Hilbrich T, Knüpfer A, Resch M*, Nagel W (eds). Tools for High Performance Computing 2016. Springer.

Schuchart J*, Nachtmann M*, Gracia J*. 2017. **Patterns for OpenMP task data dependency overhead measurements.** In: de Supinski B, Olivier S, Terboven C, Chapman B, Müller M (eds). Scaling OpenMP for Exascale Performance and Portability. Lecture Notes in Computer Science 10468. Springer.

Skvortsov P*, Schembera B*, Dürr F, Rothermel K. 2017. **Optimized secure position sharing with non-trusted servers.** arXiv:1702.08377.

Struckmann N*, Sandoval Y, HarEl N, Chen F, Fan S, Cinkelj J, Berginc G, Chronz P, Gilboa N, Scalosub G, Meth K, Kennedy J. 2017. **MIKELANGELO: MIcro KErneL virtualizAtioN for hiGh pErfOrmance cLOud and hpc systems.** Proceedings of the 6th European Conference on Service-Oriented and Cloud Computing (ESOCC2017). September 28-29. Oslo, Norway. Springer.

Trento A, Wössner U*, Kieferle JB, Cataldo A. 2017. **DSA—digital support for art—process and tools to realize a large sculpture in a heritage urban environment.** In: Fioravant A, Cursi S, Elahmar S, Gargaro S, Loffreda G, Novembri G, Trento A. (eds.) ShoCK! - Sharing Computational Knowledge! Proceedings of the 35th International Conference on Education and Research in Computer Aided Architectural Design. Rome, Italy, September 20-22. Volume 1.

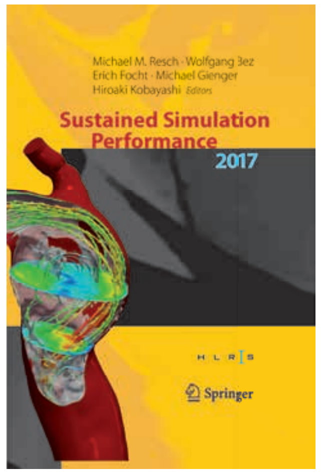
Weber J, Wackerbarth A*. 2017. **Methoden der ethischen Evaluierung digitalisierter Dienstleistungen in der Pflege.** In: Pfannstiel M, Krammer S, Swoboda W (eds). Digitale Transformation von Dienstleistungen im Gesundheitswesen III. Springer.

Zhou H*, Gracia J*. 2017. **Application productivity and performance evaluation of transparent locality-aware one-sided communication primitives.** Int J Network Comput 2017;7(2)136-153.

* denotes HLRS author or editor

HLRS Books

Sustained Simulation Performance 2017

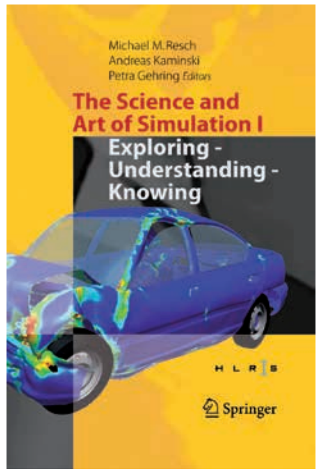


Editors:
Wolfgang Bez
Erich Focht
Michael Gienger
Hiroaki Kobazashi
Michael M. Resch

(Springer, 2017)

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, as well as the future of HPC systems and heterogeneous architectures. The contributions cover a broad range of topics, from improved system management to computational fluid dynamics, high-performance data analytics, and novel mathematical approaches for large-scale systems. In addition, they explore innovative fields like coupled multiphysics and multiscale simulations. All contributions are based on selected papers presented at the 24th Workshop on Sustained Simulation Performance, held at HLRS in December 2016 and the subsequent Workshop on Sustained Simulation Performance, held at the Cyberscience Center, Tohoku University, Japan in March 2017.

The Science and Art of Simulation I

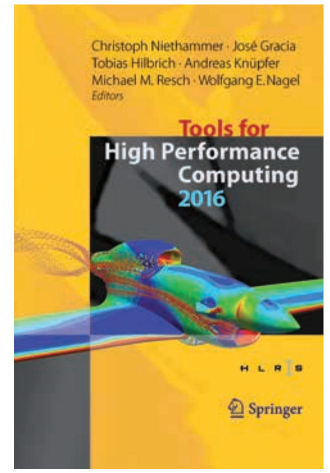


Editors:
Petra Gehring
Andreas Kaminski
Michael M. Resch

(Springer, 2017)

This new book series addresses computer simulations as a scientific activity and engineering artistry (in the sense of a technē). The first volume is devoted to three topics: the art of exploring computer simulations, the art of understanding computer simulations, and the art of knowing through computer simulations. Bringing together perspectives of both scientists and philosophers of science, it considers such questions as the implicit assumptions of simulation and the problems they entail, the capabilities and limitations of simulation in political and social contexts, and the unique kinds of knowledge that are gained in simulation that complicate our understanding of scientific method and progress.

