Looking back on the year 2016, HLRS is proud of what we have achieved. New records for research project funding, industrial income, and the number of users who participated in our training courses are signs of the increased relevance of our research and the growing demand for the unique services that HLRS provides.

At the same time, 2016 was a year of major decisions that will shape HLRS for the next decade. Our most important achievement was securing funding for our next two HPC system installations, which are planned for the years 2019 and 2023. The federal government of Germany, the state government of Baden-Württemberg, and the University of Stuttgart together agreed to spend 153 million Euro over 8 years for investment and operating costs to guarantee that HLRS and its users remain world leaders in HPC simulation.

2016 was also a year in which we massively invested in the field of data analytics. Recognizing the challenges our users face in interpreting data produced by simulations, experiments, and sensors of all sorts, HLRS added a Cray Unika to its family of HPC systems. The computer was developed in partnership with Cray and was funded by Cray, the state of Baden-Württemberg, and HLRS. This powerful new tool for analyzing large datasets is now available to users from both research and industry. Another key activity started in 2016 is MoeWE, a project to develop a series of modular “blended learning” courses in HPC. Leveraging experience gained through the extensive training program that HLRS offers, MoeWe will enable us to further increase the reach of our training activities. The project is funded by the European Social Fund (ESF) and the state of Baden-Württemberg. It is led by HLRS in collaboration with the computing centers of the universities of Freiburg and Ulm.

Industrial users have been of key importance for HLRS for decades. In 2016, we were pleased that one of our collaborations with industrial partners set a new world record. Together with Ansys and Cray, HLRS was able to run Ansys Fluent on more than 172,000 cores for a single job. Such an accomplishment offers exciting new opportunities for our industrial customers.

These highlights are just a sampling of the wealth of stories and information contained in this 2016 Annual Report. We hope that you will enjoy this glimpse into our recent activities, which shows that HLRS – a national HPC center – continues to offer state-of-the-art resources to our users and to provide the general public with an impressive return on its investment in our work.

With best regards,

Prof. Dr.-Ing. Dr. h.c. Dr. h.c. Prof. E. h. Michael M. Resch
Director HLRS
Staff at the High Performance Computing Center Stuttgart (HLRS) have begun a project to combine High-Performance Computing (HPC) and High Performance Data Analysis (HPDA) to address handling and analyzing the ever-growing amount of data generated due to the continuing progress of digitalization. Using its supercomputer Hazel Hen, the HLRS examines – with project partner Cray – the potential of a new technology and suitable software for efficient data analysis.

HPC and data analysis already plays an important role in the automotive industry, for example, where extremely large data sets need to be processed and analyzed for the field of product development. “In cooperation with selected industrial users in the Stuttgart region, we will test the capabilities of the hardware and software in an industrial environment,” explains Prof. Dr. Michael M. Resch, Director of HLRS. “It is very important to us to find a practical solution, which eventually users from all kinds of industries can benefit from.”
NEW HLRS HARDWARE FAMILY MEMBERS

HLRS welcomes its newest computer hardware family members – two Cray Urika-GX systems – which were delivered to HLRS in late November. They are currently being set up. The systems will allow HLRS to enhance its data analytics technologies, enabling users and staff to investigate how the combination of high-performance computing and data analytics will benefit industrial and academic users.
ANSYS, HLRS and Cray set new supercomputing records

ANSYS (NASDAQ: ANSS), the High Performance Computing Center (HLRS) of the University of Stuttgart and Cray Inc. have set a new supercomputing world record by scaling ANSYS Fluent to over 172,000 computer cores on the Cray XC40 Hazel Hen supercomputer at HLRS, enabling organizations to create innovative and groundbreaking complete virtual prototypes of their products faster and more efficiently than ever.

ANSYS, HLRS and Cray have pured the boundaries of supercomputing and achieved a new milestone by scaling ANSYS software to 172,032 core on Hazel Hen, running at 82 percent efficiency. This is nearly a five-fold increase over the record set two years ago when Fluent was scaled to 36,000 cores.
The High-Performance Computing Center Stuttgart, together with the University of Freiburg and Ulm University, has been designing a new training program concept to grow the HPC talent pool. The goal of the project is reducing the skills shortage in information technology (IT) space.

