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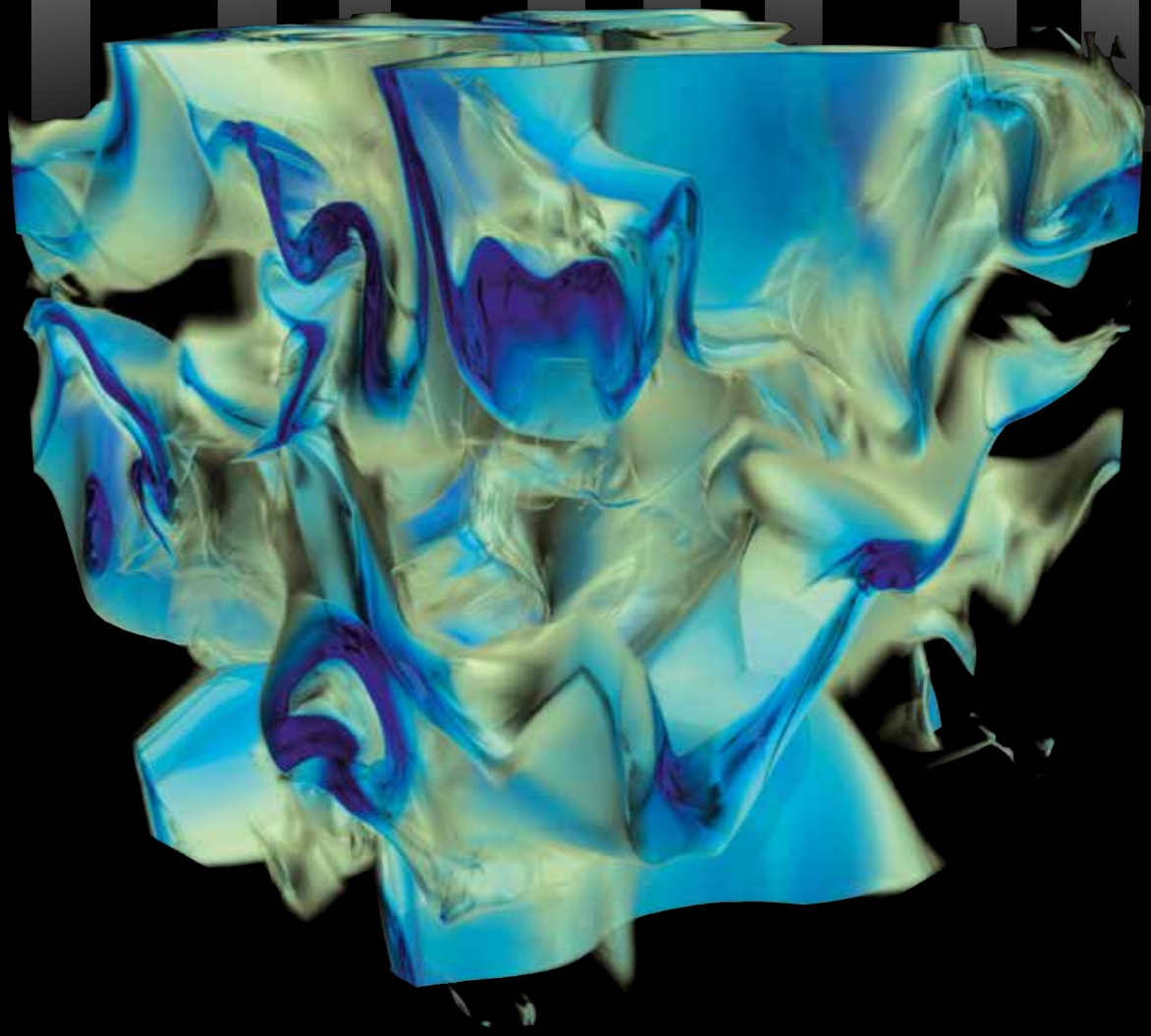

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GCS
Gauss Centre for Supercomputing

Welcome to the latest issue of InSiDE, the bi-annual Gauss Centre for Supercomputing (GCS) magazine highlighting innovative supercomputing in Germany. As we approach the end of 2019, GCS leadership feels confident that our strategy—focused on education and training, diverse architecture availability, and individualized support for users from academia and industry—is paying dividends. Our transition to next-generation, pre-exascale architectures is nearly complete, and our centres' staffs are hard at work ensuring our users are making the best-possible use of these resources while also planning for the next generation.

As the High-Performance Computing Center Stuttgart (HLRS) begins the installation process for its next-generation supercomputer, Hawk, long time users are looking forward to the possibilities to investigate science and engineering problems previously too computationally demanding for previous machines (PAGE 4). While the Jülich Supercomputing Centre (JSC) is preparing to install the next module of its JUWELS supercomputer, it also recently partnered with Google to use HPC for developing quantum computing technologies (PAGE 7). The Leibniz Supercomputing Centre (LRZ) is also focused on supporting emerging technologies, hosting its inaugural quantum computing user group meeting (PAGE 9).

Our user base and our partnerships with other institutions underscore our commitment to stewardship of HPC resources for the public good. Researchers using LRZ resources uncovered the role that earthquake motions play in creating extreme tsunamis, such as those hitting Palu Bay, Indonesia in 2016 (PAGE 10). The HiDALGO project, funded as part of the European Union's Horizon 2020 programme, is aimed at harnessing high-performance computing, data analytics, and artificial intelligence to address some of humanity's most serious global challenges. From predicting and managing forced migration to addressing pandemics, HPC can play a role in ensuring decision makers have the best information possible in order to address these challenges. Among the 12 institutions involved in HiDALGO, HLRS serves as the technical lead (PAGE 20). Researchers using JSC resources are making breakthroughs in understanding composite materials on an atomic level, paving the way for developments in cleaner, safer ways of transportation (PAGE 12).

Future generations of HPC systems offer the promise of even more scientific breakthroughs. As we move closer to the exascale threshold, GCS centres' staffs are hard at work making sure that our users are successful in solving today's biggest challenges and are prepared to take full advantage of cutting-edge technologies as they emerge.

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

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NEWS FEATURES

LOOKING FORWARD TO HAWK'S TAKE-OFF

As HLRS prepares for the installation of its next-generation supercomputer — called Hawk — a longtime power user discusses the opportunities that it will offer for science and industry.

Dr.-Ing. Wolfgang Schröder **© RWTH Aachen Aerodynamics Institute**

Early in 2020, the High-Performance Computing Center Stuttgart (HLRS) will begin installing Hawk, a new supercomputer that will offer more than 3.5 times the computing speed of its current flagship system, Hazel Hen. The computer, manufactured by Hewlett Packard Enterprise and based on the AMD Rome processor, will have a peak performance of 27 petaFLOPs, offering a powerful new tool for academic and industrial research and technology development.

As director of the Institute of Aerodynamics at RWTH-Aachen University, Dr.-Ing. Wolfgang Schröder has been a longtime user of HLRS's supercomputing facilities. He and his colleagues study turbulent flows, a category of physical phenomena that is important for the development of better, more efficient technologies in the aerospace, energy, and automotive sectors, among others. Because the models that he and his team develop represent turbulence with high precision down to its smallest scales, their simulations have often required the use of a large percentage of Hazel Hen's computing capacity. Schröder's work is thus an example of the kind of computationally intensive research that will benefit from the additional resources Hawk will offer.

In the following interview, Schröder discusses why he is looking forward to Hawk's launch and why — even with the arrival of new technologies such as artificial intelligence and quantum computing — high-performance computing will continue to be important for scientific and industrial progress.

? *Dr. Schröder, your group has been one of the heaviest users of HLRS's current supercomputer, Hazel Hen. Why is supercomputing important to your work, and what new opportunities do you anticipate once Hawk comes online?*

My lab is primarily interested in exploring fundamental questions related to turbulent flows, where it is necessary to resolve the temporal and spatial scales of the flow field. Those scales are extremely small, which means that you need very high-resolution, sophisticated algorithms. The models we develop are relevant for various fields of physics; to be more precise, computational fluid dynamics, acoustics, and combustion, etc. This also includes multiphase flows, which are even more complex because they involve interfaces between different kinds of matter in different phases (e.g., liquid and gas). We need high-performance computing to look at all of these kinds of questions.

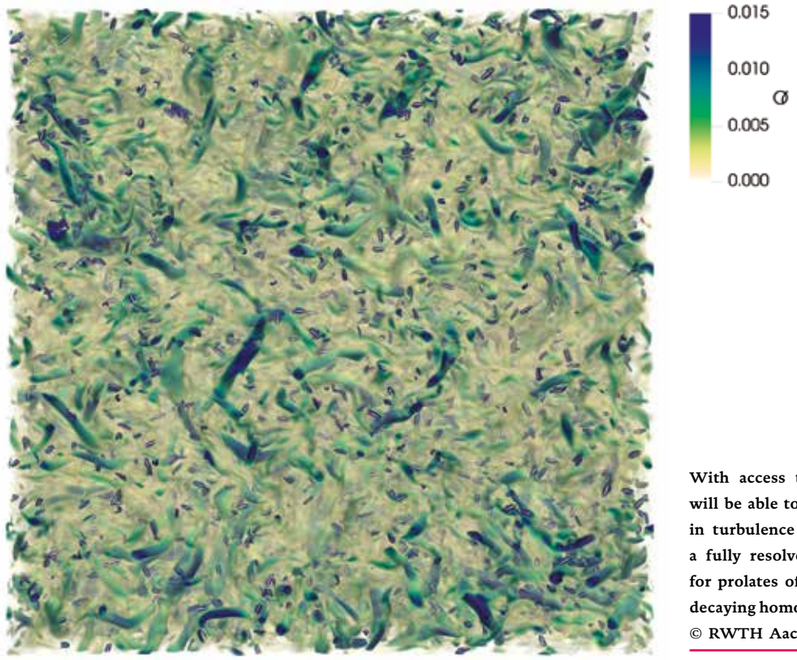
The size of the supercomputer also affects the scale of the problems that we can study, because when you do a computation, you have to store the data. We typically don't look at one time step or one instant, but at a long time period to see how the flow field develops. The smaller the temporal and spatial scales, the more data you generate.

Sometimes we have deadlines for large simulations that we need to satisfy. In these cases we often like to use 90,000-100,000 processors, which enables us to produce a result in 2 weeks or so as opposed to a couple of months, which would be required on a smaller system. I would always prefer to use 100% of the machine, but of course we have to share the computer with others. So from our perspective, we welcome the arrival of Hawk because the bigger the machine, the better for all.

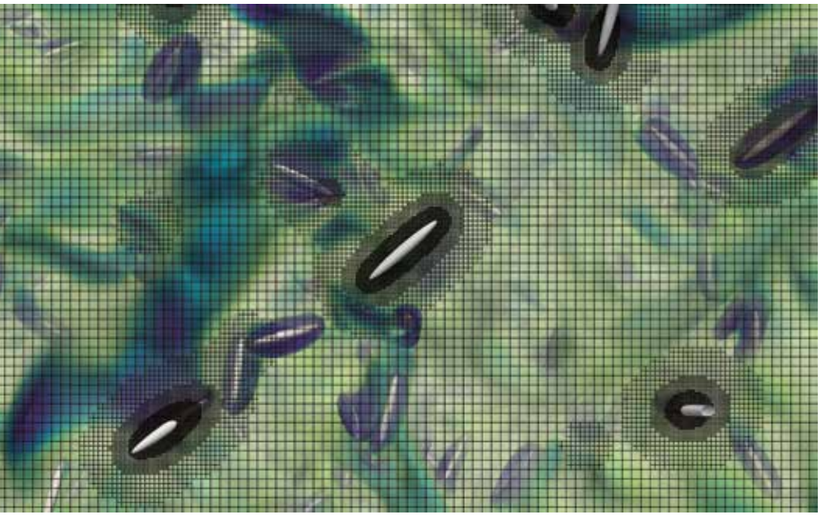
When we write a proposal and ask for funding, we also know that the reviewers know the limits of the machines. We have to make sure that what we propose is realistic with respect to the computers that are available. If there were a bigger computer, the proposal would contain different numbers, and so limits in supercomputing capacity also define the proposals we can write.

? *Although your lab is focused on basic fluid mechanics research, the models you develop are relevant for industry. How do you see industry benefiting from the new capabilities that Hawk offers?*

The goal of our lab is to understand fluid mechanics at a very fundamental level, and so we perform computations where "everything," down to the smallest parts of the physical system we are studying — within the limits of continuum mechanics — is resolved at a very high resolution. Industry does not need this kind of comprehensive model, but to develop a model for a specific, smaller problem that an engineer might have, you first need to have a complete solution. Otherwise you might develop a model that is wrong from the beginning.



With access to Hawk, Schröder's group will be able to continue to make advances in turbulence studies. This image shows a fully resolved fluid-particle interaction for prolates of Kolmogorov length size in decaying homogeneous turbulence.
© RWTH Aachen Aerodynamics Institute



The image shows a zoom of a flow field plus the mesh to emphasize the adaptive mesh refinement for each of the moving particles.
© RWTH Aachen Aerodynamics Institute

To determine the heat transfer or cooling efficiency, for example, the information for even a small part of the system has to be described by a perfect model, and that perfect model can only be developed using a supercomputer like Hawk. Then we can reduce that kind of comprehensive description to something that is simpler that can be used by industry. Instead of running one large computation, they can then use a supercomputer during their design cycle to find an optimized solution to their specific problem.

If, for example, a turbo engine is to be improved, it might need a new geometry. The more efficient that geometry is, the better the complete efficiency of the turbo engine. This reduces fuel consumption, which is better for the environment, so there is a direct link between optimization of an engineering question and our environmental interest.

***?** As new technologies like artificial intelligence and quantum computing have gained more attention, questions have been raised about the need to continue building bigger and bigger supercomputers. Why is the continued investment in HPC necessary?*

Some people seem to think that HPC belongs to the ancient times. A few years ago, there was a lot of talk about big data, and nowadays everyone is talking about artificial intelligence and machine learning. But there is a clear relationship between supercomputing and AI. Anytime you talk about AI, that kind of analysis is always based on big data sets, and when you're talking about analyzing big data sets, you need high-performance computing.