Tools for High-Performance Computing 2016

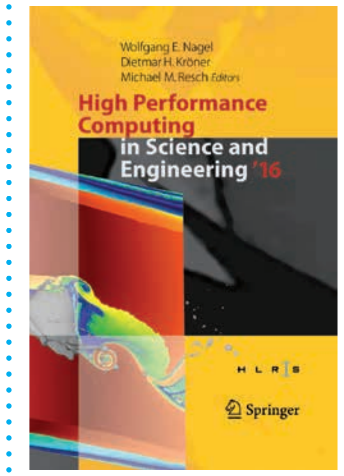


Editors:
Dietmar H. Kröner
Wolfgang E. Nagel
Michael M. Resch

(Springer, 2017)

Compiling proceedings from an October 2016 conference, this book is based on an awareness that high-performance computing is playing an increasingly important role in numerical simulation and modeling in both academic and industrial research. At the same time, however, the efficient use of large-scale parallel systems is becoming more difficult. In response, the HPC community has developed tools for parallel program development and analysis over the last decade, and what may have started as a collection of small helper scripts has now matured into production-grade frameworks. Some of these tools have been commercialized, while others are operated on an open-source basis by a growing research community. Powerful user interfaces and an extensive body of documentation also allow easy usage by non-specialists. The essays collected in the book cover recent developments aimed at helping users and tool developers to manage the unique challenges of computing on HPC systems.

High-Performance Computing in Science and Engineering '16



Editors:
Dietmar H. Kröner
Wolfgang E. Nagel
Michael M. Resch

(Springer, 2017)

Based on results discussed at the 19th Results and Review Workshop, held at HLRS in October 2016, the book covers fields of computational science and engineering including computational fluid dynamics, computational physics, chemistry, and computer science with a special emphasis on industrially relevant applications. Presenting findings generated using Hazel Hen, one of Europe's leading high-performance computing systems, this volume treats a wide variety of applications that deliver a high level of sustained performance and covers the main HPC methods. The book was published in cooperation with scientists at the Albert-Ludwig-Universität Freiburg and the Technische Universität Dresden.

SYSTEMS AND USAGE

Inside Our Computing Room

Cray XC40 Hazel Hen

Hazel Hen is at the heart of HLRS's HPC system infrastructure. With a peak performance of 7.42 Petaflops, it is one of the most powerful HPC systems in the world (position 19 in the TOP500, November 2017) and is the fastest supercomputer in Germany. Hazel Hen entered operation in October 2015, is based on the Intel Haswell Processor and the Cray Aries network technologies, and is designed for sustained application performance and high scalability.

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

Cray Urika-GX

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

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

NEC SX-ACE

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

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

NEC Cluster

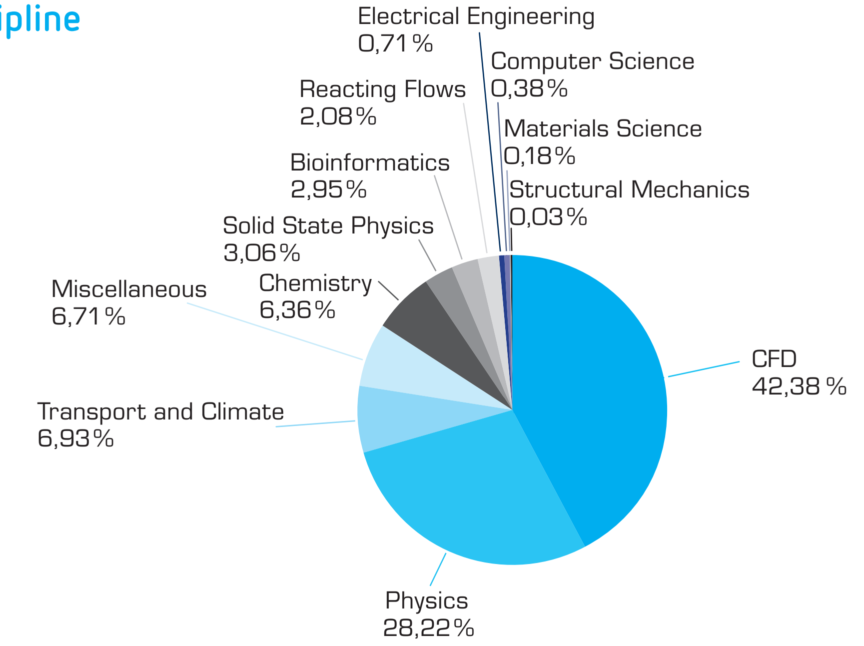
This standard PC cluster was installed in spring 2009. To meet increasing demands for compute resources, its configuration has been constantly adapted. The current configuration is as follows:

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

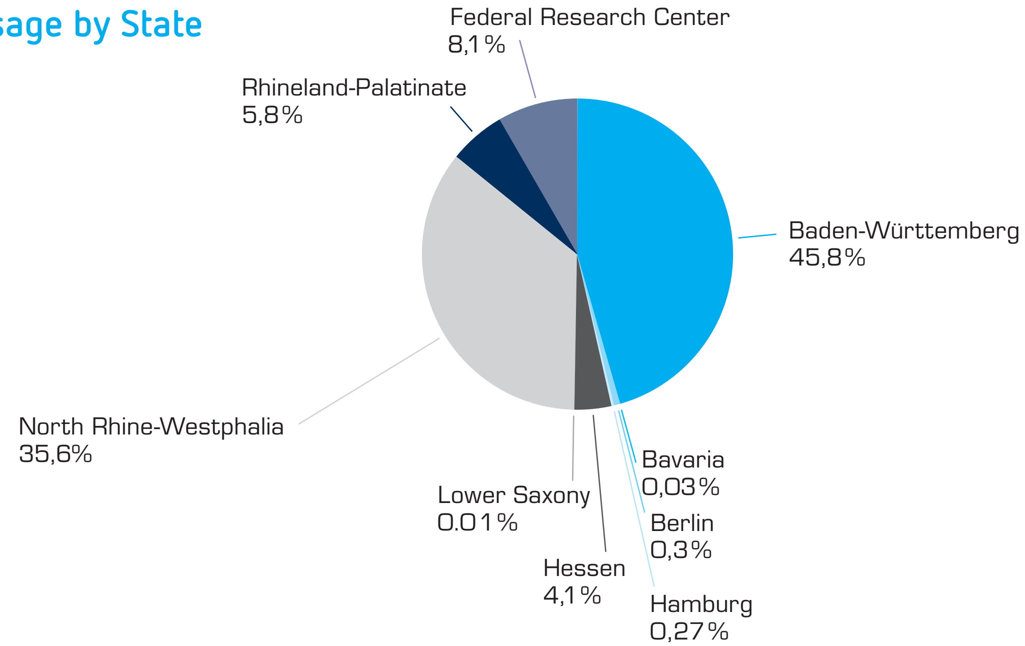
User Profile

In 2017 the Gauss Centre for Supercomputing approved 14 new large-scale projects for Hazel Hen (each project requiring more than 35 million core hours within one year), for a total of 1.28 billion core hours. The Partnership for Advanced Computing in Europe (PRACE) also approved 5 international simulation projects for HLRS, for a total of 96.7 million core hours. In total, 104 projects were active on Hazel Hen in 2017 with 1.5 billion core hours used.

System Usage by Scientific Discipline



System Usage by State



Selected User Publications

Antoniadis AF, Tsoutsanis P, Drikakis D. 2017. **Assessment of high-order finite volume methods on unstructred meshes for RANS solutions of aeronautical configurations.** Comput Fluids 146:86-104.

Babb JF, McLaughlin BM. 2017. **Radiative charge transfer in collisions of C with He⁺.** J Phys B: At Mol Opt Phys. 50:044003.

Bahe YM, Barnes DJ, Dalla Vecchia C, et al. 2017. **The Hydrangea simulations: galaxy formation in and around massive clusters.** Mon Not R Astron Soc. 470(4):4186-4208.

Bangga G, Lutz T, Dessoky A, Krämer E. 2017. **Unsteady Navier-Stokes studies on loads, wake, and dynamic stall characteristics of a two-bladed vertical axis wind turbine.** J Renew Sustain Ener. 9: 053303.

Bangga G, Lutz T, Jost E, Krämer E. 2017. **CFD studies on rotational augmentation at the inboard sections of a 10 MW wind turbine rotor.** J Renew Sustain Ener. 9:023304.

Bangga, G., Lutz, T. & Krämer, E. 2017. **Root flow characteristics and 3D effects of an isolated wind turbine rotor.** J Mech Sci Technol. 31:3839.

Bangga G, Weihing P, Lutz T, et al. 2017. **Effect of computational grid on accurate prediction of a wind turbine rotor using delayed detached-eddy simulations.** J Mech Sci Technol. 31:2359.

Barnes DJ, Kay ST, Bahe Y, et al. 2017. **The Cluster-EAGLE project: global properties of simulated clusters with resolved galaxies.** Mon Not R Astron Soc. 471(1):1088-1106.

Beinke R, Klaiman S, Cederbaum LS, et al. 2017. **Many-body effects in the excitation spectrum of weakly interacting Bose-Einstein condensates in one-dimensional optical lattices.** Phys Rev A. 95(6):063602.