To address the commitments of many IT professionals to job and family, all new courses will be organized in a “blended learning” mode, consisting of a balanced mix of workshops and online learning.
HLRS IN NUMBERS
IN NUMBERS

User Projects: 35
Industrial Costumers: 7
Core hours produced: 1,496 Billion

International Appearances: 59
Talks: 12

Third-party Funds: 3,943,156

Scientists: 71
Non Scientists: 29
Research Assistants: 11

Staff: 111
Guests: 14

Publications:
- Books: 6
- Bookchapters: 12
- Journals: 15
- Conference Papers: 16

Other: 2%
DFG: 6%
Federal Gov.: 14%
State Gov.: 38%
EU: 46%

User Workshop: 1,003 Participants
Scientific Workshops: 289 Participants
Lectures: 44 SWS

User Projects: 117 Days
Industrial Costumers: 17 Days
Core hours produced: 1,496 Billion
CRAY XC40 HAZEL HEN

The Cray XC40 Hazel hen is in production. Part of the Phase 1 filesystem (Hermit), installed in 2010, has been replaced by new hardware technology. The upgrade reduced Power consumption for this part of the system from ~140 kW to ~40kW. The resulting Filesystem provides 10PB of storage capacity with more than 200GB/s bandwidth. The configuration of Hazel Hen is as follows:

<table>
<thead>
<tr>
<th>CPU</th>
<th>Intel® Xeon® CPU E5-2680 v3</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>12 core @ 2.5 GHz</td>
</tr>
<tr>
<td>Number of Nodes</td>
<td>7,712 / 185,088</td>
</tr>
<tr>
<td>Peak Performance</td>
<td>7.42 PFLOPS</td>
</tr>
<tr>
<td>Memory</td>
<td>128 GB per node</td>
</tr>
<tr>
<td>Interconnect</td>
<td>Cray Aries</td>
</tr>
<tr>
<td>Disk Storage</td>
<td>15 PB</td>
</tr>
</tbody>
</table>

CRAY URIKA-GX

More and more projects running on the Cray XC 40 Hazel Hen generates large amounts of data. To provide a powerful tool analyzing this results a specialized Data Analytics Platform has been installed in December 2016. This research project give users the ability to adapt Data Analytics Methods into the area of engineering applications.

| Optimized Software for | Spark |
|                        | Hadoop |
|                        | CGE (CrayGraph Engine) |
| Number of Nodes | 64 |
| Cooperation with Academic and Industrial Partners | Daimler, Porsche, Sicos-BW, among others |

Hazel Hen consists of 41 cabinets à 1.5 t = 61.5 t
For applications with a strong demand for vector operations and high memory bandwidth, HLRS provides a vector computer. The NEC Vector CPU has 4 Cores @ 1.0 GHz. Number of Nodes/Cores: 64 / 256. Peak Performance: ~ 16 TFLOPS. Memory: 4 TB. Memory BW per Node: 220 GB/s (single core), 256 GB/s (4 cores). Interconnect: NEC IXS.

**NEC SX-ACE**

<table>
<thead>
<tr>
<th>CPU</th>
<th>NEC Vector CPU 4 Cores @ 1.0 GHz</th>
</tr>
</thead>
<tbody>
<tr>
<td>Number of Nodes/Cores</td>
<td>64 / 256</td>
</tr>
<tr>
<td>Peak Performance</td>
<td>~ 16 TFLOPS</td>
</tr>
<tr>
<td>Memory</td>
<td>4 TB</td>
</tr>
<tr>
<td>Memory BW per Node</td>
<td>220 GB/s (single core), 256 GB/s (4 cores)</td>
</tr>
<tr>
<td>Interconnect</td>
<td>NEC IXS</td>
</tr>
</tbody>
</table>

**NEC CLUSTER**

The standard PC cluster was installed in spring 2009. To meet the increasing demands for compute resources, the configuration of the PC – Cluster has been constantly adapted. The configuration is as follows:

<table>
<thead>
<tr>
<th>Node Type</th>
<th>Intel Xeon E5-2670 (SandyBridge)</th>
<th>102</th>
</tr>
</thead>
<tbody>
<tr>
<td>Node Type</td>
<td>Intel Xeon E5-2660 v3 @ 2.60 GHz (Haswell)</td>
<td>88</td>
</tr>
<tr>
<td>Node Type</td>
<td>Intel Xeon E5-2680 v3 @ 2.50 GHz (Haswell)</td>
<td>276</td>
</tr>
<tr>
<td>Memory per Node</td>
<td>64 / 128 / 256</td>
<td></td>
</tr>
<tr>
<td>Interconnect</td>
<td>Infiniband QDR / FDR</td>
<td></td>
</tr>
</tbody>
</table>
In 2016, user projects from different academic fields have been active on the Hazel Hen system. Users from German-based institutions are provided access through the Gauss Centre for Supercomputing. In total, 94 German national projects have been active on the system. Eleven of them have been granted access as Gauss large scale projects having a budget of at least 35 million core-hours for one year. In addition, eight projects based in different European countries – with access provided through the PRACE review process – have been using the system in the first quarter of 2016, finishing their calculations.

**System usage by state**

Figure 1+2 shows the distribution of computing time to the different states of Germany based on the location of the projects principal investigator. Federal research centres are shown independently. This graph provides an interesting picture – institutions based in North Rhine-Westphalia and Baden-Württemberg use about 40% of the system each, followed by Hessen with about 8%, Berlin with 3%, and Rhineland-Palatinate with 2%.

**System usage by field**

In Figure 1 we show the system usage of German projects by different application fields. As in the past years the strong role of engineering applications, especially CFD, is emphasized. More than 60% of produced core-hours is used by that field. The second strongest field has been again Physics, including solid-state physics, using more than 20% of the provided cycles. The fields of Chemistry and Climate are both using about 4% each, being the other fields with a significant usage.
GOLDEN SPIKE AWARD
The Golden Spike Award is given to HLRS users who present particularly excellent projects at the HLRS Results and Review Workshop.

Simulation of realistic earthquake events is currently one of the best options to better understand the complex dynamics that happen during earthquakes, and how these dynamics influence seismic hazards. SeisSol, an earthquake simulation package, is used to gain valuable insights on such complicated processes. The code couples rupture simulations with seismic wave propagation, thus also capturing secondary ruptures in complex fault zones. SeisSol uses a high order discontinuous Galerkin discretization on unstructured adaptive tetrahedral meshes. These meshes are required to resolve geometric features that can lead to localized phenomena. All element-local operations of the discontinuous Galerkin scheme are formulated as small matrix-matrix multiplications. The kernel code is generated using the high-performance library LIBXSMM as a backend and reaches about 50% peak-performance on modern Intel CPUs. Since SeisSol refrains from global communication, a similar percentage of peak performance can be achieved in petascale simulations.

To take advantage of the highly optimized kernels in realistic scenarios, a complete workflow scaling to 100,000 cores and more is required. On Hazel Hen, we focused on the high-resolution wave field output for visualization and a new checkpoint-restart implementation. Due to the close collaboration with HLRS, we had exclusive access to one of the new Lustre file systems. We evaluated the performance of different I/O libraries (MPI-IO, HDF5, SIONlib) without the interference of other codes running on the machine. Our results show that 72-84% of the theoretical peak bandwidth can be achieved with all I/O libraries. However, the libraries require careful tuning to the hardware and the I/O pattern of the application.