It's also important to keep in mind the kind of problem you are investigating. My lab works on turbulent flows, and to generate just one data set we need high-performance computers, because in order to learn something, you need lots and lots of data. When we run a big analysis on an HPC system, it can take months. If we were only using AI algorithms, it would take ages. From that point of view, we have to make sure we continue to improve our ability to generate data.

The same is true with quantum computing (QC). Many current problems that will continue to be relevant won't be able to be solved on quantum computing. You always have to match the right problem to the right architecture. Currently it doesn't make sense to solve a simple heat equation on a quantum computer.

When I talk to people in Jülich who are experts in QC, they also tell me that they need information produced using high-performance computing in order to develop their quantum computers. It's not independent. It's like in soccer — you need defense and offense or the team doesn't work. The same is true with high-performance computing and new kinds of computational technologies.

Interview by Christopher Williams

FZ JÜLICH AND GOOGLE ANNOUNCE QUANTUM COMPUTING PARTNERSHIP

Research alliance aims to improve development, benchmarking, and training related to one of the world's most intriguing emerging technologies.

Left to Right: **Prof. Wolfgang Marquardt, Chairman of FZ Jülich; Dr. Hartmut Neven, Technical Director at Google and lead of the Quantum Artificial Intelligence Labs; Dr. Markus Hoffmann, Head of quantum partnerships at Google; Prof. David DiVincenzo, Director of the Peter Grünberg Institute at FZ Jülich; Prof. Kristel Michielsen, JSC; Prof. Sebastian M. Schmidt, member of the FZ Jülich board; Prof. Thomas Lippert, Director of JSC.**
© FZ Jülich / Kurt Steinhausen

In early July 2019, Germany's Federal Minister of Economics, Peter Altmaier, visited Google headquarters in Mountain View, California to celebrate a partnership between Google and one of Germany's premier research institutions—Forschungszentrum Jülich (FZ Jülich)—with the aim of advancing quantum computing technologies. By October 2019 the collaboration had already begun to bear fruit, as Google and partners, including FZ-Jülich, released a paper in Nature demonstrating how a quantum computer was used to solve a previously intractable problem for traditional supercomputers. While it is only a proof of concept, it was an important step in the development of quantum computing technology.

The partnership with Google largely revolves around one part of the larger FZ Jülich organization, the Jülich Supercomputing Centre (JSC), one of the three centres making up Germany's premier supercomputing alliance, the Gauss Centre for Supercomputing (GCS). Between Google's lengthy experience with quantum computing and JSC's computational expertise and high-performance computing (HPC) systems, the partnership has begun pushing quantum computing to reach new heights.

"This is a symbiotic relationship," said Prof. Kristel Michielsen, Group Leader of JSC's Quantum Information Processing group. "I think we at JSC benefit from their experience with quantum computing and annealing devices, as well as their connections with industries looking to use this technology. They benefit from us due to our in-house simulation expertise in quantum computing and having access to leading high-performance computing resources. Both organizations share a strong interest in training researchers on how to program for these new compute devices."

The partnership focuses on the two organizations sharing research and benchmarking results with one another as well as collaborating on training courses for JSC's academic users and industrial researchers. Michielsen indicated that JSC would be hosting a series of hands-on workshops and "Spring Schools" in the coming year that would give attendees the opportunity to access the Jülich Unified Infrastructure for Quantum Computing (JUNIQ).

Quantum computing is an emerging technology based on the quantum theory—rather than information being encoded in long series of 1s and 0s, quantum computers store information in "qubits" that can theoretically represent both 1 and 0 at the same time. Much like how researchers can use equations to understand how atoms and their constituent particles behave without being able to observe the particles in real time, quantum computers can give researchers greater flexibility when solving open-ended, complex problems that have many variables.

Although recent announcements have made headlines and researchers have taken an important step in its development, quantum computing is still in its infancy, and the same open-ended nature that makes quantum computing intriguing for some researchers also makes it less efficient for more straight-forward series of calculations. Researchers invested in developing quantum computing technology turn to traditional HPC resources to help develop and benchmark quantum computer prototypes.

"Traditional HPC helps us in three different ways," Michielsen said. "We can simulate these quantum computing devices so we can better understand how they operate, which ultimately contributes to the design aspects of these machines. HPC can help us benchmark new quantum computing devices, where we run a simulation on a quantum device and verify the solution on traditional HPC. This contributes to efficiency as well as correctness. And finally, we think that hybrid computing—using a combination of traditional HPC and quantum computers—will be the way of the future for many researchers' workflows."

Michielsen emphasized that as quantum computing hardware technology continues to develop, HPC centres such as JSC will not only serve as laboratories for developing it as a real compute technology; they will also benefit by integrating the technology in a way that further supports the HPC user community.

"Here in Jülich, we already have a lot of expertise in quantum computing, but ultimately we are all still near the starting line," she said. "As the technology develops, it is our job to make HPC users aware that the technology is available and articulate its potential for certain applications. Now and then, I meet people who think they can skip using HPC for their research and profit from the benefits of quantum computing, but current quantum computing technology is not yet ready for production simulations, and I think this hybrid mode of operation might be the key for bringing applications into quantum computing space." *eg*

LRZ EMBRACES EMERGING TECHNOLOGIES WITH THE BAVARIAN QUANTUM COMPUTING EXCHANGE

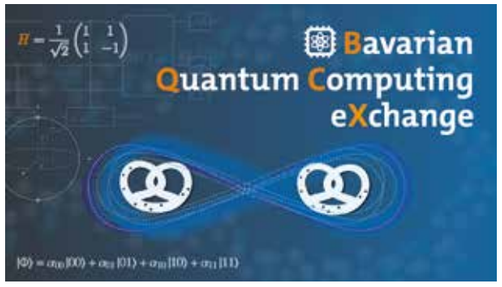
For certain tasks, they promise to solve problems much faster than current supercomputers: quantum computers are an important technology in future computing. The Leibniz Supercomputing Centre (LRZ) is driving this future topic forward backed by the Bavarian Government: On October 10th, 2019 Prime Minister Markus Söder presented the High-tech Agenda for Bavaria to the state parliament. Two billion euros are to be spent on the technology programs over the next few years. The LRZ is positioned at the "core of the new Bavarian quantum network". Its programme 'Bavarian Quantum Computing Exchange' will combine knowledge, research, and activities in academia and industry to advance this emerging technology in Bavaria.

"Bavaria is going to play a leading role in quantum technology, and there are still too many unanswered questions about quantum technology," says Laura Schulz, Head of Strategic Development at LRZ and founder of the group. "In order to answer them, we are now bringing together a wide range of specialists in the working group." As a positive side effect, the work on and with the supercomputer SuperMUC-NG will also benefit from the Quantum Computing Exchange, because many challenges of quantum technology are similar to those of supercomputers.

Concerted action from research and industry

At the kick-off event in July, representatives of the Quantum Computer Exchange from the Technical University of Munich, the Ludwig-Maximilians-Universität Munich, the Bundeswehr University, Munich, and the Deggendorf Institute of Technology met with specialists from companies such as IBM, Intel, and BMW, who are also working on quantum technologies. In the future, the group will meet the second Wednesday of every month. Researchers, students, and specialists from industry who have an interest in quantum computing or are working with the emerging technology are welcome to attend.

"The central point now is information and knowledge exchange in order to accelerate research and improve technology," explains Luigi Iapichino, team leader for LRZ's Quantum Computing group. "We discuss hardware and software solutions for quantum computers and plan workshops, trainings and lectures around the technology." At the first meeting, participants synchronized their knowledge about tasks and projects and opened mailing lists and other communication channels.



Future computing power through quantum technology

Similar to the supercomputers available today, quantum computers provide the computing capacities that contribute to the development of artificial intelligence or other data-intensive tasks.

SuperMUC-NG, one of the ten fastest supercomputers in the world (as of the June 2019 Top500 list), still works on the basis of bits and the binary system of 0s and 1s and creates billions of calculations in a very short time. Quantum computers, on the other hand, have a more open-ended path to arriving at a solution—they not only use 0s and 1s, but also their permutations 10 and 11. As a result, they can take several calculation paths in parallel. This makes them faster in certain tasks, especially when it comes to processing data.

Once quantum hardware is more widely available, enthusiasts hope that special algorithms will be able to organize complex tasks and confusing data silos faster than traditional ones.

Looking for students, researchers and supporters

Despite advancements in the field, the computing power of quantum computers is still volatile, unreliable, and difficult to standardize. Researchers in industry and academia are testing optical and mechanical methods to make them more reliable. Nevertheless, computer scientists from the Swiss Federal Institute of Technology (ETH) in Zurich are already working on the first software programs and libraries. The Quantum Computing Exchange at LRZ will also devote itself to hardware and software issues and further promote corresponding projects. Above all else, LRZ is dedicated to enabling future users of quantum computers to research and work with them as quickly and efficiently as possible. *sv*

SCIENCE FEATURES

RESEARCHERS UNCOVER CRITICAL ROLE OF DIRECT EARTHQUAKE MOTIONS IN TRIGGERING A "SURPRISE" TSUNAMI

Combining earthquake and tsunami computer models of the 2018 tsunami in Palu, researchers identified underlying causes of the deadly tsunami.

In recently published research, an international team of geologists, geophysicists, and mathematicians showed how coupled computer models can accurately recreate the conditions leading to one of the world's deadliest natural disasters of 2018, the Palu earthquake and tsunami, which struck western Sulawesi, Indonesia in September last year. The team's work was published in Pure and Applied Geophysics.

The tsunami was as surprising to scientists as it was devastating to communities in Sulawesi. It occurred near an active plate boundary, where earthquakes are common. Surprisingly, the earthquake caused a major tsunami, although it primarily offset the ground horizontally—normally, large-scale tsunamis are typically caused by vertical motions.

Researchers were at a loss—what happened? How was the water displaced to create this tsunami: by landslides, faulting, or both? Satellite data of the surface rupture suggests relatively straight, smooth faults, but do not cover areas offshore, such as the critical Palu Bay. Researchers wondered—what is the shape of the faults beneath Palu Bay and is this important for generating the tsunami? This earthquake was extremely fast. Could rupture speed have amplified the tsunami?

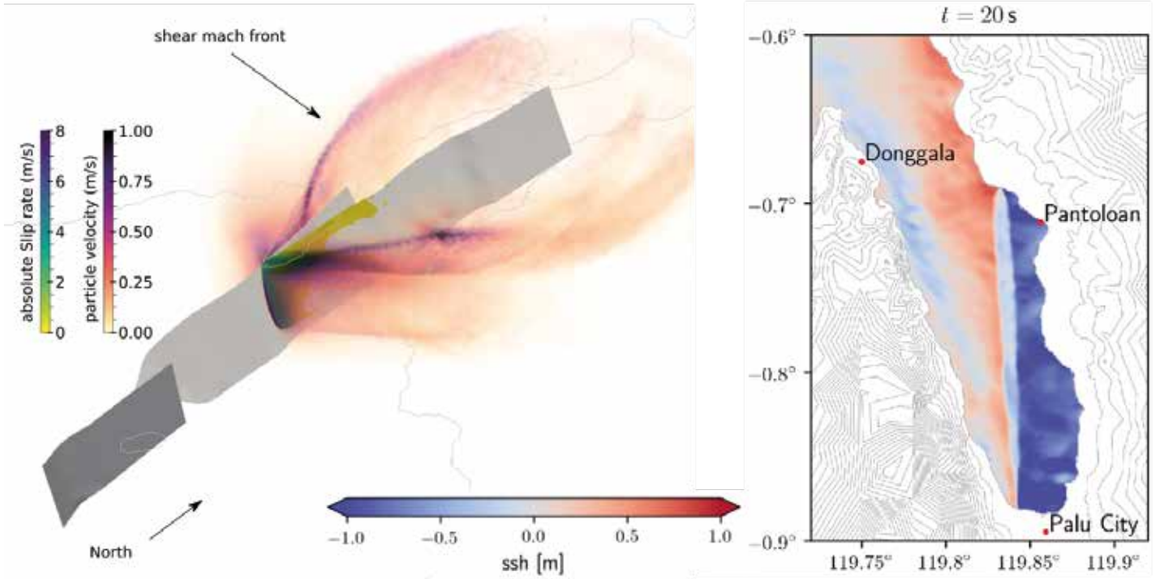
Using a supercomputer operated by the Leibniz Supercomputing Centre, a member of the Gauss Centre for Supercomputing, the team showed that the earthquake-induced movement of the seafloor beneath Palu Bay itself could have generated the tsunami, meaning the contribution of landslides is not required to explain the tsunami's main features.

The team suggests an extremely fast rupture on a straight, tilted fault within the bay. In their model, slip is mostly lateral, but also downward along the fault, resulting in anywhere from 0.8 metres to 2.8 metres of vertical seafloor change that averaged 1.5 metres across the area studied. Critical to generating this tsunami source are the tilted fault geometry and the combination of lateral and extensional strains exerted on the region by complex tectonics.

The scientists came to this conclusion using a cutting-edge, physics-based earthquake-tsunami model. The earthquake model, based on earthquake physics, differs from conventional data-driven earthquake models, which fit observations with high accuracy at the cost of potential incompatibility with real-world physics. It instead incorporates models of the complex physical processes occurring at and off of the fault, allowing researchers to produce a realistic scenario compatible both with earthquake physics and regional tectonics.

The researchers evaluated the earthquake-tsunami scenario against multiple available datasets. Sustained supershear rupture velocity, or when the earthquake front moves faster than the seismic waves near the slipping faults, is required to match simulation to observations. The modelled tsunami wave amplitudes match the available wave measurements and the modelled inundation elevation (defined as the sum of the ground elevation and the maximum water height) qualitatively match field observations. This approach offers a rapid, physics-based evaluation of the earthquake-tsunami interactions during this puzzling sequence of events.