Benson SP, Pleiss J. 2017. **Self-assembly nanostructures of triglyceride–water interfaces determine functional conformations of Candida antarctica lipase B.** Langmuir 33:3151-3159.

Bovard L, Martin D, Guercilena F, et al. 2017. **r-process nucleosynthesis from matter ejected in binary neutron star mergers.** Phys Rev D. 96:124005.

Braun C, Hogan C, Chandola S, et al. 2017. **Si(775)-Au atomic chains: geometry, optical properties, and spin order.** Phys Rev Materials 1:055002.

Breitsprecher K, Abele M, Kondrat S, Holm C. 2017. **The effect of finite pore length on ion structure and charging.** J Chem Phys. 147:104708.

Buhl S, Gleiss F, Köhler M, et al. 2017. **A combined numerical and experimental study of the 3D tumble structure and piston boundary layer development during the intake stroke of a gasoline engine.** Flow Turbul Combust. 98(2):579-600.

Carbonio EA, Rocha TCR, Yu A, et al. 2017. **Are multiple oxygen species selective in ehtylene epoxidation on silver?** Chem Sci. (Epub ahead of print)

Dörr PC, Kloker MJ. 2017. **Crossflow transition control by upstream flow deformation using plasma actuators.** J Appl Phys. 121: 063303.

Dörr PC, Kloker MJ. 2017. **Numerical investigations on Tollmien–Schlichting wave attenuation using plasma-actuator vortex generators.** AIAA J. doi:10.2514/1.J056779.

Dröske NC, Förster FJ, Weigand B, von Wolfersdorf J. 2017. **Thermal investigation of an internally cooled strut injector for scramjet application at moderate and hot gas conditions.** Acta Astronautica 132:177-191.

Ertl M, Weigand B. 2017. **Analysis methods for direct numerical simulations of primary breakup of shear-thinning liquid jets.** Atomization Spray 27(4):303-317.

Evarestov RA, Gryaznov D, Arrigoni M, et al. 2017. **Use of site symmetry in supercell models of defective crystals: polarons in CeO2.** Phys Chem Chem Phys. 19:8340-8348.

Fambri F, Dumbser M, Zanotti O. 2017. **Space–time adaptive ADER-DG schemes for dissipative flows: Compressible Navier–Stokes and resistive MHD equations.** Comp Phys Commun. 220:297-318.

Flad D, Gassner G. 2017. **On the use of kinetic energy preserving DG-schemes for large eddy simulation.** J Comput Phys. 350:782-795.

Fosser G, Khodayar S, Berg P. 2017. **Climate change in the next 30 years: What can a convection-permitting model tell us that we did not already know?** Clim Dynam. 48(5-6):1987-2003.

Greiner MT, Jones TE, Klyushin A, et al. 2017. **Ethylene epoxidation at the phase transition of copper oxides.** J Am Chem Soc. 139(34):11825-11832.

Han P, Antonov D, Wrachtrip J, Bester G. 2017. **Surface-bound states in nanodiamonds.** Phys Rev B. 95:195428.

Han P, Bester G. 2017. **Force field potentials for the vibrational properties of II-VI semiconductor nanostructures.** Phys Rev B. 96:195436.

Hanauskie M, Takami K, Bovard L, et al. 2017. **Rotational properties of hypermassive neutron stars from binary mergers.** Phys Rev D. 96:043004.

Hindmarsh M, Huber SJ, Rummukainen K, Weir DJ. 2017. **Shape of the acoustic gravitational wave power spectrum from a first order phase transition.** Phys Rev D. 96: 103520.

Hoilijoki S, Ganse U, Pfau-Kempf Y, et al. 2017. **Reconnection rates and X line motion at the magnetopause: global 2D-3V hybrid-Vlasov simulation results.** J Geophys Res. 122(3):2877-2888.

Hötzer J, Steinmetz P, Dennstedt A, et al. 2017. **Influence of growth velocity variations on the pattern formation during the directional solidification of ternary eutectic Al-Ag-Cu.** Acta Materialia 136:335-346.

Janecek I, Naar P, Stachon M, et al. 2017. **Fragmentation of KrN+ clusters after electron impact ionization. Short-time dynamics simulations and approximate multi-scale treatment.** Phys Chem Chem Phys. 19:2778-2790.

Janecek I, Stachon M, Gadea FX, Kalus R. 2017. **Fragmentation of KrN+ clusters after electron impact ionization II. Long-time dynamics simulations of Kr7+ evolution and the role of initial electronic excitation.** Phys Chem Chem Phys. 19:25434-25440.

Janzen T, Zhang S, Mialdun A, et al. 2017. **Mutual diffusion governed by kinetics and thermodynamics in the partially miscible mixture methanol + cyclohexane.** Phys Chem Chem Phys. 19:31856-31873.

