ANNUAL REPORT
2015

HIGH PERFORMANCE COMPUTING CENTER STUTTGART
Editorial

With this annual report HLRS changes its way of reporting by moving from a bi-annual report to annual reports. We further shorten the information provided. We summarize the achievements and developments and focus on a few highlights. This should make it easier for the reader to get an overview of what happened at HLRS last year.

The two most important events in 2015 were the starting of the construction work for the new HLRS training building and the final installation of the new Cray XC40 system code named Hazel Hen.

With the new training center to be finished in 2016 HLRS will be able to extend its training program substantially in the future allowing HLRS to intensify its post-graduate training programs.

The new Cray XC40 system established HLRS again as the leading center in Europe putting it on number 8 in the TOP500 list and on number 6 in the HPCG benchmark. This makes Hazel Hen the fastest production system in Europe. The system earned HLRS an HPCWire award at Supercomputing 2015 for its usage in large scale crash simulations for industrial usage.

2015 was also the year when HLRS was able to set up a European Center of Excellence for Global Systems Science. CoeGSS as the project is called is coordinated by Carlo Jäger from Potsdam with HLRS being the key HPC partner. With this project HLRS extends its application portfolio into new fields establishing new structures to support new users from areas like social sciences and financial simulations.

2015 was also the year to work out a strategy for the time after Hazel Hen. Together with its partners from the Gauss Center for Supercomputing HLRS has worked out a new concept that will carry the center into the next decade.

Providing key performance indicators for a supercomputing center this report summarizes all aspects of operation, service and research. We hope you enjoy reading!

With best regards,

Prof. Dr.-Ing. Dr. h.c. mult. Prof. E. h. Michael M. Resch
Director HLRS
ANNUAL REPORT 2015

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Visit of Mrs. Minister Theresia Bauer at the HLRS

Mrs. Minister Theresia Bauer, Science Minister of Baden-Württemberg and newly selected “Science Minister of the Year 2015”, paid the HLRS a visit in early February. Host Professor Michael M. Resch, Director of the HLRS, took Mrs. Bauer on a guided tour through the HLRS supercomputing center.

Following a visit to the data center room where Mrs. Bauer took a detailed look at the recently installed petascale supercomputer Hornet (peak performance: 3.8 Petaflops), the Minister was also introduced to Virtual and Augmented Reality.

In the HLRS simulation lab, Mrs. Bauer was given a presentation of various projects the HLRS scientists are currently working on, demonstrating the impressive visualization capabilities of the HLRS CAVE (Cave Automatic Virtual Environment). Prof. Michael M. Resch also seized the opportunity to discuss with Minister Bauer the role of High Performance Computing in science, research, and industry as well as the ever more relevant subject of education and training provided by the HLRS.
On May 8, 2015, the ceremonious laying of the foundation stone for the new HLRS Training Center took place in the presence of representatives of the State Ministries, the Building Authority of the Stuttgart University, the Rector of the University of Stuttgart, students, and employees of HLRS. The keynote address was delivered by Rolf Schumacher, Ministerial Director of the Ministry of Finance and Economics Baden-Württemberg. The new HLRS Training Center, which is conceptualized and designed as an annex to the existing HLRS research building, is scheduled to become operational in October 2016. The construction costs are borne in full by HLRS.
Hazel Hen is Europe’s fastest supercomputer on the High Performance Conjugate Gradient (HPCG) benchmark list. This was announced at the Supercomputing Conference 2015 in Austin, Texas.

The newly created HPCG benchmark represents the behavior of HPC systems running real applications. Hazel Hen, a CRAY XC40 system, captured a strong 6th position on the HPCG list by delivering a performance of 138 Teraflops and thus took the European lead amongst the world’s fastest supercomputers.

In the TOP500 list which ranks the world’s fastest supercomputers based on their performance measured by the Linpack benchmark, Hazel Hen also made it into the Top-10. The HLRS HPC system is listed as the 8th fastest supercomputer in the world with its Rmax performance of 5.64 Petaflops (5.64 quadrillion floating point operations per second).