"Finding that earthquake displacements probably played a critical role generating the Palu tsunami is as surprising as the very fast movements during the earthquake itself," said Thomas Ulrich, PhD student at Ludwig Maximilians Universität, Munich and lead author of the paper. "We hope that our study will launch a much closer look on the tectonic settings and earthquake physics potentially favouring localized tsunamis in similar fault systems worldwide." *eg*



Visualizations of the modelled coupled earthquake and tsunami across Palu Bay.
Left: **Seismic waves being generated while the earthquake propagates southward in a 'superfast' manner. Warm colours denote higher movements across the geological faults and higher ground shaking (snapshot after 15 seconds of earthquake simulation time).**
Right: **The movements of the earthquake beneath the bathtub shaped Palu Bay generate a 'surprise' tsunami (snapshot of the water waves aftee 20s of simulation time of the tsunami scenario). Image credit: Ulrich et al., 2019.** **© LMU**

MATERIALS SCIENTISTS COMBINE THEORY AND EXPERIMENT FOR STUDYING COMPOSITE MATERIAL CONTACTS

University of Freiburg researchers use JSC supercomputing resources to better understand structural material design.

From the earliest instance of smelting iron ore into metal or weaving fibers into cloth, humans have looked for ways to repurpose materials around us to use for specialized tasks. In recent decades, researchers have increasingly turned to high-performance computing (HPC) to aid in the next frontier of materials science research—in order to imbue materials with new and novel properties, scientists need to be able to understand and manipulate materials at an atomic level.

Recently, researchers led by Prof. Lars Pastewka from the University of Freiburg have been using Gauss Centre for Supercomputing (GCS) resources at the Jülich Supercomputing Centre (JSC) in order to study atomic-level material interactions of nanolaminates, specialized materials that, when combined and structured correctly, exhibit increased strength, hardness, and wear resistance, among other properties.

"Our motivation for studying nanolaminates is focused on trying to develop structural materials with enhanced mechanical properties," Pastewka said. "These types of materials can have large implications for automotive or aircraft design, but this research is trying to understand their properties at the fundamental level."

In combination with the experimental groups of Ruth Schwaiger at the Karlsruhe Institute of Technology (now at Forschungszentrum Jülich) and Guang-Ping Zhang at the Shenyang National Laboratory for Materials Science, the team unraveled their mechanical properties at the nanoscale, by combining the high-fidelity experiments with the ability to observe nanosecond, atomic interactions in molecular dynamics simulations. The team's recent work, focused on nanolaminates made of copper and gold, was published in MRS Communications.

Contact details

Nanolaminates are a class of composites, meaning they are made up of multiple materials, which exhibit properties that significantly differ from the sum of the individual parts. The interface between the individual nanolaminate layers (in many cases, only several nanometers thick) provide resistance to irreversible deformation of the atomic-level crystal structure. The composite material then exhibits larger strength than the individual components.

In order to design materials with these specialized properties, researchers need to understand how the material reacts to its environment, specifically to external stress. An elegant way of testing the mechanical properties is to manufacture small "pillars" of the material, typically by removing the material surrounding the pillar using a focused ion beam. These pillars are then deformed with a hard flat punch while researchers measure the applied force. When researchers interpret these experiments, though, they don't often take into account that surfaces—of the pillar and of the flat punch—are never perfectly flat.

While many materials look smooth to the naked eye, at the atomic level, every material exhibits rough, uneven surfaces. Peaks on these surfaces serve as the points of intimate atomic contact in situations such as when pushing down on the pillar. The contact geometry is important to understand where materials are actually touching one another at the atomic scale.

"Roughness has implications in materials science, because the force is transmitted at just the contacting peaks," Pastewka said. "Thinking about pressure, this means that the local pressure experienced by the surface can be orders of magnitude higher than the apparent applied pressure because the real area of contact is much smaller than we naively think it is. True contact between any two materials happens at the smallest scales." The point where these interactions happens, the interfaces, is the focal point for researchers.

While the fine details of surface roughness are largely uncontrolled in experiments, computer simulations allow to control the position of every atom in the system and hence creating surfaces that are perfectly flat or that have controlled roughness.

The team applied pressure to different-sized nanopillars with controlled roughness, and then compared the results with experiments. The simulations showed that perfectly flat surfaces lead to homogeneous deformation of the pillar, but introducing roughness induced failure of the pillar through "shear bands". These shear-bands are also observed in experiments. Shear bands start deforming a structure on a local level and continue deformation along "shear-bands," which leads eventually to fractures. The simulations revealed that a simple atomic step on the surface is sufficient to induce failure through shear banding. The type of deformation experienced by the material is highly sensitive to the small-scale features of the surface.

In order to simulate pillars large enough to get an accurate representation of the experimental nanolaminates, the researchers needed access to HPC. "We need to do large-scale simulations in our research so we can connect to the experiments," Pastewka said. "Our largest simulations contain around half a billion atoms and are carried out at the same scale as the experiments, something that can only be simulated on leading supercomputing resources such as those at GCS. Simulation results match the experiments both qualitatively and quantitatively." While the experiments serve to validate simulation results, the simulations allow monitoring the motion of every individual atom and to control every detail of the virtual reality of the simulation, including surface roughness.

These results are a first step to designing nanolaminate materials that avoid failure through shear-banding. The team's research helped clarify that shear-banding instability is tied to surface roughness. While surface roughness cannot be avoided, research should focus on designing materials that do not stabilize shear-bands. The team suggests that this could be achieved by looking for nanolaminates with components whose elastic constants match closely.

Material progress

The team's nanolaminate research has laid the groundwork for its next focus area—friction and wear. Pastewka indicated that studying friction adds a significant challenge for both experimentalists and computational scientists, but that the team's nanolaminate research can help inform models used in friction simulations. Nanolaminates are useful model systems for friction research because experimentally the deformation of the initially straight layers can be traced by just looking at them. Compared to the relatively straight, flat, and uniform geometry of the pillar surface, studying friction requires that the researchers focus on spherical objects' contacts with flat surfaces, a more complicated computational challenge.

That said, HPC can help enable insights into friction models that would otherwise be impossible to observe. "If you run a friction experiment, you can only observe things from the past because the interface is buried," Pastewka said. "If you have to wait to look at the surface after the experiment, most of the interesting things have already happened. We know that nanolaminates have this straight geometry, and trace while they deform. Friction experiments have shown us patterns and vortices that look almost like cloud formation. Looking at these nanolaminates experimentally has opened up very interesting questions, because we can see phenomena that aren't well understood, but then we can use computing to try and make sense of pattern formation." *eg*

Snapshot of the molecular dynamics simulation of the deformation of a Cu|Au nanolaminate pillar. The image shows the extrusion of a wedge-shaped region. The wedge is bounded by two shear-bands that are the origin of this failure mode. © Adrien Gola

UNIVERSITY OF STUTTGART RESEARCHERS USE HPC TO IMPROVE WIND TURBINE DESIGN

Researchers use a machine learning algorithm and supercomputing to improve energy efficiency.

Over the past several decades, green energy technologies have played an increasing role in nations' energy production. With the growing emphasis on sustainability and the need to fight climate change, green energy coming from solar panels, wind turbines, and geothermal sources will only become more important.

To increase clean energy production, researchers and companies in the green energy sector would like to be able to build larger, more efficient turbines that generate more power.

Until recently, engineers have designed relatively modest wind turbines. Typical turbines are anywhere from 50–150 metres tall, have roughly 120-metre blade diameters, and generate roughly 3 megawatts (MW) of power, or about enough power for 2,000 homes.

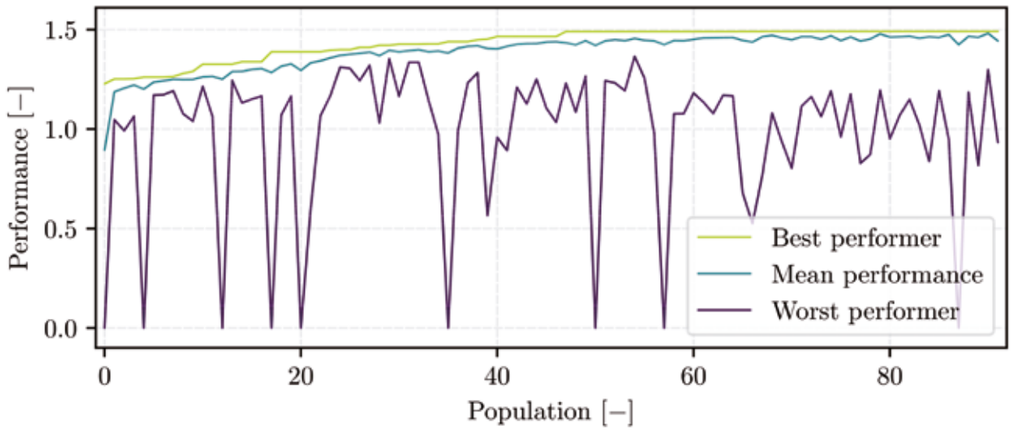
New designs are getting bigger, though. Engineers are designing wind turbines that have 200-metre blade diameters and are capable of generating 10–20 MW. At such large scales, designers have to make sure these large investments are generating energy as efficiently as possible, including mitigating inefficiency introduced by environmental factors.

To that end, a group of researchers at the University of Stuttgart has been using high-performance computing (HPC) resources at the High-Performance Computing Center Stuttgart (HLRS) to help design more energy efficient wind turbines. "When we are talking about more than 10 megawatts of power, even a one-percent increase in efficiency means a lot of additional energy and a lot of money saved," said Dr. Galih Bangga, post-doctoral researcher at the University of Stuttgart's Institute for Aerodynamics and Gas Dynamics (IAG). The team's recent research was published in the Journal of Renewable and Sustainable Energy.

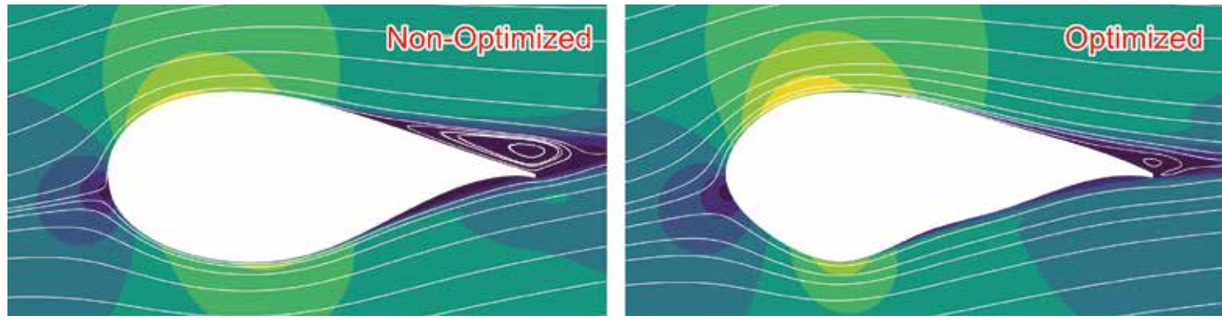
Survival of the sleekest

As wind turbines get larger in order to generate more electricity, so too must their constituent parts. Specifically, wind turbine blades need to have thicker bases, or airfoils, that attach to the main body and ultimately ensure the turbine's structural integrity. While these thicker airfoils result in a safe, stable wind turbine, they also reduce efficiency due to reduced aerodynamic performance.

The IAG team wanted to figure out how to make blades more aerodynamic without compromising a turbine's structural integrity. Unfortunately, building prototypes of many different blade designs and then running experimental tests on all models would be prohibitively expensive and time consuming.



Evolution of the optimized airfoil performance over the generation number within the genetic algorithm scheme.



Total velocity field comparison between the baseline and optimized airfoil. The optimized airfoil shows weaker separation with improved aerodynamic performance.

Computer simulation offers a much more efficient and cost-effective way to optimize blade designs. In this case, the researchers virtually created many different variations of airfoils, then ran them through a genetic algorithm—an algorithm based on the same genetic laws that, for example, an agricultural researcher might use to maximize crop yields and resilience by breeding plants with the best traits.

Much like Gregor Mendel detailed how cross pollinating pea plants with the best traits would lead to better pea plants, the team's genetic algorithm takes dozens of turbine blade designs and runs rough turbulence simulations to compare how the models perform, continuing the process until the "most optimized" candidate emerges.

Once the algorithm helps the team identify the best candidate, they turn to HPC to run a higher resolution computational fluid dynamics (CFD) simulation to verify that the algorithm was correct. In the team's paper, they were able to identify and improve the aerodynamic performance on very thick blade-root airfoil by anywhere from 2.5–7 percent. In practical terms, Bangga noted that the optimization would save roughly 195,000 Euro per year in energy savings on each 10-megawatt wind turbine using this design.

While the team can run its genetic algorithm on personal computers, the high-resolution CFD simulations needed to verify the model would be impossible without HPC. "HPC is absolutely needed to verify the huge number of databases through the use of high-fidelity simulations," Bangga said. "The access to HLRS resources is a huge benefit to us and our work."

Engineering the future

In the coming months, Bangga will be presenting the team's airfoil findings, as well as other recent simulation work they have done related to controlling airflow at the blade level, at several conferences and workshops. In addition to discussing the airfoil, the team is also discussing the role that active flow controls (AFC) can have in improving wind turbine efficiency.

While making subtle design changes to wind turbine blades' airfoils bring modest, but noticeable changes in energy efficiency, AFC is a more involved and expensive process that can lead to even greater energy efficiency. Active flow controls are similar to the flaps influencing the airflow on an airplane wing—they are controllable parts that influence how air flows around a structure or machine at a local level.

"We want our work to help engineering communities at a variety of scales, not just those that can afford large research and development budgets," Bangga said. "We want to be able to find ways that improve energy efficiency that smaller companies or local governments can afford, but we also want to find ways to maximize energy efficiency as much as possible.

In the next phase of its work, the team wants to expand the level of detail while running the genetic algorithm, allowing them to achieve a higher level of confidence in their optimization recommendations. *eg*

JÜLICH SUPERCOMPUTING CENTRE CONTINUES COORDINATION OF 6TH PRACE IMPLEMENTATION PHASE PROJECT

PRACE-6IP is the sixth in a series of the pan-European supercomputing infrastructure Partnership for Advanced Computing in Europe (PRACE) implementation phase projects. It is funded as part of the European Union's H2020 framework programme and started on 1 May 2019. Like its predecessors, PRACE-6IP is coordinated by Forschungszentrum Jülich. It has a budget of 29 million Euro, a duration of 32 months and is comprised of 30 partners. Over 220 researchers from 58 organisations (including third parties) in 26 countries will assist the PRACE Research Infrastructure (PRACE-RI) and support the PRACE users. The PRACE-6IP project continues and extends the scope of the PRACE-5IP project, based on the long-running programme's core principles:

Provision of Tier-0 service based on excellence and innovation

Regular PRACE access calls continue and constitute the bulk of the audited allocation of resources. A rigorous and proven peer-review model that meets or exceeds the standards of comparable processes in participating countries, and indeed globally, will be further enhanced. Other paths to explore are elastic/cloud services, linking with European Open Science Cloud (EOSC), and providing PRACE services to large-scale instruments (e.g. ESRF, CERN and SKA/AENEAS). PRACE-6IP will also consider how to accommodate for both existing and new Tier-0 resources (a class of leading HPC resources in Europe) in the EuroHPC framework.