Käpylä PJ, Käpylä MJ, Olspert N, et al. 2017. **Convection-driven spherical shell dynamos at varying Prandtl numbers.** Astron Astrophys. 599:A4.

Kellner M, Sprenger I, Steinmetz, et al. 2017. **Phase-field simulation of the microstructure evolution in the eutectic NiAl-4Cr system.** Comput Materials Sci. 128:379-387.

Klaiman S, Streltsov AI, Alon Oe. 2017. **Uncertainty product of an out-of-equilibrium Bose-Einstein condensate.** J Phys: Conf Ser. 826:012020.

Knist S, Goergen K, Bonomo E, et al. 2017. **Land-atmosphere coupling in EURO-CORDEX evaluation experiments.** J Geophys Res-Atmospheres 122(1):79-103.

Knodel MM, Reiter S, Targett-Adams P, et al. 2017. **3D spatially resolved models of the instracellular dynamics of the hepatitis C genome replication cycle.** Viruses 9(10):282.

Knop-Gericke A, Pfeifer V, Velasco-Velez JJ, et al. 2017. **In situ X-ray photoelectron spectroscopy of electrochemically active solid-gas and solid-liquid interfaces.** J Electron Spectrosc. 221:10-17.

Kohns M, Horsch M, Hasse H. 2017. **Activity coefficients from molecular simulations using the OPAS method.** J Chem Phys. 147:144108.

Kohns M, Werth S, Horsch M, et al. 2017. **Molecular simulation study of the CO2-N2O analogy.** Fluid Phase Equilibr. 442:44-52.

Koß P, Statt A, Virnau P, Binder K. 2017. **Free-energy barriers for crystal nucleation from fluid phases.** Phys Rev E. 96:042609.

Köster A, Mausbach, Vrabec J. 2017. **Premelting, solid-fluid equilibria, and thermodynamic properties in the high density region based on the Lennard-Jones potential.** J Chem Phys. 147:144502.

Kotomin EA, Merkle R, Mastrikov YA, Kuklja MM, Maier J. 2017. **The effect of (La,Sr)MnO3 cathode surface termination on its electronic structure.** ECS Transactions 77(10):67-73.

Koutsou G. 2017. **Nucleon structure and the neutron electric dipole moment from twisted mass lattice QCD.** Few-Body Syst. 58:104.

Kronenburg A, Stein OT. 2017. **LES-CMC of a partially premixed, turbulent dimethyl ether jet diffusion flame.** Flow Turbul Combust. 98:803.

Lakehal D, Metrailler, Reboux S. 2017. **Turbulent water flow in a channel at ReT = 400 laden with 0.25 mm diameter air-bubbles clustered near the wall.** Phys Fluids 29:065101.

Landmann M, Rauls E, Schmidt WG. 2017. **Understanding band alignments in semiconductor heterostructures: composition dependence and type-I—type-II transition of natural band offsets in nonpolar zinc-blende AlxGa1-x/AlyGa1-yN composites.** Phys Rev B. 95:155310.

Lautenschlaeger MP, Stephan S, Urbassek HM, et al. 2017. **Effects of lubrication on the friction in nanometric machining processes: a molecular dynamics approach.** Appl Mech Mater. 869:85-93.

Lechte C, Conway GD, Görler T, Tröster-Schmid, ASDEX Upgrade Team. 2017. **X mode Doppler reflectometry k-spectral measurements in ASDEX Upgrade: experiments and simulations.** Plasma Phys Contr F. 59(7).

Lintermann, A. & Schröder, W. 2017. **A hierarchical numerical journey through the nasal cavity: from nose-like models to real anatomies.** Flow Turbul Combust.

Lode AUJ, Bruder C. 2017. **Fragmented superradiance of a Bose-Einstein condensate in an optical cavity.** Phys Rev Lett. 118:013603.

Loosem S. Statmolpv V, Meinke M, Schröder W. 2017. **Modal analysis of passive flow control for the turbulent wake of a generic planar space launcher.** CEAS Space J. (ePub ahead of print)

Lücke A, Gerstmann U, Kühne TD, Schmidt WG. 2017. **Efficient PAW-based bond strength analysis for understanding the In/Si(111)(8x2) - (4x1) phase transition.** J Comput Chem. 38(26)2276-2282.

Luitz DJ, Bar Lev Y, Lazarides A. 2017. **Absence of dynamical localization in interacting driven systems.** SciPost Phys. 3:029.

Luitz DJ, Huveneers F, de Roeck W. 2017. **How a small quantum bath can thermalize long localized chains.** Phys Rev Lett. 119:150602.

Mitza A, Nizenkov P, Pfeiffer M, Fasoulas S. 2017. **Three-dimensional implementation of the low Diffusion method for continuum flow simulations.** Comput Phys Commun. 220:269-278.