The HPCG benchmark has recently enjoyed growing attention in the HPC community as it tries to reflect changed customer requirements. It has been developed to provide a benchmark for performance of the fastest supercomputers measured in real applications. While the Linpack benchmark, which serves as metrics for the well known TOP500, measures the speed and efficiency of full matrix linear equation calculations of a system, the HPCG benchmark does not focus on raw CPU performance but stresses the system balance, e.g. floating point operations versus bandwidth and latency of the memory system and the communication network. In addition, it tightens the focus on messaging, memory, and parallelization. All these parameters add up to an "averaged" yet from the users’ perspective more beneficial and thus more important system performance.

"Being listed in the Top-10 of the TOP500 is an honor for us. However, our focus at HLRS has always been on user performance. Everything else comes second," stresses Prof. Michael M. Resch, Director of the HLRS. "As a consequence, we are all the more delighted to take the lead in Europe for this realistic application benchmark. This is the result of the work of many people at HLRS, and we would like to thank all colleagues from Cray and from the University of Stuttgart as well as the State of Baden-Württemberg and the Federal Government of Germany for their continued and ongoing support. Today, we have shown that our focus on the users pays off."

The2015HPCwireReaders’andEditors’Choicewasmade fora challenging simulation project run on the HLRS High Performance Computing (HPC) system Hornet, a Cray XC40-system. In cooperation with its partner DDN and supported by the ASCS, HLRS ran more than 1,000 car crash simulations within 24 hours. Exploiting the peta-scale computing power of the HLRS supercomputer, DDN storage was leveraged to overcome the Input/Output bottleneck challenges that previously limited the ability to increase simulations in Computational Fluid Dynamic (CFD) workflows.
Apart from providing HPC resources and services to the scientific community, the High Performance Computing Center Stuttgart (HLRS) offers a variety of services to the industry. The "Hochleistungsrechner für Wissenschaft und Wirtschaft GmbH" (HWW) was founded in 1995 as a public private partnership. Founding members are Dr. Ing. h.c. F. Porsche AG, debis AG (today represented by T-Systems and T-Systems SfR), the University of Stuttgart, the Karlsruher Institute of Technology (KIT), and the State of Baden-Württemberg. HWW was founded to promote and support productive cooperations between science and industry in Baden-Württemberg.

The HWW is proud of its successful past and held an Anniversary Colloquium on December 1, 2015. On this occasion, HWW reflected on the 20 years of successful cooperation. In the presence of a selected group of guests, the HWW managers elaborated on the partnership’s highlights: “Retrospective 20 Years of HWW”, M. Heib / T-Systems, and a Celebration Talk was given by Prof. N. Kroll / DLR and Dr. K. Becker / Airbus on “Perspectives of HPC in the Field of Aircraft Engineering.”
HLRS in Numbers
Cray XC40 Hornet

Configuration of the system as it was run in production until August 2015.

- **CPU**: Intel Haswell 12 core @ 2.5 GHz
- **Number of Nodes**: 3,944
- **Peak Performance**: 3,786 TFLOPS
- **Memory**: 128 GB per node
- **Interconnect**: Cray Aries

Cray XC40 Upgrade Hazel Hen

Upgrade of Hornet started in August 2015 by adding more Compute cabinets. The most challenging part of the upgrade procedure was to minimize the downtime - the time which was necessary to renew the cabling of the dragonfly network and testing time. The configuration is as follows:

- **CPU**: Intel® Xeon® CPU E5-2680 v3 (12 core, 2.50 GHz)
- **Number of Nodes / Cores**: 7,712 / 185,088
- **Peak Performance**: 7,420 TFLOPS
- **Memory**: 128 GB per node
- **Interconnect**: Cray Aries

Hazel Hen consist of 41 cabinets $\times 1.5 \, \text{t} = 61.5 \, \text{t}$
NEC SX-ACE

For applications with a strong demand for vector operations and high memory bandwidth, a vector computer has been installed.