In addition to checkpointing, we improved the wave field output with a novel asynchronous implementation using so-called staging nodes. With this approach, visualization data is transferred to a small subset of the compute nodes (the "I/O nodes") using the high bandwidth network. All other nodes continue with the computation without waiting for the data to be written to disk. Combining the asynchronous I/O with local time-stepping, we were able to simulate the 1992 Landers earthquake with 96 billion degrees of freedom within 3 h on 2,112 Hazel Hen nodes. The simulation generated 1 TB of output data which we use for visualization and further analysis.

contact: Sebastian Rettenberger, rettenbs@in.tum.de
Proper atomization of liquid fuel is the key issue for controlling and minimizing emissions of aircraft engines. Therefore, in order to further optimize the engine, a detailed knowledge of the spray generation and droplet propagation inside the combustion chamber is indispensable. However, numerical predictions of the spray formation process are computationally extremely expensive. The length- and time-scales to be resolved cover at least 4 orders of magnitude. This inherently leads to simulations with a huge number of required discretization points and time-steps.

The relatively new simulation method Smoothed Particle Hydrodynamics (SPH) has an excellent performance and is able to very efficiently make use of massively parallel computer systems. Using SPH, accurate and fast predictions of air assisted atomization have become possible.

contact: Samuel Braun, samuel.braun@kit.edu
The project MoeWE meets the increasing digitalization needs and demands of professionals in the area of high-performance computing. Digitization in our society is a major challenge and requires professionals to handle these future requirements. The demand for high-performance computing experts in the area of simulation, modeling, programming, and performance optimization, is high and will continue to grow with further expansion of digitalization. In order to meet long-term needs and to provide employees professional developmental opportunities outside of work and their respective personal lives, MoeWE offers a modular and flexible training to become a high-performance computing expert.

The training concept is based on a blended learning concept which combines E-learning and face-to-face learning. Our approach takes advantage of both learning forms. Therefore, the participants are flexible to study when and where it best suits their work and family life.

The target audience is professionals and executives from small and medium-sized enterprises, as well as from the industry. An academic degree is not required.

The project aims to setup and conduct nine modules each with a duration of ten studying hours a week for three months. After the basic and principle courses as well as the specialization courses, the attendees, who successfully complete the required modules, will get a certificate which confirms the status of a high-performance computing expert.

The project is set up for four years and funded by the European Social Fund in Baden-Württemberg and the Baden-Württemberg Ministry for Science, Research, and the Arts.

The following projects were successfully completed within the MoeWE project:

- Automotive Simulation (Cluster of Excellence)
- Automotive Simulation (Cluster of Excellence) Phase 2
- BEAM-IE
- bwDataArchiv
- bwHPC-2S
- bwVissu
- COE GSS
- EU POP
- DREAMCLoud
- EuroLab4 HPC
- ExaFLOW
- Exasolvers
- Exasolvers 2
- EXCESS
- HPC Data Analytics (BigData)
- HPC II (BW-Stiftung)
- HPC Outreach “Simulierte Welten”
- iWindow
- MIKELANGELO
- MoeWe
- MontBlanc3
- MSC Media Solution Center Vorpunkt
- MyITOS
- NaHa HPC-Centren
- PaSaSage
- PHANTOM
- POLCA
- PRACE-4IP
- Reallabor Stadtquartiere 4.0
- SIMTECH IHR PNI:2-S
- StaSim
- Smart-DASH_SCOPE
- SmartDASH SPMT
- TelPAS
- TranSim
- VISDRAI
- VRCITYPLAN

Funded by:
- BMBF
- BMWi
- MWK
- BMBF
- DFG
- EU
- MWK
- EU
- EU
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- EU
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- EU

Webpage:
- www.reallabor-stadtquartiere.de
- www.prace-ri.eu/
- www.phantom-project.eu
- www.mikelangelo-project.eu
- www.iwindow.info
- www.simulierte-welten.de
- www.montblanc-project.eu/
- msc-bw.de
- www.realabor-stadtquartiere.de
High-performance computing (HPC) is a key driving factor for both academic and industrial innovation. HPC technology is well-established and actively applied in various areas of applications including modelling and simulation. Results obtained from simulation are constantly increasing, and it has become a challenge for domain experts to manually analyze the data in a reasonable amount of time. Data analytics is the perfect tool to automate these processes; data analytics can support experts in decision-making.