Müller A, Schippers S, Hellhund J, Kilcoyne ALD, Phaneuf RA, McLaughlin BM. 2017. **Photoionization of tungsten ions: experiment and theory for W4^{+}.** J Phys B: At Mol Opt Phys. 50(8).

Müller A, Schippers S, Phaneuf RA, et al. 2017. **Photoionisation of Ca+ ions in the valence-energy region 20-56eV: experiment and theory.** J Phys B: At Mol Opt Phys. 50:205001.

Munoz-Munoz YM, Hsieh CM, Vrabec J. 2017. **Understanding the differing fluid phase behavior of cyclohexane + Benzene and their hydroxylated or aminated forms.** J Phys Chem B. 212(21):5374-5384.

Neuber G, Kronenburg A, Stein OT, Cleary MJ. **MMC-LES modelling of droplet nucleation and growth in turbulent jets.** Chem Eng Sci. 167:204-218.

Nizenkov, P., Noeding, P., Konopka, M. et al. 2017. **Verification and validation of a parallel 3D direct simulation Monte Carlo solver for atmospheric entry applications.** CEAS Space J. 9:127.

Nozaki D, Lücke A, Schmidt WG. 2017. **Molecular orbital rule for quantum interference in weakly coupled dimers: low-energy giant conductivity switching induced by orbital level crossing**. J Phys Chem Lett. 8(4):727–732.

Nozaki D, Schmidt WG. 2017. **Current density analysis of electron transport through molecular wires in open quantum systems.** J Comput Chem. 38(19):1685-1692.

Nozaki D, Toher C. 2017. **Is the antiresonance in meta-contacted benzene due to the destructive superposition of waves traveling two different routes around the benzene ring?** J Phys Chem C. 121:11739-11746.

Ogata T, Johnson SJ, Schiemann R, et al. 2017. **The resolution sensitivity of the Asian summer monsoon and its inter-model comparison between MRI-AGCM and MetUM.** Clim Dynam. 49(9-10):3345-3361.

Palmroth M, Hoilijoki S, Juusola L, et al. 2017. **Tail reconnection in the global magnetospheric context: Vlasiator first results.** Ann Geophys. 35(6):1269-1274.

Pandey S, Chu X, Laurien E. 2017. **Investigation of in-tube cooling of carbon dioxide at supercritical pressure by means of direct numerical simulation.** Int J Heat Mass Transfer 114:944-957.

Pandey S, Laurien E, Chu X. 2017. **A modified convective heat transfer model for heated pipe flow of supercritical carbon dioxide.** Int J Therm Sci. 117:227-238.

Pfeiffer M, Gorji MH. 2017. **Adaptive particle–cell algorithm for Fokker–Planck based rarefied gas flow simulations.** Comp Phys Commun. 213:1-8.

Pfeifer V, Jones TE, Velez JJV, et al. 2017. **In situ observation of reactive oxygen species forming on oxygen-evolving iridium surfaces.** Chem Sci. 8:2143-2149.

Reitzle M, Kieffer-Roth C, Garcke H, Weigand B. 2017. **A volume-of-fluid method for three-dimensional hexagonal solidification processes.** J Comput Phys. 339:356-369.

Riefer A, Schmidt WG. 2017. **Solving the Bethe-Salpeter equation for the second-harmonic generation in Zn chalcogenides.** Phys Rev B. 96:235206.

Riefer A, Weber N, Mund J, et al. 2017. **Zn-VI quasiparticle gaps and optical spectra from many-body calculations.** J Phys: Condensed Matter 29:215702.

Rohrmüller M, Schmidt WG, Gerstmann U. 2017. **Electron paramagnetic resonance calculations for hydrogenated Si surfaces.** Phys Rev B. 95:125310.

Rutkai G, Thol M, Span R, Vrabec J. 2017. **How well does the Lennard-Jones potential represent the thermodynamic properties of noble gases?** Mol Phys. 115(9-12):1104-1121.

Santos-Santos IME, Dominguez-Tenreiro R, Granato GL, et al. 2017. **Diversity of dwarf galaxy IR-submm emission patterns: CLUES from hydrodynamical simulations.** Astron Astrophys. 603:A4.

Schiemann R, Demory ME, Shaffrey LC, et al. 2017. **The resolution sensitivity of Northern Hemisphere blocking in four 25-km atmospheric global circulation models.** J Climate Jan 1.

Schlottke-Lakemper M, Yu H, Berger S, et al. 2017. **A fully coupled hybrid computational aeroacoustics method on hierarchical Cartesian meshes.** Comput Fluids 144:137-153.

Schneiders L, Meinke M, Schröder W. 2017. **Direct particle-fluid simulation of the Kolmogorov-length-scale size particles in decaying isotropic turbulence.** J Fluid Mech. 819:188-227.

Schneiders L, Meinke M, Schröder W. 2017. **On the accuracy of Lagrangian point-mass models for heavy non-spherical particles in isotropic turbulence.** Fuel 201:2-14.