Support a functional European HPC Ecosystem

The primary service provision at Tier-0 level is dependent on a well-functioning Tier-1 service at national level. This is exemplified in the domain of training where PRACE extended its Training Centres to ten PRACE Training Centres (PTCs). This will not only provide a service to the wider community but will also raise the profile of PRACE and prompt Tier-1 users to look beyond their borders in due course. In addition to training, PRACE collaborators also understand that code development is needed. PRACE will continue such work with programmes such as Preparatory Access and expert technical effort on selected codes. PRACE has also a functional programme at Tier-1 level which operates the DECI Calls. To promote industrial take-up of HPC services, in particular by small and medium enterprises (SMEs), and to broaden the use of HPC, PRACE-6IP is enhancing the SHAPE programme (SME HPC Adoption Programme in Europe).

Provide and develop tailored training and skills development programmes

PRACE-6IP will strengthen training offers that the EuroHPC Joint Undertaking—a consortium of European research organisations collaborating on developing European technology solutions for exascale computing and beyond—can rely on. The PRACE Training Centre brand will be further developed with a comprehensive training strategy, coordinated curriculums, and emerging HPC disciplines such as artificial intelligence and deep learning to be added to the training portfolio. Additionally, PRACE-6IP will produce material that can either be used directly by end-users or to support teaching staff. In particular, the project will continue to support Massively Open Online Courses (MOOCs) or blended on-site courses with some MOOC elements.

A sustainable governance and business model

PRACE 2 achieved an important step towards a viable business model by introducing the cost-sharing model, relying on contribution of all PRACE partners, with the long-term objective of providing a sustainable infrastructure. PRACE-6IP will continue to provide support and to oversee and monitor the evolution and effect of the refined and enhanced governance and business models. An expert team in business analysis and organisational support for the PRACE RI will provide support for organisational issues.

Coordination with European Technology Platform for HPC (ETP4HPC) and Centres of Excellence in HPC

PRACE's complementary working relationship with ETP4HPC is exemplified by its commonly executed Horizon 2020 project EXDCI-2. Furthermore, PRACE and ETP4HPC have eight common partners. Within the collaboration with ETP4HPC, staff will produce specific technical reports addressing emerging user requirements along with exascale performance and usability testing. In the context of the Centres of Excellence (CoEs), PRACE-6IP will further develop coordination with the CoEs, ultimately hoping to make excellent HPC activities in Europe less fragmented.

Group Picture of the 6th PRACE implementation phase kick-off Meeting in Bratislava on May 28, 2019. © PRACE

PRACE

Runtime (Funding Period):
1 May 2019 – 31 December 2021

Funding Source:
H2020

Funding:
29 Million Euro

Collaborators:
26 institutions

Support Tier-0 users and communities with novel software solutions

PRACE-6IP introduces a new Work Package to enable strategic software development that allows for implementing a long-term vision and to modernize existing software, aiming for a separation of concern between the various software layers as well as software reuse. PRACE-6IP is heavily focused on the preparation for exascale computing by developing forward-looking software solutions for exploiting massively parallel systems. The first selection process identified seven promising projects which will be supported with more than 900-person month of effort from PRACE-6IP.

Support the strategic development of a rich HPC environment

PRACE-6IP aims to support the strategic development of a rich HPC environment by delivering relevant information and guidance to the EuroHPC implementation process and to national HPC strategies in Europe. The project will deliver a comprehensive view of the world-wide HPC technology and market competition by gathering information from major systems and technology vendors.

Support new user needs, new user communities, and new applications

The extended and enhanced SHAPE programme and the Preparatory Access work are targeting new user communities, with the SHAPE programme specifically promoting industrial usage of HPC services. The PRACE training and skills development programmes offer training on all levels and with an extended range of topics in the training portfolio, new communities and user needs are well supported. The intent to develop more tailored training and on-demand events in PRACE-6IP is another way to answer to new and diverse user communities and user needs. The ambition to support Tier-0 users and communities with novel software solutions, will open up the PRACE RI to an increased number of new users and applications.

International HPC cooperation policy

The objective is to develop an international HPC cooperation policy, which will contribute to the development of an advanced research computing ecosystem both inside and outside Europe. It will include activities such as joint training events, possibly joint calls for computational resources and joint service/software development projects to address interoperability between infrastructures and identify common services.

Veronica Teodor and Florian Berberich

DCDB: MODULAR, CONTINUOUS, AND HOLISTIC MONITORING FOR ENERGY-EFFICIENT HPC

Datacenter Data Base aims at reducing energy consumption through measurement and integration.

Flagship high-performance computing (HPC) systems—such as the SuperMUC at the Leibniz Supercomputing Centre (LRZ) in Garching near Munich and its successor, SuperMUC-NG, which is almost an order of magnitude faster—consume up to 3MW of power.

"At the moment, we can do very little to decrease the power consumption of the machines, perhaps only a few percentage points," said Michael Ott. He deals with the supercomputer efficiency, measuring and recording consumption data, and leads the data analysis team in the Energy Efficiency High Performance Computing Working Group (EE HPC WG)."Working on the computer infrastructure, such as the cooling system, or optimizing programs and applications promise to help increase efficiency. In supercomputing, we need to look at all aspects to increase energy efficiency," he said.

New measurement tool, better interfaces

LRZ is involved in several projects exploring how to run supercomputers more energy efficiently. For example, LRZ's flagship supercomputer, SuperMUC-NG, is cooled with an innovative warm-water cooling solution. Now Ott and his team presented their monitoring program Datacenter Data Base (DCDB) funded in part through the H2020-supported DEEP-EST project. In addition to data from the hardware components of the system and sensors in the immediate vicinity of the computer, the program now also records metrics from the operating system and the runtime of the computer itself. Such data, in turn, indicates possibilities for adjustments that can be used to optimize the supercomputers and their energy consumption.

Optimize an application before using

In addition to data on the building infrastructure—such as water or air temperature and power consumption—the open source software DCDB collects information directly from components of the SuperMUC-NG such as processors, network cards, and storage systems, as well as operating systems, libraries and programs or applications. "If we know which components the applications use and how, we can begin to optimize the execution of these programs and thus increase the efficiency of the computer," Ott explains. "The holy grail in optimizing the operation of a supercomputer would be to know the properties of an application before it is used."

Better management, lower consumption

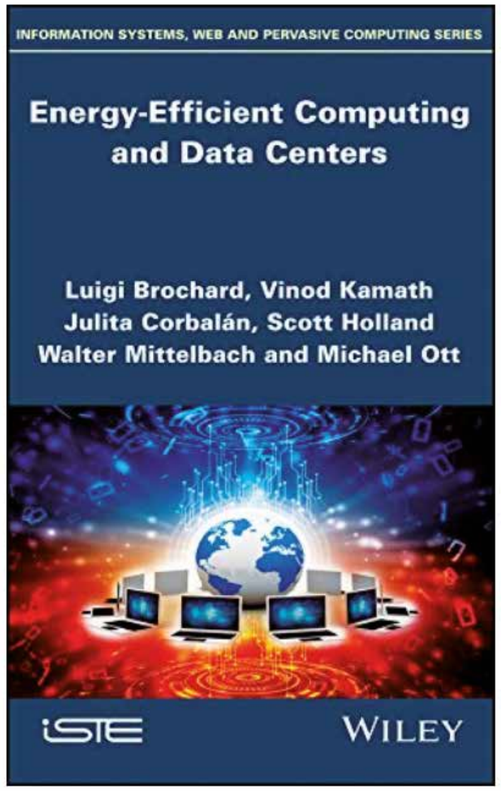
The challenge is to better coordinate the performance of supercomputers and reduce the energy consumption of applications without slowing them down. The problem is that they simultaneously access various programs and codes, most of which are not standardized and have been programmed by scientists for their own specific research goals. At LRZ, researchers each have up to 48 hours of computing time to analyse huge amounts of data or create simulations and models from their datasets. "Scientists want to use computing time to solve their research questions," Ott says. "Optimizing the runtime or reducing energy consumption is of secondary importance to them. But if data centres like LRZ understand which codes and programs work efficiently and which don't, they could help their users improve applications. They could also use this knowledge to develop and build even more efficient components for their super machines."

Preparation for Exascale

Integration also plays a role in the DCDB monitoring program: the program connects various data silos and harmonizes measured values that were previously collected from various sources. "The modular structure was important to us because it creates flexibility and allows us to connect other databases or software tools without much effort," says Ott.

The program has been made available to computer centres and researchers as open source software. Ott indicated that there is still a lack of visualization capabilities, but DCDB is already collecting information from the supercomputers like the SuperMUC-NG with the idea to apply this tool in more supercomputers and collect the experiences with it.

These data and the interfaces for optimizing energy management systems also lay the foundations for the next generation of supercomputers, the so-called exascale generation. They help to improve the tendering of technical components, IT systems, and programs through new requirements and criteria.



As part of his energy efficiency work, Ott recently contributed to Energy Efficienct Computing and Data Centers. Published by Wiley. **© Wiley**

Save energy with artificial intelligence

At LRZ the team also experiments with artificial intelligence: DCDB is not only installed on the new SuperMUC-NG, but has also been running for a longer time on the CoolMUC-3, a Linux cluster. The two computer scientists Alessio Netti and Daniele Tafani are experimenting with the first DCDB data sets produced on CoolMUC-3. Their teams are investigating whether it is possible to derive forecasts of how much power computers and applications consume in individual work steps. "If we analyse the behaviour of applications on computers, we can use artificial intelligence and machine learning to intervene and optimize energy consumption," Netti said.

Early returns are encouraging: The DCDB data not only shows energy requirements of processors in storage and computing, but also where and when applications consume particularly large amounts of power. With this knowledge, the first software and tools are being developed that analyse and optimize the DCDB data and prepare it for smart decisions. "There is a cycle of smart systems with which we can build machine learning for energy efficiency," noted Tafani. "It is quite possible to intervene in the performance of a supercomputer and coordinate individual work steps in a new or different way."

Knowledge about the work of supercomputers

It won't be long before artificial intelligence and machine learning actually control a computer's power requirements. Although the data on the machines, applications, and work steps is far from comprehensive, DCDB is busy collecting data. "The data used to estimate the computing time of applications and plan the job mix for the machine are still unreliable," Ott noted. But the good news remains: The next generation of supercomputers can be set up and controlled with the help of data in such a way that they consume significantly less energy. By then, the functionality of applications will also have been researched: Computer science has thus come a step closer to the holy grail of energy efficiency. *sv*

DCDB

Runtime:
Ongoing

Funding Organisation:
DEEP-EST Project through H2020 under grant agreement no. 754304

Funding:
500,000 Euro

Collaborators:
JSC & EPCC

HIDALGO: MERGING HPC AND HIGH-PERFORMANCE DATA ANALYTICS TO ADDRESS GLOBAL CHALLENGES

HLRS is technical lead for an EU-funded project that is exploring how simulation can address Global Challenges related to migration, air pollution, and the spread of information through social media.

As transportation and communications networks have grown, they have brought the world closer together. Whatever positive effects this has had for human development, it has also created a situation in which many local or regional challenges that societies now face have become global. Addressing climate change, fighting disease pandemics, and managing forced migration, for example, are all issues that not only profoundly affect individual nations but also cross international boundaries.

With the arrival of more powerful computing technologies, demand has been growing among governments and other decision-making entities for tools that provide real-time forecasts they can use to manage sudden challenges. As more data related to these kinds of problems becomes available, high-performance computing (HPC) incorporating simulation, data analytics, and artificial intelligence holds the potential to provide such tools. However, it can only do so if it can rise up to a range of technical challenges, such as in creating and adopting the frameworks needed to manage and analyze the large, complex datasets involved.

Late last year, the High-Performance Computing Center Stuttgart (HLRS), in collaboration with project coordinator ATOS and 11 other institutions from seven countries, began a new research project called HiDALGO aimed at achieving this goal. Funded under the Horizon 2020 Framework Programme of the European Union, HiGALGO is developing novel computational methods, algorithms, and software for modelling complex processes that arise in connection with global challenges. This includes improving simulation quality by incorporating more data sources — including collections of batched data as well as real-time streamed data — and combining existing models into more comprehensive coupled models.

A key scientific focus of HiDALGO is on the integration of high-performance data analytics with high-performance computing. As large, multidimensional data sets representing different facets of global challenges become available, it is clear that HPC will play an essential role in their processing and analysis. Developing methods to efficiently manage and analyze the enormous data sets necessary to represent such problems, as well as coupling a diverse set of data sources and computational models, are formidable challenges that HiDALGO is addressing.

At the same time, HiDALGO is supporting pilot projects in which these methods could have a practical impact. One, led by Dr. Derek Groen in the Computer Science department at Brunel University London, is focused on developing realistic models of forced migration during war.

Groen, along with colleagues Diana Suleimenova and David Bell, has been developing an open source simulation code called Flee, which predicts the destinations of refugees escaping conflict situations. Using a computational approach called agent-based modelling, Flee inserts virtual displaced persons into a simulated conflict situation; each agent moves through the virtual world based on a set of predefined rules until it reaches a safe location. Their goal is to develop a tool that decision makers could use—along with up-to-date data from conflict zones—to predict refugee movements and allocate relief resources to locations closest to a humanitarian crisis.

Although Flee was initially run on a local desktop, Groen's group is now working with staff at HLRS and the Institute of Communications and Computer Systems (Greece) to optimize the code for large-scale supercomputers, and have already been able to run it efficiently using over 400 compute cores. More computing power should enable them to develop increasingly realistic models that incorporate greater numbers of factors—such as an individual's ethnicity and language, weather conditions, or dynamic situations on the ground like border closures—that affect refugees' movements. Groen's group also works with HLRS and the KNOW Center in Austria to develop visualization tools that present the results of HPC simulations in a format that would quickly enable decision-makers to forecast and react to sudden population movements.