This project aims at developing a concept to combine HPC with data analytics. In cooperation with Cray, HLRS have extended the current HPC cluster with specific data analytics hardware. During the course of the project, the hardware will be evaluated in order to develop practical solutions for various areas. The project will investigate, for example, operation in industrial areas by cooperating with the Daimler AG.

**Fortissimo**

Fortissimo/Fortissimo 2 is a project, funded by the European Commission to foster the uptake of high-performance computing for manufacturing small and medium enterprises (SMEs). While big industrial players have the capacity of evaluating technologies such as HPC, SMEs often are hindered by the investments to do so and also suffer from uncertainty about potential benefits of this technology. Fortissimo thus tries to overcome these hurdles by providing simulation services and tools over an HPC-Cloud solution, combined in a single entry point – the Fortissimo marketplace.

To set this up properly, Fortissimo uses an experiment-driven approach, thus starting from a set of experiments with end-users, delivering requirements and testing the results (and the marketplace as a whole). This set of experiments has run since the start of Fortissimo and now in the framework of the I4MS activity of the European Commission. HLRS is a core partner and operates the marketplace, whilst also bringing in its expertise on applications and optimization to the I4MS Initiative.

**Big Data**

High-performance computing (HPC) is a key driving factor for both academic and industrial innovation. HPC technology is well-established and actively applied in various areas of applications including modelling and simulation. Results obtained from simulation are constantly increasing, and it has become a challenge for domain experts to manually analyze the data in a reasonable amount of time. Data analytics is the perfect tool to automate these processes; data analytics can support experts in decision-making.

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CONFERENCES
The ISC is the most important conference for HPC in Europe.

The US-based SC is one of the largest internationally.

HLRS, together with JSC and LRZ, was a co-exhibitor at ISC’16 at the Gauss Centre for Supercomputing booth. The three national supercomputing centres presented their wide-ranging HPC activities supported by their HPC systems and showcased the results achieved.

The virtual reality (VR) presentation set up at the booth by the HLRS visualization team turned out to be a true eye catcher for ISC attendees. The HLRS scientists had used a 3D tiled display in table configuration to interactively investigate data acquired from CT or MRI scans in combination with bio-mechanical simulations of bone implant compounds, blood flow simulations, anatomical structures, and forensic data. One of the demonstrations displayed clinical CT-data of a trauma patient. A second demonstration displayed the 3D-image acquired from the torso of a crime victim who had been shot three times and killed. Visitors were able to observe the virtually recreated body structures from all different angles and follow the explanations by the HLRS scientists regarding the analysis and derived insights of the bio-mechanical simulation results or the reconstruction of the crime scenario.

HLRS representatives hosted and participated in a number of workshops, birds-of-a-feather sessions, tutorials, and other ISC events.

HLRS AT SC’16

HLRS participated in the SC’16 supercomputing conference, which took place in Salt Lake City, Utah, USA, November 13-18, 2016. The event corresponds with the annually recurring International Exhibition and Conference on High-Performance Computing, Networking, Storage, and Analysis. As always, the HLRS booth (number 1743) was worth a visit. Staff welcomed visitors to a booth that featured a brand new layout and design and were excited to answer visitors’ questions about the manifold research activities connected to HLRS. They also provided visitors with information about HLRS’ flagship supercomputer, the Cray XC40 Hazel Hen, one of Europe’s fastest supercomputers. Indeed, “fast” was the theme of the HLRS exhibition. Members of the visualization department prepared an augmented reality demonstration of an airflow simulation around a Porsche 911 driving at the speed of 318 km/h. Additionally, the scientists presented current research projects in parallel visualization, remote hybrid rendering, and scientific visualization in virtual reality on a 3D back projection. Visitors could see, for example, how high-performance computing helps city planners design better and safer cities and how virtual reality can be of assistance in the participation process.
1. Why philosophy at a High-Performance Computing Center?