- **CPU**: NEC Vector CPU 4 Cores @ 1.0 GHz
- **Number of Nodes/Cores**: 64 / 256
- **Peak Performance**: ~ 16 TFLOPS
- **Memory**: 4 TB
- **Memory BW per Node**: 220 GB/s (single core) 256 GB/s (4 cores)
- **Interconnect**: NEC IXS

NEC Cluster

The standard PC cluster has been 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:

- **Node Type**: Intel Xeon E5560 (Nehalem) 2.8 GHz
- **Node Type**: Intel Xeon E5-2670 (SandyBridge) 102
- **Node Type**: Intel Xeon E5-2660 v3 @ 2.60 GHz (Haswell) 88
- **Memory per Node**: 12 / 32 / 64 / 128 / 256
- **Interconnect**: Infiniband DDR / GDR
In the reporting period different kinds of academic user projects have been active on the system. European users are provided access through the PRACE proposal evaluation procedure. Users from Germany based institutions are provided access through the GAUSS Centre for Supercomputing. In 2015, 15 PRACE projects and 108 German projects have been active on the system. Nine of the German projects have been provided access as Gauss large scale projects.

**Usage of systems**

**System usage by field**

Figure 1 shows the system usage of German projects by different application fields. Here, the strong role of CFD is emphasized as more than 50% of the allocated computing power is going into this field. The second strongest field has been Physics which includes solid state physics which has used more than 20% of the provided cycles.

**System usage by State**

As laid out in Figure 2, the distribution of computing time to the different institutions within the different states show an interesting picture. Both, Baden-Württemberg and Nordrhein-Westfalen use a bit more than 40% of the system. The remaining 16% are distributed between institutions of other states and the Federal Research Centres.
Golden Spike Award
AEROCOUSTIC SIMULATION OF COMPLETE HELICOPTER SIMULATION USING CFD (PATRICK KRANZINGER)

In the past years, the aeroacoustic noise emission of helicopters became one of the most important, but also challenging issues in helicopter development. The Blade Vortex Interaction (BVI) phenomenon is one of the dominant phenomena characterizing the helicopter’s aeroacoustic footprint. Everybody who witnessed a helicopter’s landing approach will remember a strong impulsive noise emission for quite a long time during the whole maneuver. In particular, people living in the entry lane of a heliport or a hospital suffer from increased noise exposure. Often, helicopters are deployed in search and rescue, and security (such as police) missions, which require flight routes above populated areas, and are in conflict with night time banning.

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LARGE SCALE NUMERICAL SIMULATIONS OF PLANETARY INTERIORS (DR. ANA-CATALINA PLESA)

Mantle convection describes the slow creep of rocky materials caused by temperature-induced density variations and compositional heterogeneities inside planetary bodies. This process is ultimately responsible for the heat transport from the deep interior and for the large-scale dynamics inside the Earth and other terrestrial planets thus influencing surface geological structures like volcanoes, rifts and tectonic plates as well as the magnetic field generation.

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THEORY OF DYNAMICAL PROCESSES IN SEMICONDUCTOR NANOSTRUCTURES VIA LARGE SCALE AB INITIO CALCULATIONS (PROF. DR. GABRIEL BESTER)

To unravel the effects of temperature (lattice vibrations) on the electronic and optical properties of semiconductor nanostructures known as quantum dots, we perform large scale ab-initio Density Functional Theory (DFT) calculations on realistic structures with diameters ranging from 2 to 3 nm, which contain up to one thousand atoms and several thousand electrons. The scientific interest resides not only on the understanding of fundamental physics (“How does matter behave at the nanometer scale?”) but also on a reliable assessment of the process of carrier relaxation — how do excited electrons relax to their ground state, and how fast — which is most relevant for semiconductor nanodevices. Specifically for the design and control of nanomaterials in the fields of optoelectronics, spintronics, photovoltaic, biolabeling, and the next generation of displays.