In other pilot projects underway as part of HiDALGO, researchers are developing tools and sensor networks to forecast and minimize air pollution in cities, and to identify and prevent the spread of false or malicious messages over online social networks. In each case, the goal is not only to address a specific global challenge, but also to produce advances in the science of high-performance computing that will improve the use of high-performance data analytics in an HPC framework.

In conjunction with the pilot projects, HiDALGO is also investigating how artificial intelligence could support the development of more realistic models. Although the specific methods are still in development, the project is exploring how AI could help simulation researchers to identify and tune parameters within their algorithms that are most significant for particular problems they are investigating; this could help accelerate the development of more realistic models.

"HiDALGO is showing that high-performance computing and high-performance data analytics are not only useful for scientific research or optimizing engineering designs," says Bastian Koller, Managing Director of HLRS. "Instead, the project demonstrates that HPC also has an important role to play in helping to address some of the most difficult challenges that we as a society are facing." *cw*

HIDALGO

Runtime (Funding Period):
1 December 2018 -- 30 November 2021

Funding Source:
H2020 (H2020-INFRAEDI-2018-1)

Funding:
7,991,500 Euro in total
1,052,375 Euro for HLRS

Collaborators:
ATOS, ECWMF

JSC HOSTS INAUGURAL EARTH SYSTEM MODELLING SYMPOSIUM

Climate and earth modelling experts converge on JSC for knowledge exchange.

Prof. Thomas Jung of the Helmholtz Centre for Polar and Marine Research was one of several researchers who gave presentations during the inaugural Earth System Modelling Symposium. © FZ Jülich

More than 40 researchers representing 6 different Helmholtz Centres converged on the Jülich Supercomputing Centre (JSC) at the Forschungszentrum Jülich (FZ Jülich) from May 27–29 for the inaugural Earth System Modelling (ESM) symposium. The ESM project started in 2017, bringing 8 different German research organizations together to better couple climate models to address grand challenges in the realm of climate modelling.

As one of the partner institutions heavily involved in the computations aspects of the project, JSC hosted the event in order to bring together researchers using the ESM partition of the JSC supercomputer JUWELS with computer scientists and JUWELS system administrators. FZ Jülich is one of the largest centres making up the Helmholtz Association of German Research Centres and JSC has a partition on JUWELS dedicated specifically to ESM work.

The symposium began with an overview on the structure, objectives, and accomplishments of the ESM project to date. Dr. Norbert Attig from JSC informed attendees about the current state of the ESM partition and explained JSC's plans to expand JUWELS in 2020.

Four ESM researchers—Prof. Thomas Jung from the Alfred Wegener Institute, Prof. Johanna Stavena from the Helmholtz Centre for Material and Coastal Research, Prof. Olaf Kolditz from the Helmholtz Centre for Environmental Research, and Prof. Stefan Kollet from FZ Jülich—gave lectures on ESM simulations representing several different scientific disciplines that all required access to the ESM partition of JUWELS. The presentations underscored the integrative aspects of ESM and the need for high-end high-performance computing (HPC) resources for earth system modelling.

During the second day of the symposium, conference attendees focused on computer architecture. The attendees held discussions about how different architectures can best support the ESM project's goals, with a special emphasis on graphics processing units (GPUs) being used in conjunction with traditional CPUs. JSC employee Dr. Andreas Herten detailed to attendees how they could make best use out of GPUs for their research. There were also two extensive hands-on sessions throughout the symposium.

As the symposium came to an end, attendees focused on additional, forward-looking aspects of the ESM project. Dr. Martin Schultz of JSC presented the Pilot Lab Exascale Earth System Modelling (PL-ExaESM) project as well as the Joint Lab ExaESM project. As a pilot lab, PL-ExaESM is funded through September 2021, and the joint lab has funding approved through 2027, and are focused on expanding current earth system modelling capabilities as well as ensuring these models are prepared for next-generation HPC architectures. *eg*

DIGITAL TOOLS FOR URBAN PLANNING

Interdisciplinary meeting explores how to better use technology to better plan cities.

Sabine Kurtz, vice president of the Baden-Württemberg state parliament, highlighted the potential of new digital tools to improve many dimensions of society during her address at the Urban Systems, Global Challenges, Digital Tools symposium. © Fabian Dembski.

In the past, locations such as a town hall, a market, or a church were places where the citizens of a city gathered, exchanged news and ideas, made decisions, and managed the tasks necessary for a community to function. As digital technologies have become more powerful and ubiquitous, however, cities have begun to take new forms. New tools for communication are changing the way we live, work, and interact with one another, while new digital methods for observation, measurement, and analysis give city planners and managers new ways to understand and address these changes.

Today, cities face the important questions of how to adapt to this new digital reality, and of how to better integrate digital technologies into planning and management. Doing so could lead to better ways to address the needs and desires of the people who live there, even if they also present new kinds of challenges.

On May 29–30, 2019, the High-Performance Computing Center Stuttgart (HLRS) hosted an international symposium titled "Urban Systems, Global Challenges, Digital Tools" to exchange insights surrounding these key questions. Held in conjunction with the conclusion of the project Reallabor Stadt:Quartiere 4.0 and in cooperation with the bwHPC-S5 Competence Center for Global Systems Science, the workshop brought together academic researchers, representatives of city governments and public utilities, citizen activists, and others with experience using new digital tools for city planning.

"Digital twins" enable visualization and improve communication

Opening the gathering, Sabine Kurtz, vice president of the Baden-Württemberg state parliament, highlighted the potential of new digital tools to improve many dimensions of society, including urban development. "In the future it is conceivable that city planning will no longer take place at the drawing board," she remarked. "This is because city planners through their research now have the ability to base their proposals on data that reflect individual lives in practical ways. They can collect, record, and analyze information about everyday life."

One such application of digital tools for city planning occurred in the project Reallabor Stadt:Quartiere 4.0, an

Prof. Claudia Yamu of the University of Groningen in the Netherlands, gave a keynote lecture and joined HLRS's Fabian Dembski and Uwe Wössner for a workshop on space syntax. **© HLRS**

experiment in using digital technologies to improve citizen engagement in city planning processes. HLRS's contribution included creating and testing a "digital twin" of Herrenberg, a city south of Stuttgart. Digital twins are digital representations of real-world objects or environments that contain models, simulations, and algorithms describing their physical counterparts. To make it easier to understand complex processes, digital twins can be implemented in virtual reality (VR).

The realistic digital twin of Herrenberg facilitated communication among city managers, architects, community members, and other stakeholders, turning abstract facts and figures into observable virtual activity. During their presentation at the symposium, Reallabor participants shared some practical lessons they learned about the challenges of communicating with city governments and community members.

Ulrich Grommel of energy company EnBW underlined the value of using digital twins in planning, describing a collaboration with the HLRS Visualization Department that took place as part of an upgrade of a hydropower plant in the Black Forest. The detailed model enabled the company to better explain to the power plant's neighbors how the project would impact the area, including its effect on noise levels, and facilitated more productive interactions with them.

Additional talks by Willi Wendt and Günter Wenzel (Fraunhofer IAO), Keynote speaker Claudia Yamu (University of Groningen), Tobias Schiller (Internationale Bauausstellung 2027), and conflict management and planning specialist Piet Sellke focused on additional examples of efforts to use digital tools to model environments, and to engage stakeholders in city planning.

The interactive city

Other kinds of technologies such as sensor networks and mobile apps can also offer tools for empirical data collection, delivering insights about how a city is experienced based on real-time feedback from city residents as they move through their urban environments.

Peter Zeile of the Karlsruhe Institute of Technology, for example, presented an overview of his research on tracking "urban emotions." By strapping on biosensors to individuals as they move through a city, his team can measure physiological changes that indicate places where people feel comfortable or anxious. This approach, he suggested, could help planners identify changes to city design that could improve feelings of wellbeing.

Using simulation to address global challenges

The growing capabilities of high-performance computing also promise opportunities to study and address economic and social problems that societies are now facing. In a talk about HiDALGO — a collaborative European project that is exploring how digital technologies could be used to better understand global systems — HLRS's Michael Gienger introduced the idea of the synthetic information system, an approach that integrates multiple data types to simulate dynamic activity patterns in populations. Participants in HiDALGO are testing this approach to assess its utility in modelling things such as forced migration. Gienger described how scientists develop synthetic information systems, as well as some challenges of developing system-level models of human behavior.

In another talk focusing on global challenges, Zoltán Horváth of the University of Györ described another HiDALGO case study, focusing on air quality modelling and management. Nikola Sander of the German Federal Institute for Population Research looked at the question of migration, presenting her latest research focused on internal movement of populations within Germany. HLRS Director Michael Resch also provided an overview of HLRS's engagement with Global Challenges, focusing on the potential use of simulation to study problems related to climate change, the development of pandemics, and the spread of fake news.

Participants in the workshop "Digital Twin Case Study: Herrenberg. Traffic Simulation in Realtime in VR Environments" were given a VR demonstration by HLRS visualization staffers Uwe Wössner and Thomas Obst. **© HLRS/Fabian Dembski**

Experiencing virtual cities

In addition to numerous lectures, the symposium also offered hands-on sessions in which participants engaged with virtual reality tools being used for city planning at HLRS. Visualization Department head Uwe Wössner led a demonstration of HLRS's 3D city modelling capabilities in the CAVE, its facility for virtual reality. Keynote speaker Claudia Yamu also joined Wössner and HLRS's Fabian Dembski for a workshop on "space syntax"; that is, how the physical shape and street grid of an urban environment affect the movement of individuals through that environment. *cw*

BAVARIA'S BILLION BILLION – THE 2019 LRZ NEXT-GEN HPC SYMPOSIUM

International high-performance computing (HPC) experts convened at Leibniz Supercomputing Centre (LRZ) on July 21, 2019 to discuss the state and future of supercomputing in the centre's annual post-International Supercomputing Conference (ISC) symposium in Garching near Munich, Germany. Titled, "Bavaria's Billion Billion: A Symposium on Exascale, Extreme-Scale AI and the Future of Science," an afternoon of presentations and discussion delved into the worldwide preparations underway for exascale-class computing, the needs and expectations of computing at that scale, the interplay of traditional modelling and simulation with emerging data-intensive workloads and workflows, and what this all means for the future of science in general, and supercomputing in particular.

It's about the users

In his introductory remarks, Prof. Dieter Kranzlmüller, host of the symposium and director of LRZ, stressed a supercomputer's top priority and purpose is to facilitate science.

"Of course it's great to have our system be among the top machines in the world," he said. "That kind of recognition attracts the talent to work on and with these systems, and, in our case, it propels the Bavarian HPC community forward. But as a center with a broad user base and application mix, our forefront concern must always be on ensuring usability."

The balance and value of achieving a Top 20 system while focusing on delivering user value was punctuated by Andrew Jones from NAG (UK) and further noted by Jeff Hittinger, both staff members at the Center for Applied Scientific Computing at Lawrence Livermore National Laboratory (LLNL) in the USA. "You can be a large center and leader in the field of supercomputing for more than 25 years without seating a first-place machine for a while, but having various machines in the Top 20 or even Top 50 that are geared towards the different requirements of different user groups at a centre is paramount to the science," Hittinger stated.

Diversity of architecture has both up and downsides

The current architectural diversity present in the community led attendees to discuss factors driving the increase in heterogeneous architectures and the pressures predicted to cull the processor and accelerator landscape spawned several thoughts.

Prof. Martin Schulz of the Technical University of Munich named the end of Moore's law, power limits, and frequency limits as just a few of the challenges in reaching exascale computing. He noted that the HPC community has to better understand what kinds of architectures applications will be needed and how important it is to find the best architectural fit for a certain centre.

Dr. Fred Streitz of LLNL added that artificial intelligence and machine learning have created a lot of space for specialization.

Deal with the data

Prof. Dr. Sean Smith of the National Computational Infrastructure in Australia underlined examples highlighting the emergence of huge amounts of data in research projects and how this affects the interplay of HPC and data storage and data analytics. Earth observation data, genome data, and climate model data are growing at exponential rates at his facility. However, the complexity in deawwling with it comes not only from storing it. Smith explained that more effort needs to be put into the management of the data, and the data services which allow analytic processes to access and manipulate it.

It takes a supercomputing village

Following the discussion about accelerator-based systems, the integration of artificial intelligence and machine learning methods, as well as data analytics and data storage challenges, guests in the audience wondered how to deal with the ever-growing complexity of future systems. Schulz expects a shift in the balance of power between vendors and the HPC centres. For the centres to be better equipped for fulfilling their new role, intensifying international collaboration will be key. Another aspect all speakers and panelists could agree on—there is still room for closer collaboration.

Supercomputing is a people business

Attendees had a lot to consider after detailed discussions on future systems, potential architectural changes, the convergence of HPC with data analytics and AI as well as application readiness.

Supercomputing and emerging technologies surrounding the field do not add value on their own—it is a field driven by human innovation, Kranzlmüller said, drawing a large circle of people to include. He continued, noting that the HPC community knows the need for more highly qualified computational scientists and there were already programs in place to help address this need. However, many in the HPC community rarely think about the entire HPC ecosystem and the staff needed to develop it. Kranzlmüller added that building this ecosystem is one of the three pillars of the German national HPC strategy.

Laura Schulz and Sabrina Schulte

Distinguished presenters and panelists from the USA and Europe took part in discussion on the future promise and challenges of HPC as part of the Bavaria's Billion Billion event, hosted at LRZ. **© Alessandro Podo**

GERMAN AEROSPACE AND HPC JOIN FORCES FOR GLOBAL CHANGE RESEARCH

On May 27, representatives from the German Aerospace Agency (DLR) and the Leibniz Supercomputing Centre (LRZ) signed an agreement to partner on the Terra_Byte project. The multidisciplinary project focuses on interpreting data coming from sources ranging from satellite imaging data to social media. The project is focused on better recording and understanding global change in a broader sense. Researchers use imaging data from satellites to study natural disasters, for instance, but understanding large-scale ecological change requires information coming from the ground as well—social media posts, for instance, provide a huge potential for information about these events on a local level. In both cases, though, researchers must be able to efficiently sift through massive amounts of loosely connected data coming from myriad sources.
In the partnership DLR will be primarily focused on research and algorithm development, and LRZ will be focused on implementing large-scale, reliable IT services, optimizing data analysis and data management processes, and incorporating artificial-intelligence and big-data-related processes. The partner organizations plan to analyze 40 petabytes of data across thousands of cloud-based computing cores, and will be implementing the first stage of expansion by the end of 2020.