At first glance, it is quite unusual. But from my point of view, it is not surprising because the HLRS has a tradition of being avant-garde. See, philosophy is concerned with our relationship to the world and ourselves. These relations are shaped by concepts like "truth," "goodness," "justice," "reason," "action," and many more. These concepts have two exceptional features. On the one hand, they are necessary both in everyday life and in science. We cannot do science, or anything else, without any idea of what "truth" or a "good reason" is. But on the other hand, these concepts cannot be investigated empirically. This can be demonstrated with a simple argument: Every empirical investigation requires the concept of truth in order to distinguish a false statement from a true one. Therefore, notions like truth (and justice, reason and so on) cannot be researched in a straightforward empirical manner, but are required in order to conduct empirical studies. This is where philosophy comes into play (and also why philosophy can't be replaced by empirical sciences). Philosophy models concepts like truth, reason, and goodness, and explores the limits and benefits of different models.

Computer simulation is now changing the way science is done. Philosophy is interested in questions like: What kind of truth models are implicitly involved simulations studies? What counts as a good reason for believing in the results? Why do simulationists speak astonishingly often about "trust" in simulation models? These phenomena (and more) are part of their everyday practice and we would like to explore this collaboratively with them to understand what is at stake in this deep transformation of science and society.

2. Speaking of collaboration: How is working with your colleagues?

First of all, it is great to able to study computer simulations right where the expertise is gathered. This gives my colleagues and me the opportunity to come to a...
deeper understanding of scientific practices. By no means is everything documented in simulationists’ publications, because these are concerned with presenting results and justifications. The HLRS has proven to be a paradise for philosophers studying computer simulations. Many colleagues who are scientists, mathematicians, or engineers are interested in better understanding this relatively new (in the history of science) and still rapidly developing methodology. This interest is evident by the many ways we collaborate: We publish and we teach together; we write joint research applications and we organize conferences, workshops and colloquia. So we are really a part of HLRS.

Currently, I am working with Michael Resch and Uwe Küster on a paper about mathematical opacity in computer simulations; we’ve just published a volume on computer simulation (Science and Art of Simulation, published by Springer). But I am not alone; the philosophers in my team collaborate also with scientists, engineers, and mathematicians. Most of them have a dual professional background: Hildrun Lampe, a philosopher and environmental scientist, examines different kinds of uncertainty in computer simulation; Nico Formanek, a philosopher and physicist, is exploring how computer simulation changes the theory construction in quantum chromodynamics; Alena Wackerbarth, a sociologist and philosopher, is investigating the use of medical simulations for parental decision-making; Michael Herrmann, a philosopher and mathematician, studies the role of mathematics in computer simulation, and Juan Duran, philosopher and computer scientist, analyzes normativity in modeling and simulation. All of them work closely with computer scientists and engineers at HLRS like Colin Glass, Björn Schembera, and Ralf Schneider, to name just a few.

3. You said before that you would like to understand the impact of computer simulation on science and society. What is the significance of HPC for society?

You can imagine how the assumed fundamental transformation of scientific methods that comes along with computer simulation is of great relevance to our lives. Until the 20th century, there were two sources of knowledge: experience and theory. Computer simulation changes this situation in a way we do not yet understand. In addition, computer simulations are used in other contexts, like forensics and medicine. Furthermore, the political system is interested in the achievements and limitations of computer simulation for decision-making. Computer simulation will become a part of our everyday life. This is what I had in mind when I said HLRS has a tradition of being avant-garde. It recognized the societal relevance early on.
1. Much of your research is focused on the use of simulation technologies in biomechanics. How is the integration of information and communications technologies (ICT) — and especially simulation technologies — into the health sector progressing?

In the 20th century, as a result of globalization, organizations across the world began dedicating enormous intellectual and financial resources to advance all aspects of information and communication technologies.

These efforts made it feasible to develop enormous communication infrastructures, which are — like in the case of industry 4.0 — supposed to enable innovation and improve the efficiency with which we use sustainable resources. Several years ago, one ICT sector already proved itself capable of delivering these promised features: the field of simulation technology.

Another sector that requires more and more financial and intellectual capacities is health and well-being. Society’s interest in this area was triggered by the realization that as a society we are aging, a fact that requires us to address health problems and is consuming a growing portion of our resources. Cardiovascular disease, for example, causes 2 million deaths annually in the E.U. and costs 192 billion Euros.