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Research Projects
The evaluation, assessment and forecast of social, economic and ecological developments forms the basis of the Centre of Excel-
lence for Global Systems Science (CoeGSS). In order to understand and improve global analyses and decision processes in a more
efficient way, the CoeGSS project builds on synthetic populations that reflect the behaviour of the human mankind.

Based on static degrees of relationships and social as well as health habits, an anonymized population dataset including
millions or even billions of people will be created in order to understand global problems like pandemic, urbanization or even market growth. As most of the time various factors and relations need to be taken into account, the considered data-
sets grow drastically and therefore require HPC and in addition, High Performance Data Analytics (HPDA). Thus, bridging the gap between those two paradigms will be one of the key findings of the project.

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The digitalization of economy and society is one of the most comprising revolutions of our time. Apart from the industrial transformation of an industry 4.0, the change of living environments and the working worlds has to be shaped significantly in the future. At the same time, the impact of digitalization on cities as our central habitat is hardly known and there is no public understanding due to the complexity and the interlinking of topics. Planning and decision-making processes are often conducted with very conventional and highly regulated methods and tools which can hardly keep pace with the current challenges. However, the fields of innovation of digitalization and planning and decision-making processes are supposed to be viewed in combination with more and more complex demands under consideration of all relevant players as well as the central location for living in urban space.

With this project, which is set up for three years, the Research Association relies on a strategy of co-design of research and of the common knowledge acquisition with citizens. With the help of a series of real-world experiments and inventions, innovative and future-oriented procedures for city district planning are supposed to be developed with early shaped citizen participation and tested in cooperation with the cities Stuttgart and Heidelberg.

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BEAMMe

The liberalization of the energy sector and the increasing decentralization of country wide electrical power supplies cause a high complexity of techno-economical systems in terms of production, distribution and storage of electrical power when realizing renewable energy technologies. Against the background of the desired creation of a European internal energy market and the ongoing transformation of the Renewable Energy – Energy-Supply-System (RE-ESS), the application of system analytical models gains more and more significance to answer arising questions that concern the identification of sustainable investment strategies to ensure supply safety, in connection with the constantly increasing share of renewable energy production.

During the past years it became obvious that the application of energy-system models for focused investment- and deployment-optimizations requires more computational power than even a modern workstation can deliver.

Facing these challenges the target of this research project is to harvest the potential that parallelized computations on High-performance computing systems provide for the high resolution optimization strategies of the energy-system analysis.

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STADTQUARTIERE 4.0
The Augmented Reality (AR) demonstration of the air flow around a Porsche sports car was a true show stopper at this year’s International Supercomputing Conference in Frankfurt a. M. (July 12-16, 2015). With visualizations showing how air behaves when colliding with and flowing around the car, visitors were given the chance to experience AR live, i.e. the mixture of reality (the car) and virtual reality (the simulated air flow). This interesting presentation was brought to the ISC visitors by members of the HLRS visualization staff who supported a special exhibit in ISC’s CAE Pavilion focusing on Computer Aided Engineering in the Automotive Industry.

Like in previous years, HLRS was a partner on the booth of the Gauss Centre for Supercomputing where the three national supercomputing centres presented their wide-ranging HPC activities supported by their HPC systems and the results achieved. Interested parties were able to receive information e.g. about the recently completed so-called XXL Projects at HLRS - large scale simulation projects which challenged the endurance of the new HLRS system “Hornet” by testing the readiness of its hardware and software for extreme-scale compute jobs during its early installation phase. HLRS also offered 3D visualizations on a tiled 3D display wall. The highlight was the interactive remote visualization of the water flow in a pump turbine simulated by the Institute of Fluid Mechanics and Hydraulic Machinery of the University of Stuttgart.

HLRS representatives hosted and participated in a number of workshops, Birds-of-a-feather sessions, tutorials and other ISC events. In the Industry track of the conference program, Prof. Dr. Wolfgang Schröder of the Institute of Aerodynamics and Fluid Dynamics of RWTH Aachen introduced one of the aforementioned Hornet XXL projects to the interested audience of ISC participants: for project “Prediction of the Turbulent Flow Field Around a Ducted Axial Fan” 110 machine hours on 92,000 of Hornet’s compute cores had been used.