SENSATIONAL IMAGES FROM SPACE

Blue clouds and green clumps embodying gas structures, or magnetic fields in silver and orange: these stunning images illustrate the evolution of interstellar turbulence. A team of researchers led by astrophysicist Salvatore Cielo from the Leibniz Supercomputing Centre (LRZ) illustrates with unprecedented resolution what happens when the explosions of supernovae and stellar winds form stars. The 5-minute film produced in Garching, with its fascinating images and physical formulas, has been shortlisted as Best Scientific Visualisation Showcase at SC19 conference in Denver, running November 17–22 2019.
This is the largest visualization of such a cosmic event ever shown, produced at the LRZ based on simulations by the astrophysicist Christoph Federrath of the University of Canberra. The LRZ computing experts and astrophysicists Salvatore Cielo and Luigi Iapichino used SuperMUC-NG for the renderings, which were then assembled and edited for the final video by visualization specialists Elisabeth Mayer and Markus Wiedemann.

PROF. KRANZLMÜLLER APPOINTED TO GAUSS ALLIANZ BOARD OF DIRECTORS

Professor Dieter Kranzlmüller, Director of the Leibniz Supercomputing Centre in Garching near Munich, was appointed to the Board of Directors of the German “Gauß-Allianz” in Autumn 2019. The Gauß-Allianz is a non-profit association based in Berlin and represents 21 scientific high-performance computing centres of the Tier-2 category in Germany. Being also Chair of the Board of Directors for the Gauss Centre for Supercomputing, Germany’s alliance of the three leading supercomputing facilities, Kranzlmüller’s main task lies in integrating the activities and strategies of Germany’s Tier-1 and Tier-2 high performance computing centres.

SECURE AND SERVICE-ORIENTED: LRZ ISO CERTIFIED

The Leibniz Supercomputing Centre is ISO certified: The data stored on the LRZ servers in Garching is secure, and its IT services are processed efficiently and transparently. As the first scientific supercomputing centre in Germany, the LRZ has been certified according to the criteria of the International Organization for Standardization (ISO) with regard to two standards: “In such an information-driven area as science and research, security and confidentiality of sensitive data have top priority,” says Professor Dieter Kranzlmüller, Director of the LRZ. “With the ISO certifications, we are sending a strong signal to the users of our services, our partners, and our employees.” The LRZ spent a year and a half refining the technology and processes for the ISO 27.001 and ISO 20.000 certificates, and also had around 250 employees trained in data protection and security.

HAICU LOCAL UNIT AT FORSCHUNGSZENTRUM JÜLICH: COOPERATING ON MACHINE AND DEEP LEARNING

With the Helmholtz Artificial Intelligence Cooperation Unit (HAICU), the Helmholtz Association aims to build a future-oriented network for basic and applied artificial intelligence (AI) research. As an interdisciplinary AI platform, HAICU will integrate the Helmholtz Association’s outstanding science portfolio, excellent infrastructures, unique data sets, and extensive methodological competence in order to position the Helmholtz Association at the forefront of AI research. HAICU’s central unit is located at Helmholtz Zentrum München. Other Helmholtz centres have been selected as hosts for the five local HAICU units, with one of them located at Forschungszentrum Jülich. Two teams from the Jülich Supercomputing Centre (JSC) will work close together in the HAICU Local unit at Jülich. The research focus of Cross-Sectional Team Deep Learning (CST-DL) will be on enabling large-scale continual learning on modular supercomputers, which includes integrated simulation-learning closed-loop systems, methods for transferable, multi-task unsupervised and reinforcement learning, and distributed neural architecture search. High-Level Support Team (HLST) will focus on software development, data set creation and maintenance and research support for machine/deep learning. www.haicu.de

HAICU HELMHOLTZ ARTIFICIAL INTELLIGENCE COOPERATION UNIT

INTERNATIONAL INDUSTRIAL SUPERCOMPUTING WORKSHOP 2019

On September 25–26, the High-Performance Computing Center Stuttgart (HLRS) welcomed representatives of supercomputing centers and industrial users of supercomputing for the seventh International Industrial Supercomputing Workshop. In addition to HLRS, the meeting attracted representatives from the Barcelona Supercomputing Center (Spain), Edinburgh Parallel Computing Center (UK), Bosch (Germany), CINECA (Italy), SICOS-BW (Germany), KISTI (South Korea), Toyo University (Japan), Oak Ridge National Laboratory (USA), National Center for Supercomputing Applications (USA), Leibniz Supercomputing Centre (Germany), and PDC Center for High Performance Computing (Sweden). The participants exchanged insights about how their organizations facilitate the integration of HPC into industrial R&D, pointed to opportunities that data generating technologies offer for the private sector, and highlighted unique challenges that industry faces as supercomputers approach exascale. Also discussed were emerging needs in industry for support with artificial intelligence and high-performance data analytics.

‘OUMUAMUA – OUTER SPACE’S SHORT VISIT TO OUR SOLAR SYSTEM

In 2017, ‘Oumuamua became the first recorded object from interstellar space to pass through our solar system. It immediately triggered considerable speculation due to its extraordinary characteristics: was it more like an asteroid, a comet, or something else? In a study recently published in Nature Astronomy, an international team of scientists from Europe and the USA, including Susanne Pfalzner from JSC, analysed data collected on ‘Oumuamua. What is particularly baffling is that while ‘Oumuamua appears to accelerate along its trajectory—behaviour typical of comets—the astronomers were unable to detect the gas emissions usually associated with this acceleration. The authors assume that the physical processes observed here are common throughout the universe,universal, but that they have simply not yet seen anything like ‘Oumuamua in our solar system. However, this study showed that ‘Oumuamua is of completely natural origin.

HLRS PARTICIPATES IN STUTTGART'S FIRST-EVER "SMART AND CLEVER" SCIENCE FESTIVAL

HLRS had an active role in Stuttgart's first-annual "Smart and Clever" science festival, which ran June 26–July 6, showcasing 75 different Stuttgart-based research organizations across 78 different events. The event aimed at showcasing the important role of scientific research in Stuttgart and highlight solutions researchers in Stuttgart are developing to address pressing societal problems. Prof. Michael Resch, Director of HLRS, participated in a discussion on artificial intelligence with Baden-Württemberg Minister for Science and the Arts Theresia Bauer and experts in the field. Dr. Andreas Kaminski, Group Leader of HLRS's Philosophy of Science and Technology of Computer Simulation, participated in a panel discussion after a public viewing of Friedrich Dürrenmatt's classic play The Physicists, focusing on themes surrounding ethical responsibilities of scientific research and disruptive technologies. The HLRS visualization department also presented an exhibit in Stuttgart's city hall that demonstrated how they are using virtual reality to help improve public engagement in city planning.

ON4OFF PROJECT – ARTIFICIAL INTELLIGENCE TO SUPPORT REGIONAL RETAILERS

The ON4OFF project, funded by the state of North Rhine-Westphalia for three years, wants to create smarter links between brick-and-mortar retailers and their online offerings, and thus make the regional retail sector more competitive with online shops. The plan is to make this possible through the use of artificial intelligence intertwined with a systematic use of adaptive case management algorithms developed by the University of Duisburg-Essen. JSC, together with Adesso AG, is responsible for the development of machine learning algorithms that will improve customers' shopping experience in the retail sector. The ON4OFF project will take advantage of JSC's modular supercomputing approach to gain customer insights faster. It will also enable a new culture of data sharing between retailers and consumers, and a smooth transition of data flows between online and offline customer data and shopping processes. Project partner Parfümerie Pieper will implement the concepts in its flagship stores, while the overall project will work on broadening concepts for application in other commercial sectors. www.on-4-off.de

NEUROSCIENCE STUDENTS INTRODUCED TO THE WORLD OF SUPERCOMPUTING AT HPC FOR NEUROSCIENCE WORKSHOP

Neuroscience research has become increasingly interdisciplinary in recent years. New imaging technologies deliver ultra-high resolution images, and new simulation technology enables scientists to simulate larger and more detailed neural networks. Therefore, HPC and good data management strategies are becoming indispensable for this community. The SimLab Neuroscience at JSC organised the workshop "HPC for Neuroscience" in July as part of the education programme of the European Union-funded Human Brain Project, which offers interdisciplinary training for students. The workshop taught supercomputing basics to start using HPC systems for (neuroscience) research and to prepare students for more advanced training courses offered by JSC. In addition to general HPC-related lectures and hands-on sessions, the programme included introductions to community-specific simulators and visualisation tools. The workshop was very well received by the participants and will likely be repeated.

BAVARIA'S MINISTER FOR SCIENCE SIBLER VISITS LRZ

On September 11, 2019, the Bavarian Minister for Science, Bernd Sibler, visited the Leibniz Supercomputing Centre and immersed himself in virtual worlds at the Centre for Virtual Reality and Visualization (V2C). LRZ Director Prof. Dieter Kranzlmüller informed Sibler about the modern technologies and project installations being developed in the V2C, as well as about the diverse fields of application of the new supercomputer SuperMUC-NG - one of the nine fastest computers in the world as of the June 2019 Top500 list. Further topics discussed during the visit were the next generation of supercomputers—so-called exascale computing—and future computing, which deals with emerging technologies, artificial intelligence, and quantum computing. Sibler was impressed: "Bavaria's digital future is being shaped here! The Leibniz Supercomputing Centre is one of the internationally visible beacons of the Bavarian research landscape. It is doing pioneering work in the field of AI research and quantum computing technologies," he said.

HLRS STRENGTHENS COLLABORATIONS IN ASIA

This summer, HLRS deepened its collaborations with Chinese research institutions, signing memoranda of cooperation with the supercomputing center of the University of Science and Technology of China (USTC) and the National Supercomputing Center Guangzhou (NSCC-GZ) at Sun Yat-sen University in Guangzhou, China. The agreement with USTC, which runs for three years, will facilitate information sharing on topics of common interest through exchange of scientists, periodic meetings, and collaborative research projects. NSCC-GZ is home to Tianhe 2A, one of the fastest supercomputers worldwide, and is a leader in high-performance computing in China. The Guangzhou center and HLRS pledged to exchange researchers and hold workshops together in the coming years.

NEW SUPERCOMPUTING-AKADEMIE COURSE FOR IT ADMINISTRATORS IN INDUSTRY

On September 16, the Supercomputing-Akademie launched a new continuing education training module focused on the planning and operation of high-performance computing (HPC) cluster systems. Titled "HPC Clusters: Plan, Build, Run," it addresses the needs of IT managers, administrators, computer scientists, and others involved in the coordination of HPC resources in industrial settings, either on their own HPC clusters or in the cloud. The new course, organized in a blended learning format that combines in-person and online learning, is the third in a growing portfolio of training offerings being developed by the Supercomputing-Akademie — a collaboration among HLRS, the University of Freiburg, and Ulm University that is supported by the Baden-Württemberg Ministry for Science, Research and the Arts and the European Social Fund. Past courses offered by the Supercomputing-Akademie have provided training in parallel programming and simulation, while additional course modules addressing performance optimization, sustainability in HPC, and visualization are currently in development.

STAFF SPOTLIGHT: PASSION FOR TRAINING AND EDUCATION

Dr. Volker Weinberg, Leibniz Supercomputing Centre

From early on in his education, Volker Weinberg had eclectic learning interests—he began learning Japanese at eight years old, developed a passion for training and education working for the Munich Volkshochschule (adult education centre) during his year of civil service between high school and university, got inspired to study physics by similarities between the Asian worldview and modern quantum field theory, and found an interest in scientific computing shortly after beginning his university studies.

Ultimately his passion for educating others has proven to play the major part in his role at the Leibniz Supercomputing Centre (LRZ) in Garching near Munich. As the HPC Training and Education Coordinator at LRZ, Weinberg uses not only his background in elementary particle physics research, but also his deep interest in training and education to help coordinate and bolster the LRZ and Gauss Centre for Supercomputing (GCS) training programs, ensuring users are making the best use possible of their allocations on GCS supercomputing resources.

"From early on, I was interested in education and training in general," Weinberg said. "Even during my civil service year at the Munich Volkshochschule, I was involved in the course program organization for seniors and did some teaching myself."

As a physics student at the Ludwig-Maximilians-Universität, Munich he worked for the faculty's computer cluster, leading to many interactions with IT experts at LRZ.

Weinberg's interests in physics, computing, and education merged during his PhD studies at the Free University of Berlin (FU) and the research center DESY. In his research Weinberg explored the vacuum structure of lattice quantum chromodynamics (LQCD) a theory focused on using advanced numerical simulations to understand how quarks and gluons, as building blocks of matter, behave and interact. His research team had large allocations on the supercomputers at the Jülich Supercomputing Centre (JSC) and LRZ, and a lot of expertise in high-performance computing (HPC). Not only did LQCD help make Weinberg aware of the world of HPC early in his career, but it also informs how he approaches the GCS training program. "I think it is really important for someone responsible for coordination of the training program to go through all those difficulties of highly demanding and challenging real-world simulations on different platforms in order to understand the needs of our users and offer courses on relevant topics," he said.

Between his experience with cutting-edge LQCD simulations at DESY, teaching undergraduate students in computing at the FU, and his time organizing adult education, Weinberg sees value in having education programs touch on a variety of knowledge levels and skill sets, and he brought that view to the GCS and LRZ training programmes. He pointed out that the three GCS centres have a wide variety of educational offerings, and that there is strength in that diversity.

As a hosting member of the Partnership for Advanced Computing in Europe (PRACE), GCS offers advanced training courses for European researchers looking to further refine and improve their HPC knowledge and code performance. On the other hand, the individual centres partner with local universities and industries to regularly host workshops aimed at training working professionals how to incorporate simulation into their workflows.