Schröder M, Meyer HD. 2017. **Transforming high-dimensional potential energy surfaces into sum-of-products form using Monte Carlo methods.** J Chem Phys. 147:064105.

Schwitalla T, Bauer HS, Wulfmeyer V, Warrach-Sagi K. 2017. **Continuous high-resolution midlatitude-belt simulations for July–August 2013 with WRF.** Geosci Model Dev. 10(5):2031-2055.

Seidl MJ, Aigner M, Keller R, Gerlinger P. 2017. **CFD simulations of turbulent nonreacting and reacting flows for rocket engine applications.** J Supercrit Fluid. 121:63-77.

Seino K, Sanna S, Schmidt WG. 2017. **Temperature stabilizes rough Au/Ge(001) surface reconstructions.** Surf Sci. 667:101-104.

Selvam PK, Kulenovic R, Laurien E, et al. 2017. **Thermal mixing of flows in horizontal T-junctions with low branch velocities.** Nucl Eng Des. 322:32-54.

Smyth RT, Johnson CA, Ennis DA, et al. 2017. **Relativistic R-matrix calculations for the electron-impact excitation of neutral molybdenum.** Phys Rev A. 96:042713.

Statnikov V, Meinke M, Schröder W. 2017. **Reduced-order analysis of buffet flow of space launchers.** J Fluid Mechan. 815:1-25.

Tebi S, Paszkiewicz M, Aldahhak H, et al. 2017. **On-surface site-selective cyclization of corrole radicals.** ACS Nano. 11(3):3383-3391.

Vo S, Stein OT, Kronenburg A, Cleary MJ. 2017. **Assessment of mixing time scales for a sparse particle method.** Combust Flame 179:280-299.

Vovchenko V, Pasztor A, Fodor Z, et al. 2017. **Repulsive baryonic interactions and lattice QCD observables at imaginary chemical potential.** Phys Lett B. 775:71-78.

Watermann T, Sebastiani D. 2017 **Liquid water confined in cellulose with variable interfacial hydrophilicity.** Z Phys Chem. (ePub ahead of print)

Weiner SE, Tsatsos, Cederbaum LS, Lode AUJ. 2017. **Phantom vortices: hidden anfular momentum in ultracold dilute Bose-Einstein condensates.** Sci Rep. 7:40122.

Weir DJ. 2017. **Acoustic waves and the detectability of first-order phase transitions by eLISA.** J Phys Conf Ser. 840:012031.

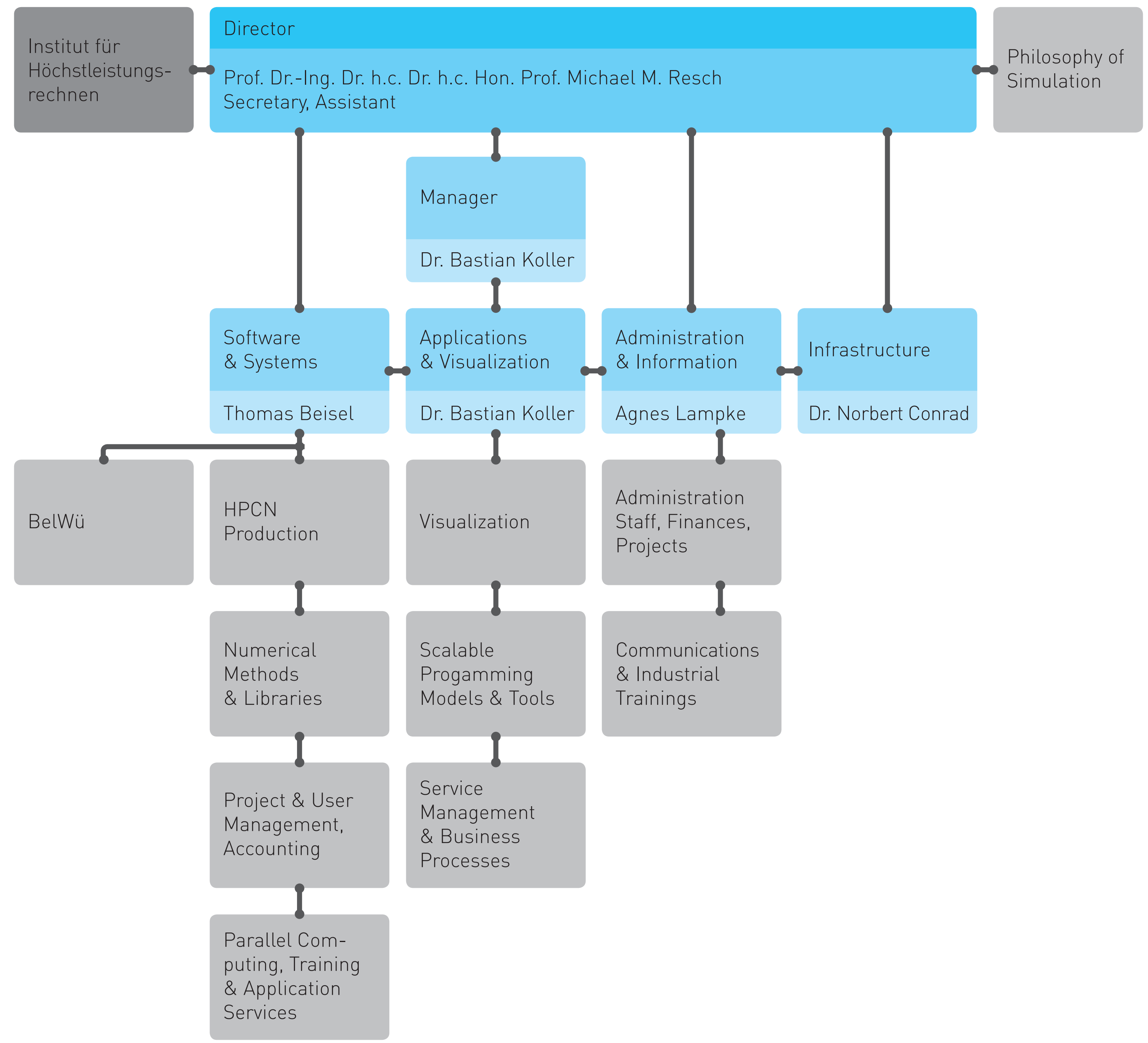
Zhang F, Baust T, Zirwes T, et al. **Impact of infinite thin flame approach on the evaluation of flame speed using spherically expading flames.** Energy Technol-Ger. 5(7):1055-1063.