HLRS participated in this year’s Supercomputing Conference (SC15), which took place in Austin, Texas, USA, from November 15 - 20, 2015 at the annually recurring international exhibition and conference on High Performance Computing (HPC), Networking, Storage, and Analysis. One topic of major interest to the HPC community was certainly HLRS’s recently installed HPC-System Hazel Hen (peak: 7.42 PFlops), while Virtual Reality presentations on a 3D rear projection on the HLRS booth drew the attention of SC visitors. In particular the HLRS staff showcased how HPC is getting increasingly more important in the reconstruction of crime scene scenarios: on site, they analyzed blood stains using interactive simulations and visualized the results using Augmented Reality.

Furthermore, HLRS staff gave presentations, speeches, and participated in special interest group sessions. For example, Dr. Rolf Rabenseifner acted as co-speaker at the SC15-tutorial on “MPI+X - Hybrid Programming on Modern Compute Clusters with Multicore Processors and Accelerators”, and Vladimir Marjanovic was one of three presenters at the BoF session “High Performance Geometric Multigrid (HPGMG): an HPC Benchmark for Modern Architectures and Metric for Machine Ranking”. 

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

International counts the SC in the USA.
Supercomputing, High Performance Computing, Quantum Computing: Our world is turning digital faster and faster.

Lothar Späth made HPC possible 30 years ago. What computing power did the supercomputer have back then?

In 1986, the vector computer Cray-2 with four processors (today cores) was installed at the University of Stuttgart, a machine with the, back then, amazing amount of 4 GB of memory, more than all Cray machines had had before. People today might smile because their Smartphone has a larger memory. The same applies for the processor frequency of 244 MHz, high at that time. They would not smile about the physical density of the packaging of the machine. The modules of 1 x 4 x 8 inches consist of up to 768 chips, where a memory chip had only 256 Kbit instead of 16 MB memory.

The current computer at HLRS, Hazel Hen, is on 8th place in the TOP500 ranking of the fastest Supercomputers. What distinguishes the present day Parallel Computer from the Vector Computer back then?

HLRS’ current Cray XC40 machine has 61,696 DIMMs (memory modules) with 38 chips (= 2.34 Mill) and 0.99 PetaByte memory in 7,712 nodes. The footprint is much larger, also the power consumption with 2 MW instead of 180 KW. We have 185,000 cores instead of 4, the peak performance is 7.4 PetaFlop instead of 1 GigaFlop. The core frequency varies around 2.5 GHz, ten times as high. However, the peak bandwidth peak performance relation, which is important for the efficiency of many important algorithms, is 0.16 Byte/Flop today compared to 8 B/F for the Cray-2. The processor architecture is much more complicated. Vectorization as a special parallel paradigm has been reanimated after being said to be dead 15 years ago.

Blood analysis, flow calculations, driving simulations, climate research are all not a problem for a supercomputer of the present. What developments in technology can we expect in the next years?

Higher chip density is getting more expensive, the processors frequencies are getting smaller to save energy. The number of cores per processor is getting larger at a small rate. Vector mechanisms will be typical. We will see steps to push integration to the third dimension, first for memory, then for the processors, if the cooling problems can be solved. Limited Input/Output and storing capabilities might involve difficulties for simulation of unsteady problems. There is a promise in getting more and more cores. There is no promise that these could be used efficiently for homogeneous tasks as for Computational Fluid Dynamics.

Instead scaling programs by increasing the computational load to millions of cores, which involve larger and larger job run times as long as the solution effort scales worse than linear with the problem size (e.g. multi grid techniques might help), it will be more important to decrease (!) the efficiently solvable problem size per active unit. To reach this, faster synchronization of the active units by common register sets is needed, faster handling of mixing data as assembling a distributed stiffness matrix, faster handling of randomly distributed data.