Weinberg also noted that while staff members at the three centres excel at providing training for their own unique architectures on their respective leading (Tier 0) HPC systems, a lot of training focuses on parallelizing and optimizing codes for HPC environments generally. This encourages the GCS centres' training staffs to collaborate and coordinate in their training activities. Weinberg especially enjoys the fruitful collaboration in training within GCS, but also with other European supercomputing centres, especially in Austria, Czech Republic and Finland.

There is more to a successful HPC training program than just making sure users are prepared to use a centre's current supercomputer, though—HPC centres want ensure that users can navigate and take advantage of new and emerging technologies as well. The GCS centres are at the frontline of emerging technologies' developments, including the rise of artificial intelligence (AI), machine learning, and data analytics applications as well as relatively new HPC architectures, such as those employing GPUs or other accelerators.

"In the last two years, the rise of AI, machine learning, and data analytics has been one of the biggest changes in how we think about HPC training," he said. "There is an immense interest from our users in these fields. Four LRZ colleagues, including myself, were recently certified by NVIDIA as University Ambassadors to teach GPU programming and deep learning. When we offer courses on these topics, we usually get more than 100 responses. These topics have gotten so hot that we are regularly being invited to HPC centres and universities internationally."

While it is important to grow and respond to user needs related to training for new and emerging technologies, Weinberg also emphasized that one of the most important aspects of continued success for the GCS training program revolved around sticking to parallel computing fundamentals. "Emerging technologies, they are always coming and going," he said. "Having well-established courses on programming standards like MPI and OpenMP, while also following current trends, is really important. Even with new and emerging technologies, it is important to adapt these programming models for these new architectures." Recently he became LRZ representative in the OpenMP architecture review board (ARB) and language committee to actively influence the future of the OpenMP standard in this direction. Learn more about the GCS training program and schedule on pages 38-39. *eg*

EXTREME-SCALE HPC EXPERT TALKS NEXT-GENERATION ARCHITECTURES, PROMISES AND CHALLENGES OF EXASCALE

Long-time GCS collaborator and user Prof. Ulrich Rüde discusses his views on the future of supercomputing.

In his 30-year career as a computer scientist, applied mathematician, and professor, Ulrich Rüde has worked with scientists and engineers from many different research backgrounds, helping them use simulation in their work as efficiently as possible. Regardless of the science domain, though, Rüde knows that researchers want to spend most of their time solving science problems rather than figuring out how to best compile or port their respective codes to a specific high-performance computing (HPC) environment.

Rüde and his closest collaborators work on the frontiers of computer science. Recently, for example, he helped a team from his home university, the Friedrich-Alexander-Universität Erlangen-Nürnberg (FAU) and researchers at the Technical University of Munich (TUM) to solve the largest-ever finite element system on a supercomputer. The calculation included more than 10 trillion (10^{13}) unknowns in the simulation, requiring 80 terabytes of data for the solution vector alone. Finite element systems are central to many computational engineering and science applications.

Rüde has also recently collaborated with numerical analysts from TUM and geophysicists from the Ludwig Maximillians University Munich (LMU) in using Gauss Centre for Supercomputing (GCS) high-performance computing (HPC) resources at the Leibniz Supercomputing Centre (LRZ), the Jülich Supercomputing Centre (JSC), and the High-Performance Computing Center Stuttgart (HLRS). His collaborations have focused on developing new codes for studying the dynamics below the Earth's surface. Specifically, the team is studying mantle convection, the process through which the Earth's mantle moves. Such motion, driven by enormous subsurface pressures and forces, takes place at speeds of centimeters per year, and can eventually lead to the formation of mountains and earthquakes.

As the GCS centres transition to computing architectures that are scaling toward exascale computing—that is, computers capable of at least one quintillion (a 1 followed by 18 zeroes) calculations per second—we spoke with Prof. Rüde to get his thoughts on the challenges and the promises of the future of HPC.

? GCS: Prof. Rüde, as a computer scientist you have focused on HPC, but have never restricted your work to a single application. What advantages does this provide in terms of solving problems of efficiency, scalability, and portability?

UR: Computer science expertise is necessary to design the application frameworks of the future. Those who are coming from an application background or mathematics alone often do not have knowledge about computer architectures and algorithms; they often lack expertise in software engineering. When working with a research team, we try to pull in a lot of technology, whether that is advanced algorithms, compilers, performance engineering, or novel code generation techniques.

Of course, some disciplines have invested heavily in these directions as well, but our work is special, as we approach applications not purely in terms of code development. We want to understand the application and the models behind it, and to find the most efficient algorithms that serve the needs of the target discipline. Computational science is the combination of all of these things. It is neither a sub-branch of the target discipline, nor mathematics, nor computer science. We create new HPC simulation methods by integrating all these components.

? GCS: Why do you think science needs exascale computing, and what do you see as the biggest challenges associated with being ready for exascale?

UR: One example that illustrates the need for exascale computing can be seen in geophysics applications such as the ones I have been working on recently, which rely on a lot of uncertain data. Ideally we would like to resolve the whole planet with 1-kilometre resolution. But since Earth has a volume of one trillion cubic kilometres, this would mean using computational meshes in our simulations with this many cells. In every time step a system of this size must then be solved, which is an enormous undertaking. To handle the uncertainties of available input data and the need to compute backwards in time, we will need even more computing power. For this reason, I would say that exascale is the next step, but it is not the last step.

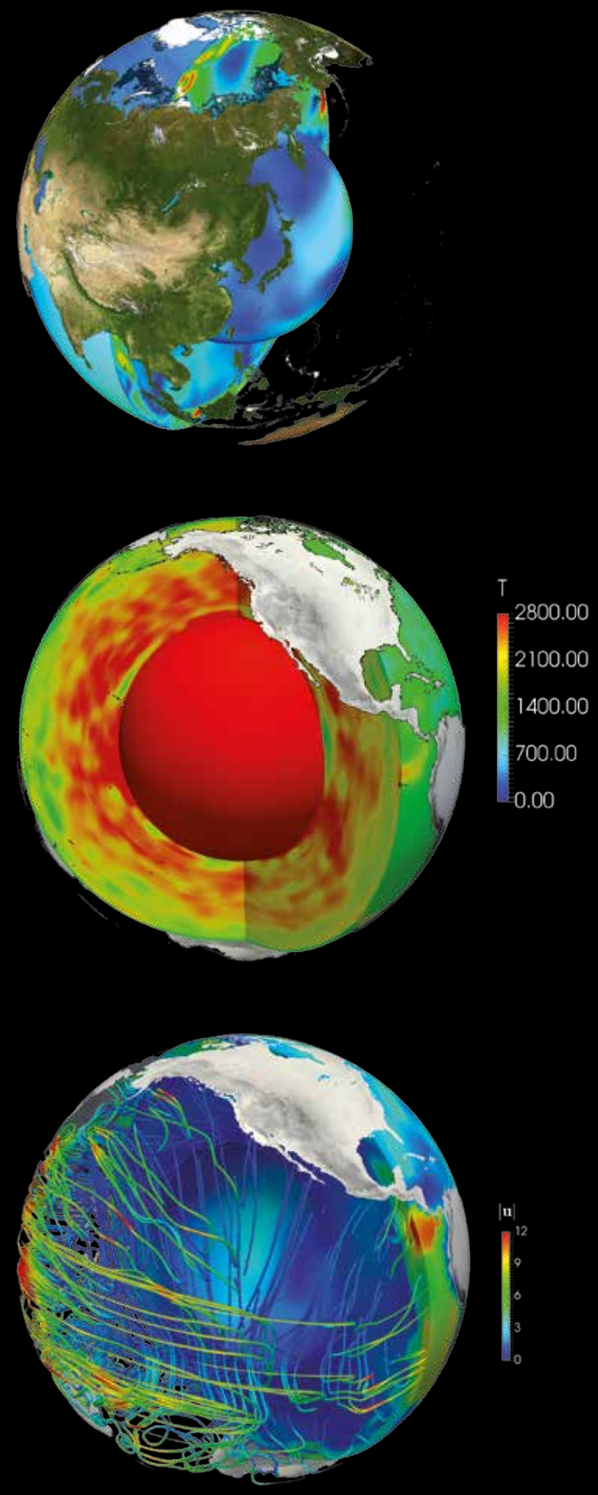
In my view, one of the biggest challenges to exascale stems from the shift in architectures from classical CPU-only models to accelerator-based architectures. I have been involved in several projects about exascale computing preparedness, for example under the auspices of the DFG priority program SPPEXA, but what I often see is that, despite talking about how exascale is fundamentally different from what we have been doing, most projects are making incremental changes to their codes. New architectures can demand significant reworking of codes, and people understand that if they have an old code, they need to do something about it, but hardly anyone is starting to write completely new code.

The end of Moore's Law [a 1960s-era theory noting that the number of transistors on a circuit board was doubling every year, leading to a steady, exponential increase in computing power] may lead to a more fundamental shift in computing than exascale. To use an analogy from economics, we have developed HPC applications in a state of constant deflation. We haven't spent as much effort developing better algorithms because next-generation hardware will seemingly always be cheaper and faster than the current generation. Some people think there will be a replacement for Moore's Law, such as quantum computing or another avenue, but I think computer science is going to become more like traditional engineering fields, where much more effort must be put into making the most efficient use of the resources that are available, even when the gains are only modest.

? GCS: What do computing centres, such as the GCS member centres, need to be doing to support their users during this transitional period in HPC?

UR: First of all, I think that in terms of access to computing power, we have been doing well in Germany. Due to demand, researchers may not always get as much time as they hope for, but we have up-to-date machines and researchers can focus on their work. The GCS centres also seem to work well together, and I think it helps to have the centres taking turns when it comes to investments in hardware. Our goal should always be to have all relevant architectures at an internationally competitive level. And efforts must be undertaken to stay competitive with what is happening in the USA and Asia.

If I am right in my thinking about the end of Moore's Law, though, the centres are going to have to make a bigger shift to focusing on software and algorithms rather than hardware. The distributed research funding in Europe means that often a lot of money goes into method and code development, but if nothing else happens and, for example, a project isn't renewed, then the knowledge gained over the course of the project can get lost. In the coming years an alliance of HPC centres and GCS must develop a new kind of infrastructure to support further developing software and retaining the knowledge base that went into the development of scientific software. This is a very fundamental issue that will only be resolved through a combined effort of research institutes, computer centres, and funding institutions. I see an increasing awareness of the problem, but not yet a good solution. There are many focused application communities that could benefit from institutional support for HPC software sustainability. *Interview by Eric Gedenk*



Recently, Prof. Rüde has been collaborating with researchers to run extreme-scale simulations of inner-Earth dynamics. © FAU

FAREWELL SUPERMUC

The recently decommissioned supercomputer SuperMUC helped researchers in Bavaria and beyond reach new computational heights.

Between 2012 and 2018, SuperMUC phase 1 and phase 2 enabled over 2,000 researchers from 23 nations to achieve scientific breakthroughs in countless research fields. The machine was decommissioned this year. **© LRZ**

It weighs as much as 42 elephants and is now a thing of the past: After computing more than nine billion core hours and completing 6.3 million jobs for researchers, the 250-ton SuperMUC is being decommissioned. The Free State of Bavaria and the German federal government invested 83 million Euro in SuperMUC Phase 1 and Phase 2 at the Leibniz Supercomputing Centre (LRZ) in Garching near Munich. "Information Technology (IT) has developed into a backbone service for science during SuperMUC's service," says Professor Dieter Kranzlmüller, director of the LRZ. "As an IT service provider, we support and advise scientists in the modelling of data and the development of applications."

6 Computer Years Replace 24,000 Human Years

Between 2012 and 2018-2019, SuperMUC was used by 2,230 researchers from 23 nations for 820 different projects. The largest project, "Observable Nucleons as a Test Case for (Particle) Physics Beyond Standard Models," computed almost 212 million core hours. As a comparison, at least 300 people would have had to have calculated for 80 years in order to evaluate the motion data of neutrons and protons. These calculations help to determine the existence of dark matter provide ideas for high-tech materials.

SuperMUC (Phase 1 and 2 combined) was built from 12,525 nodes and around 240,000 computing cores. Arranged in 238 racks and networked with more than 250 kilometers of fiber-optic cable and 46 kilometers of copper tubing, the computer achieved 6.8 petaflops of peak performance. In 2012, the first implemention of SuperMUC– SuperMUC Phase 1– was ranked the fourth fastest computer in the world, in 2018 it only reached 64th place. Computer records are more volatile than sports records.

Big Data in Science

When SuperMUC was installed, computational fluid dynamics (approx. 2.16 billion core hours), astrophysics (1.9 billion hours) or bioinformatics (1 billion hours) produced so much data, that only a supercomputer was able to evaluate them. Digitalisation has led to an explosion in the volume of data in other domain sciences as well. SuperMUC calculated for climatologists (153 million computing hours), plasma physicists (80 million), engineers (structural mechanics) and materials experts (about 35 million each) and most recently even for economic specialists (10,000 hours) and chemical physicists (42,239 hours).

During SuperMUC's years of operation, LRZ supported the researchers in their endeavours—over the course of 150 workshops and courses, 4,000 specialists were qualified to work on SuperMUC. In addition, science and research have become more international and diverse: SuperMUC processed almost 5.4 million runs from within Germany, mainly from Bavaria (4.5 million) and North Rhine-Westphalia (171,426). But 10 percent of its computing time was awarded to researchers abroad, mainly Italy (34,381 jobs) and France (34,170).