Zhang F, Zirwes T, Habisreuther P, Bockhorn H. 2017. **Effect of unsteady stretching on the flame local dynamics.** Combust Flame 175:170-179.

Zhang F, Zirwes T, Nawroth H, et al. 2017. **Combustion-generated noise: an environment-related issue for future combustion systems.** Energy Technol-Ger. 5(7):1045-1054.

ORGANIZATION

Structure



HLRS IN NUMBERS

System Usage

- 1.515 BILLION — CORE HOURS PRODUCED
- 104 — USER PROJECTS
- 25 — INDUSTRIAL CUSTOMERS
- 98 — USER PUBLICATIONS

Education and Training

39 CONTINUING EDUCATION COURSES
- 1,007 Participants
- 126 Course-Days

9 SCIENTIFIC WORKSHOPS
- 397 Participants
- 23 Days

21 UNIVERSITY LECTURES
- 2,320 Participants
- 44 SWS

Staff

136

- 80 SCIENTISTS
- 36 NONSCIENTISTS
- 20 RESEARCH ASSISTANTS

Visiting Researchers

28

Visitors at HLRS

1,363

Talks

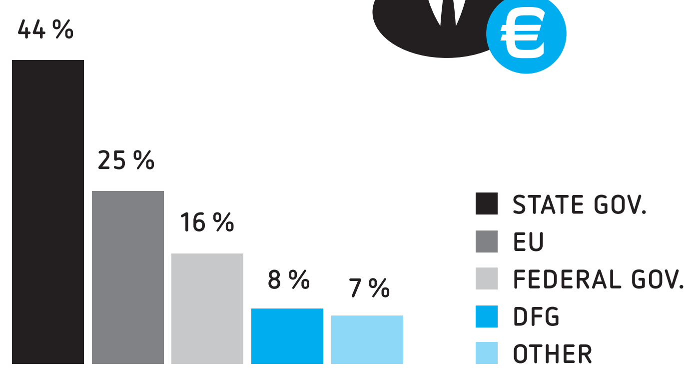
89

Publications

- 39 PAPERS IN JOURNALS, BOOKS, AND CONFERENCE PROCEEDINGS
- 4 BOOKS

Third-Party Funds

3,970,530



Divisions and Departments

Administration & Information

➜ Leader: Agnes Lampke

Administration
Leader: Agnes Lampke

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

Communications and Industrial Trainings
Leader: Dr. Jutta Oexle

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

Applications & Visualization

➜ Leader: Dr. Bastian Koller

Visualization
Leader: Dr.-Ing. Uwe Wössner

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

Scalable Programming Models and Tools
Leader: Dr. José Gracia

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

Service Management and Business Processes
Leader: Michael Gienger

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

Software and Systems

➜ Leader: Thomas Beisel

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

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

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

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

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

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

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

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

Infrastructure

➜ Leader: Dr. Norbert Conrad

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 scientists and administration, 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.

Staff Unit: Related Research

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

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

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

This annual report is printed on paper that has been certified by the Blue Angel ecolabel.