Three questions for Uwe Küster, Head of the Department of numerics at HLRS

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Dr.-Ing. Ralf Schneider, Analysis of continuum mechanical anisotropic material parameters of micro-structured volumes using direct mechanical simulation.

The simulation of bones and fractures is about to become a relevant tool for surgeons to be able to predict the impact of their work on the patients treated. In his PhD thesis Ralf Schneider puts the focus on finding the right material parameters that will allow to make such simulations as realistic as possible. Using direct mechanical simulations and working with experimental data he can identify such parameters for micro-structured volumes which form the basis for bone simulations. Ralf Schneider works with data received from μ-CT scans which allows to identify the micro-structure of bones. He uses the Finite Element Method (FEM) for his simulations. Based on this he was able to simulate fractured bones and implants to allow for the prediction of the healing process.

Dr.-Ing. Adrian Reber, Process migration in a parallel environment.

Large scale HPC systems consist of hundreds of thousands of nodes. Even though hardware reliability is usually high the huge number of components dramatically increase the probability of a failure. Usage of such large scale systems have to respond to this regardless of whether an application runs on a large scale highly integrated supercomputer or in a large scale distributed environment. Adrian Reber presents an approach that is based on checkpointing and restarting. Virtual machines – as are often used in distributed environments – would come with too high an overhead to be useful in HPC. The method developed is integrated in OpenMPI to cover a large variety of applications that rely on MPI for parallelization. A number of test cases are run to show both the feasibility of the approach and the performance.

Dr.-Ing. Florian Seybold, Numerische Methoden mittels eigentlicher Bewegung in der Geometrischen Algebra.

Modelling or simulating machines like the numerical control of industrial robots requires the parametrization of rigid motions, as well as composing them efficiently on modern HPC processor architectures. Geometric Algebra is a promising tool for parametrising motion. Common definitions of Geometric Algebra are based on an axiomatic system for the Geometric Product. Just like that, the derivation from this axiomatic system to an explicit definition of the product as a sum of coordinate multiplications is only partially possible. Common implementations of the geometric product are based on such partially explicit definitions; they do not fully consider the structure of the Geometric Product. In the first part of this thesis, Geometric Algebra is introduced by a novel construction, which defines the Geometric Product in a totally explicit manner. Properties of the Geometric Algebra are discussed, with the aim of parametrising and composing motion within Geometric Algebra. In the second part, a vectorization strategy is developed, which can be implemented on modern SIMD processor architectures by applying certain coordinate permutations. Furthermore, an efficient alternative for evaluating the sign of base vector products is described. The third part covers as a sample application the solution of inverse kinematics for industrial robots. Concerning runtime behavior on modern SIMD processor architectures, advantages of using the vectorization strategy for the Geometric Product described here as opposed to matrix algebra are shown.
Publications
High Performance Computing in Science and Engineering ’15

Transactions of the High Performance Computing Center, Stuttgart (HLRS) 2015
Editors: Nagel, W. E., Kröner, D. H., Resch, M. M.

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 2015. 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 2015

Proceedings of the Joint Workshop on Sustained Simulation Performance, University of Stuttgart (HLRS) and Tohoku University, 2015
Editors: Resch, M. M., Bez, W., Focht, E., Kobayashi, H., Qi, J., Roller, S.

The book presents the state-of-the-art in High Performance Computing and simulation on modern supercomputer architectures. It covers trends in hardware and software development in general, and the future of high-performance systems and heterogeneous architectures specifically. The application contributions cover Computational Fluid Dynamics, material science, medical applications and climate research. Innovative fields like coupled multi-physics or multi-scale simulations are also discussed. All papers were chosen from presentations given at the 20th Workshop on Sustained Simulation Performance in December 2014 at the HLRS, University of Stuttgart, Germany, and the subsequent Workshop on Sustained Simulation Performance at Tohoku University in February 2015.
### Overview Trainings 2015

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