Excellent Results Efficiently

SuperMUC needed an average of 30 TWh per year—about as many as 7,500 four-person households or about twice the city of Garching. Nevertheless, SuperMUC recycled water and heat in as many ways as possible—it saved Bavaria and the federal government more than 12 million Euro in electricity costs due to award-winning innovative technology. *eg*

POWER & ENERGY EFFICIENCY

30 TWh
power consumption per year

Energie consumption of a city with 30,000 inhabitants

1,06
Power Usage Effectiveness

SYSTEM OVERVIEW

6.8 PFlop/s peak performance
245,512 cores
25,428 processors
12,525 nodes
238 racks

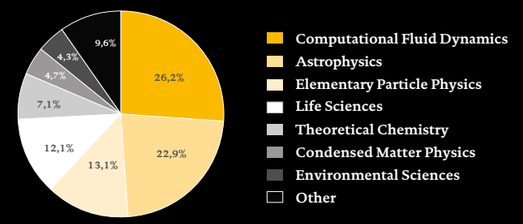
TRIVIA

Weight: 250 tons = 42 African elephants
150 courses taught on SuperMUC
more than 4,000 people educated

CABLE TANGLE

4 km of plastic hose
46 km copper pipes
250 km optical fibre cable

DOMAIN SCIENCE



ACHIEVEMENTS

9.5 billion core hours in total
= 1,099,537 years
6.3 million jobs processed
820 research projects
2,230 scientists
Largest research project:
– 7,200,000 core hours
– 115 terabyte of data
– 32,768 Cores used

COSTS

€83 MIO
=1,900 kilo of gold

€2 Mio Year

Power savings = €2 Mio per year
or €12 Mio over the entire time

TRAINING CALENDAR
HPC COURSES AND TUTORIALS

Course / Workshop Title	Location	Date
Software Development in Science	Jülich	Nov 19-20, 2019
Advanced C++ with Focus on Software Engineering	Garching	Nov 20-22, 2019
C++ Language for Beginners	Garching	Nov 25-29, 2019
HPC & ANSYS Fluent	Jülich	Nov 26-28, 2019
Advanced C++ with Focus on Software Engineering	Stuttgart	Nov 26-29, 2019
Introduction to the programming and usage of the supercomputer resources at Jülich	Jülich	Nov 28-29, 2019
Advanced Parallel Programming with MPI and OpenMP	Jülich	Dec 2-4, 2019
Python for Beginners	Garching	Dec 3, 2019
Node-Level Performance Engineering (PRACE course)	Garching	Dec 3-4,2019
Molecular Modelling with Schrödinger-Suite	Garching	Dec 4-5, 2019
Fortran for Scientific Computing	Stuttgart	Dec 9-13, 2019
Programming in C	Jülich	Jan 13-22, 2020
Introduction to Hybrid Programming in HPC and Scaling Workshop	Stuttgart	Jan 27-31, 2020
Parallel I/O and Portable Data Formats (PRACE course)	Jülich	Jan 27-29, 2020
Introduction to parallel programming with MPI and OpenMP	Jülich	Feb 3-7, 2020
ESM user forum	Jülich	Feb 4-6, 2020
Parallel Programming with MPI & OpenMP and Tools	Dresden	Feb 10-14, 2020
Fundamentals of Accelerated Computing with CUDA and OpenACC	Ostrava	Feb 10, 2020
Programmierung in Fortran	Jülich	Feb 10 - Mar 6
Parallel and Scalable Machine Learning (PRACE course)	Jülich	Feb 17-19, 2020
Introduction to Computational Fluid Dynamics	Siegen	Feb 24-28, 2020
Programming with Fortran	Garching	Feb 26-28, 2020
NIC Symposium 2020	Jülich	Feb 27-28, 2020
Usage of VTK for scientific-technical visualisation	Jülich	Mar 2020 (tbc)
Introduction to Python	Jülich	Mar 2020 (tbc)
Intermediate C++ with Focus on Software Engineering	Stuttgart	Mar 3-6, 2020
Parallel Programming of High Performance Systems	Erlangen	Mar 9-13, 2020
Introduction to ParaView for the visualization of scientific data	Jülich	Mar 12, 2020
Introduction to Cluster Filesystems	Stuttgart	Mar 12, 2020
Introduction to ANSYS Fluid Dynamics (CFX, Fluent) on LRZ HPC Systems	Garching	Mar 16-20, 2020
CFD with OpenFOAM®	Stuttgart	Mar 16-20, 2020
Iterative Linear Solvers and Parallelization	Stuttgart	Mar 23-27, 2020
Parallelization with MPI and OpenMP	Mainz	Mar 30-Apr 2
Introduction to Hybrid Programming in HPC (PRACE course)	Garching	Apr 20-21, 2020
Fortran for Scientific Computing (PRACE course)	Stuttgart	Apr 20-24, 2020
Interactive High-Performance Computing (PRACE course)	Jülich	Apr 21-22, 2020
Deep Learning and GPU programming workshop (PRACE course)	Espoo	Apr 22-24, 2020
From zero to hero, Part I: Understanding and fixing on-core performance bottlenecks	Jülich	Apr 28-29, 2020
Advanced C++ with Focus on Software Engineering	Stuttgart	May 5-8, 2020
Programming in C++	Jülich	May 11-14, 2020
VI-HPS Tuning Workshop (PRACE course)	Stuttgart	May 11-15, 2020
Introduction to Deep Learning Models (PRACE course)	Jülich	May 12-14, 2020
Introduction to the usage and programming of supercomputer resources in Jülich	Jülich	May 18-19, 2020

VISIT INSIDE ONLINE
FOR DETAILS

Course / Workshop Title	Location	Date
Data Analysis and Plotting in Python with Pandas	Jülich	May 26, 2020
Deep Learning and GPU programming using OpenACC	Vienna	Jun 3-5, 2020
High-performance computing with Python (PRACE course)	Jülich	Jun 8-10, 2020
High-performance scientific computing in C++ (PRACE course)	Jülich	Jun 15-17, 2020
Cluster Workshop	Stuttgart	Jun 16-17, 2020
Introduction to hybrid programming in HPC	Vienna	Jun 17-18, 2020
Deep Learning and GPU programming Workshop (PRACE course)	Garching	Jun/Jul (tba)
Node-Level Performance Engineering and Scaling Workshop (PRACE course)	Stuttgart	Jun 29-Jul 3

For a complete and updated list of all GCS courses, please visit:
http://www.gauss-centre.eu/training

The German HPC calendar (organized by the Gauss Allianz in cooperation with all German HPC centres) provides an extensive list of training all taking place German HPC centres. More information can be found at:
http://hpc-calendar.gauss-allianz.de/

Further training courses and events can be found on GCS member sites:
http://www.hlrs.de/training/
http://www.lrz.de/services/compute/courses/
http://www.fz-juelich.de/ias/jsc/events

The Rühle Saal at HLRS in Stuttgart **© HLRS**

JÜLICH SUPERCOMPUTING CENTRE
FORSCHUNGSZENTRUM JÜLICH

The Jülich Supercomputing Centre (JSC) at Forschungszentrum Jülich is committed to enabling scientists and engineers to explore some of the most complex grand challenges facing science and society. Our research is performed through collaborative infrastructures, exploiting extreme-scale supercomputing, and federated data services.

Provision of supercomputer resources: JSC provides access to supercomputing resources of the highest performance for research projects coming from academia, research organizations, and industry. Users gain access for projects across the science and engineering spectrum in the fields of modelling and computer science.

- Supercomputer-oriented research and development in selected fields of physics and other natural sciences by research groups and in technology, e.g. by doing co-design together with leading HPC companies.
- Higher education for master and doctoral students in close coperation with neighbouring universities.
- Implementation of strategic support infrastructures including community-oriented simulation laboratories and cross-sectional teams, e.g. on mathematical methods and algorithms and parallel performance tools, enabling the effective usage of the supercomputer resources.

The Cluster module of JSC's Modular Supercomputer "JUWELS". **© Forschungszentrum Jülich**

CENTRE DESCRIPTIONS

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Compute servers currently operated by JSC

System	Size	Peak Performance (TFlop/s)	Purpose	User Community
Atos BullSequana X1000 Cluster "JUWELS"	10 cells, 2,567 nodes 122,768 cores Intel Skylake 224 graphics processors (NVIDIA V100) 275 Tbyte memory	12,261	Capability Computing	European (PRACE) and German Universities and Research Institutes
T-Platforms Cluster + Intel/Dell Booster "JURECA"	Cluster: 1,884 nodes 45,216 cores Intel Haswell 150 graphics processors (NVIDIA K80) 281 TByte memory Booster: 1,640 nodes 111,520 cores Intel Xeon Phi (KNL) 157 TByte memory	2,245 4,996	Capacity and Capability Computing	German Universities, Research Institutes and Industry
Fujitsu Cluster "QPACE 3"	672 nodes, 43,008 cores Intel Xeon Phi (KNL) 48 TByte memory	1,789	Capability Computing	SFB TR55, Lattice QCD Applications

A detailed description can be found on JSC's web pages: www.fz-juelich.de/ias/jsc/systems

LEIBNIZ SUPERCOMPUTING CENTRE

Leibniz Supercomputing Centre
of the Bavarian Academy of Sciences and Humanities

For nearly six decades, the Leibniz Supercomputing Centre (Leibniz-Rechenzentrum, LRZ) has been at the forefront of its field as a world-class high performance computing centre dedicated to providing an optimal IT infrastructure to its clients throughout the scientific community–from students to postdocs to renowned scientists—and in a broad spectrum of disciplines–from astrophysics and engineering to life sciences and digital humanities.

Leadership in HPC and HPDA
Located on the research campus in Garching near Munich, the LRZ is a leadership-class HPC and HPDA facility delivering top-tier supercomputing resources and services on the national and European level. Top-notch specialists for HPC code portability and scalability support the LRZ' broad user base and ensure to run operations in the most energy-efficient way.

Future Computing at LRZ
The LRZ is leading the way forward in the field of Future Computing focusing on emerging technologies like quantum computing and integrating AI on large-scale HPC systems. A robust education program for HPC, machine learning, artificial intelligence and big data is complementing the LRZ offer.

IT backbone for Bavarian science
In addition to its role as national supercomputing centre, the LRZ is the IT service provider for all Munich universities as well as research organizations throughout Bavaria.

SuperMUC NG at the Leibniz Supercomputing Centre. **© LRZ**

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Compute servers currently operated by LRZ

System	Size	Peak Performance (TFlop/s)	Purpose	User Community
"SuperMUC-NG" Intel/Lenovo ThinkSystem	6,336 nodes, 304,128 cores, Skylake 608 TByte, Omni-Path 100G	26,300	Capability Computing	German universities and research institutes, PRACE (Tier-0 System)
	144 nodes, 8,192 cores Skylake 111 TByte, Omni-Path 100G	600	Capability Computing	
"SuperMUC Phase 2" Lenovo Nextscale	3,072 nodes, 86,016 cores, Haswell EP 197 TByte, FDR 14 IB	3,580	Capability computing	German universities and research institutes, PRACE (Tier-0 System)
"CooLMUC-2" Lenovo Nextscale	384 nodes, 10,752 cores Haswell EP 24.6 TByte, FDR 14 IB	447	Capability computing	Bavarian Universities (Tier-2)
"CoolMUC-3" Megware Slide SX	148 nodes, 9,472 cores, Knights Landing, 17.2 TByte, Omnipath	459	Capability Computing	Bavarian Universities (Tier-2)
IvyMUC	Intel Xeon E5-2650 ("Ivy Bridge")	13	Capability Computing	Bavarian Universities (Tier-2)
Teramem	1 node, 96 cores, Intel Xeon E7-8890 v4 ("Broadwell"), 6 TByte RAM	13	Big Data	Bavarian Universities (Tier-2)
DGX-1, DGX-1v Machine Lerning Systems	2 nodes, Nvidia Tesla, 8 x P100, 8 x V100	1,130 (Mixed Precision)	Machine Learning	Bavarian Universities (Tier-2)
Compute Cloud for SuperMUC-NG	64 nodes, 3,072 cores, Intel Xeon ("Skylake"), 64 Nvidia V100	128, 8,000 (Mixed Precision)	Cloud	German Universities and Research Institutes, PRACE

A detailed description can be found on HLRS' web pages: https://doku.lrz.de/display/PUBLIC/Access+and+Overview+of+HPC+Systems

HIGH-PERFORMANCE COMPUTING CENTER STUTTGART

Based on a long tradition in supercomputing at University of Stuttgart, HLRS (Höchstleistungsrechenzentrum Stuttgart) was founded in 1996 as the first German federal centre for high-performance computing. HLRS serves researchers at universities and research laboratories in Europe and Germany and their external and industrial partners with high-end computing power for engineering and scientific applications.

Service for industry
Service provisioning for industry is done together with T-Systems, T-Systems sfr, and Porsche in the public-private joint venture hww (Höchstleistungsrechner für Wissenschaft und Wirtschaft). Through this cooperation, industry always has access to the most recent HPC technology.

Bundling competencies
In order to bundle service resources in the state of Baden-Württemberg HLRS has teamed up with the Steinbuch Centre for Computing of the Karlsruhe Institute of Technology. This collaboration has been implemented in the SICOS BW GmbH.

World class research
As one of the largest research centres for HPC, HLRS takes a leading role in research. Participation in the German national initiative of excellence makes HLRS an outstanding place in the field.

View of the HLRS Cray XC40 “Hazel Hen”. © Boris Lehner for HLRS

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Compute servers currently operated by HLRS

System	Size	Peak Performance (TFlop/s)	Purpose	User Community
Cray XC40 "Hazel Hen"	7,712 nodes 185,088 cores 1 PB memory	7,420	Capability Computing	European (PRACE) and German Research Organizations and Industry
NEC Cluster (Laki, Laki2) heterogenous compunting platform of 2 independent clusters	826 nodes 17,420 cores 88 TB memory	726	Capacity Computing	German Universities, Research Institutes and Industry
NEC SX-ACE	64 nodes 256 cores 4 TB memory	16	Vector Computing	German Universities, Research Institutes and Industry

A detailed description can be found on HLRS’ web pages: www.hlrs.de/systems

InSiDE magazine (German: Innovatives Supercomputing in Deutschland) is the bi-annual publication of the Gauss Centre for Supercomputing, showcasing recent highlights and scientific accomplishments from users at Germany's three national supercomputing centres. GCS was founded in 2007 as a partnership between the High-Performance Computing Center Stuttgart, Jülich Supercomputing Centre, and the Leibniz Supercomputing Centre. It is jointly funded by the German Ministry of Education and Science (Bundesministerium für Bildung und Forschung – BMBF) and the corresponding ministries of the three states of Baden-Württemberg, North Rhine-Westphalia, and Bavaria.

www.gauss-centre.eu

Cover image: © LRZ. Researchers from LRZ, Intel, and the Australian National University collaborated to visualize the largest interstellar turbulence simulations ever performed. More information on page 28. To see the image in motion, scan the QR code.

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