In this context, ICT’s promises of innovation and the sustainable reduction of resource consumption make sense for the health sector. Nevertheless, the fusion of these two fields is not as mature as one might hope.

2. What are the critical problems that should be addressed to overcome the missing integration of ICT and health care?

From my point of view, what has to be seen critically is the current tendency of “data harvesting by every means.” The mining of “large amounts of data,” as targeted in the eHealth Action Plan, is really just the extension of the trial and error approach seen in classical clinical trials. As detailed in the recently released Avicenna roadmap, the crucial deficit in this approach is that it is not able to reveal internal mechanisms that Early signs of this integration can be found in solutions related to the eHealth sector. Here, the goal is to improve diagnostics, treatment, and follow-up care by fully connecting medical devices and patient data locally, across facilities, and/or even via the Internet. However, these targets have only recently been met. As Estonian President Toomas Hendrik Ilves, Chair of the independent high-level eHealth Task Force, said in the eHealth Action Plan, “Healthcare lags at least 10 years behind virtually every other area in the implementation of IT solutions.”
connect global measures like drug delivery or usage of a new device to secondary effects, such as screw loosening in implants.

For example, a study by Ohtori et al. published in 2013 reported 12 month follow up data for three groups of patients who had undergone instrumented mono- and bisegmental fusion of the lumbar spine by means of screw-rod fixation systems. The data were collected from one control group and two groups treated with teriparatide or bisphosphonate, respectively. The study showed a reduction of screw loosening for the teriparatide group but no effect for the bisphosphonate group when compared to the control group. This was surprising because both medications were supposed to improve bone quality and so one would have expected an increase of positive outcomes in both groups. The question of what prevented the bisphosphonate from being effective could not be answered because the system's internal processes, such as the connection between the local strain field and local bone remodeling, which are supposed to have an influence, were not accessible.

Even if data harvesting were improved by extending ICT to devices that observe the patient's vital statistics, this situation would not improve because the collected data will suffer from the same problem as the one described above. That is, they will only describe global physical parameters, which are not useful in providing a deeper understanding of the causal chain of internal mechanisms that lead to screw loosening.

3. What could be an approach to overcome the problem of classical physical clinical trials?

In my lab we think that simulation could address these problems. Detailed, holistic simulation of devices and how they interact with the human body promises deeper insight for health research. In addition, applying virtual design principles in medical device development — like those already widely used in the engineering domain — holds the potential to accelerate innovation processes and development cycles.

Even though numerical simulation technology is widely applied in various fields of academic health research — like orthopedics and osteosynthesis — the challenge that needs to be tackled in the years to come is to lift deterministic simulation approaches from the engineering domain to a state in which they are able to account for the full variation of human diversity. This will mean developing simulations that can quantify uncertainty not just in the parameter variations that go into creating a model of the device itself, but also with respect to physiological variation in patients.

This will especially hold true for devices and procedures that are well established and are considered mature by virtue of having been extensively tested in classical clinical trials. For example, although total hip replacement has been done for a long time, success rates are stagnating at about 90%. With only 10% improvement left to achieve, the stakes in terms of modeling effort and statistical significance are higher, as it will be important to capture the details that distinguish negative outcomes while also considering the additional costs to the health care system that would be necessary to improve the success rates.
THREE RECENT PHD THESSES AT HLRS

Dr. phil. Stina Kjellgren

Simulations play a key role in a variety of fields. One field in which simulation is getting increasingly important is the assessment of risks in planning processes. In this PhD thesis, risk management and the usage of simulation is explored. The focus on flooding, which plays an increasingly more important role in Germany.

Given that simulation can provide a better foresight in this field, it is an open question whether and how much simulations can play a role in the planning processes to reduce the risk of flood damage. The investigations give first insight into how simulations are perceived by decision makers in the planning process and how simulation results can be used in the planning process.

Dr.-Ing. Axel Tenschert
Ontology Matching in a Distributed Environment

Ontologies in computer science are used for storing, updating and utilizing semantic data. Usage of such ontologies allows users to process data and find answers to questions related to these data.

Through the matching of several ontologies relevant semantic data containing information are identified or the validity of data structures is proven. Ontology matching is thus a measure to better explore and use large amounts of data.

However, it requires high-performance computing. Hence, reduction of compute time by improving ontology matching methods is a key question for big data applications. In this thesis a matching approach is developed and a prototype implementation is presented that allows scalable ontology matching.

Dr.-Ing. Huan Zhou (with honors)
Communication Methods for Hierarchical Global Address Space Models in HPC

Efficient communication is a key to high sustained simulation performance on supercomputers. The Message Passing Interface (MPI) provides the necessary means to optimize communication. However, for an average user it is getting increasingly complicated to optimize the communication of an application to best exploit the features of MPI.

In this thesis, Huan Zhou first explores a way of hiding the complexity of MPI in Partitioned Global Address Space (PGAS) applications, taking away the complexity for the user but providing a maximum level of performance. By implementing an intuitive and efficient layer on top of MPI, she can show for real-world engineering applications that such a method can simplify programming and increase performance at the same time.
HIGH PERFORMANCE COMPUTING IN SCIENCE AND ENGINEERING ‘16

Transactions of the High Performance Computing Center, Stuttgart (HLRS) 2016

Editors: Nagel, W. E.; Kröner, D. H.; Resch, M. M. (Eds.)

This book presents the state-of-the-art in supercomputer simulation. It includes the latest findings from leading researchers using systems from the High Performance Computing Center Stuttgart (HLRS) in 2016. The reports cover all fields of computational science and engineering ranging from CFD to computational physics and from chemistry to computer science, with a special emphasis on industrially relevant applications. Presenting findings of one of Europe’s leading systems, this volume covers a wide variety of applications that deliver a high level of sustained performance.

The book covers the main methods in high-performance computing. Its outstanding results in achieving the best performance for production codes are of particular interest for both scientists and engineers. The book comes with a wealth of color illustrations and tables of results.

SUSTAINED SIMULATION PERFORMANCE 2016

Proceedings of the Joint Workshop on Sustained Simulation Performance, University of Stuttgart (HLRS) and Tohoku University, 2016

Editors: Resch, M. M.; Bez, W; Focht, E.; Patel, N.; Kobayashi, H. (Eds.)

The book presents the state of the art in high-performance computing and simulation on modern supercomputer architectures. It explores general trends in hardware and software development, and then focuses specifically on the future of high-performance systems and heterogeneous architectures. It also covers applications such as computational fluid dynamics, material science, medical applications and climate research and discusses innovative fields like coupled multi-physics or multi-scale simulations. The papers included were selected from the presentations given at the 20th Workshop on Sustained Simulation Performance at the HLRS, University of Stuttgart, Germany in December 2015, and the subsequent Workshop on Sustained Simulation Performance at Tohoku University in February 2016.
30 various HLRS-related titles have been published by Springer since 1998.

TOOLS FOR HIGH PERFORMANCE COMPUTING 2016


This book presents the proceedings of the 10th International Parallel Tools Workshop – held October 4-5 in Stuttgart – a forum to discuss the latest advances in parallel Tools for HPC2016.

High-performance computing plays an increasingly important role for numerical simulation and modelling in academic and industrial research. At the same time, using large-scale parallel systems efficiently is becoming more difficult. A number of tools addressing parallel program development and analysis have emerged from the high-performance computing community over the last decade, and what may have started as collection of small helper script has now matured to production-grade frameworks. Powerful user interfaces and an extensive body of documentation allow easy usage by non-specialists.
TRAININGS AND WORKSHOPS
### OVERVIEW TRAININGS 2016

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

### OVERVIEW WORKSHOPS 2016

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Visualization of an epithelial cell culture on a Cytodex microcarrier, rendered as a volume using a photo stacking approach based on images produced with light sheet fluorescence microscopy. The image was generated at HLRS in conjunction with Visionair, a European Commission-funded project to create a world-class visualization research infrastructure. Image courtesy of Dr. Emmanuel Reyraud (Centre for Biomedical Engineering, University College Dublin).