

Preface

The Cray supercomputer HERMIT—installed in October 2011—is still the working horse at HLRS. It is a large Cray XE-6 with a peak speed of more than 1 PFLOP/s, based on the AMD Interlagos chip with overall more than 113,000 cores, integrated into 38 water-cooled cabinets. Additionally, the system is tightly integrated with external servers for pre- and postprocessing to support complex workflows. The system entered the Top500 list already in November 2011 and was—at that time—ranked number 12 on a worldwide level, achieving a Linpack value of 831,4 TFLOP/s. In the list published in November 2013, this system still is ranked on spot 39. Having Hermit as an infrastructure, and together with the new research buildings for VISUS, SimTech, and HLRS, the Universität Stuttgart is well positioned to become one of the leading science nodes for simulation technology in Germany, as well as abroad.

In 2014, the second delivery phase will follow, and the final Cray system will then have a peak performance of roughly 5 PFLOP/s. The plan is to have a Tier-0 HPC system within the GCS operating at any time within the 5-year period.

The HLRS participates in the European project PRACE (Partnership for Advances Computing in Europe) as part of the GCS, extending its reach to all European member countries, and has provided hundreds of millions of cpu hours to the European user community. Additionally, HLRS participates with partners in Germany in two Exascale Software Initiatives on European Level, namely TEXT and CRESTA where the challenges on the efficient use of current and future computing systems are investigated.

While the GCS has successfully addressed the high end computing needs, it was clear from the very beginning that an additional layer of support is required to maintain the longevity of the center, via a network of competence centers across Germany. This gap is addressed by the Gauß-Allianz (GA), in which regional and local centers teamed up to create the necessary infrastructure, knowledge, and the required methods and tools. The mission of the Allianz is to coordinate the HPC-related activities of its members. By providing versatile computing architectures and by combining the expertise of the participating centers, the necessary ecosystem for computational science has been created. Strengthening the research and increasing

the visibility to compete at the international level are the further goals of the Gauß–Allianz. To disseminate information about its activities, the Gauß–Allianz is publishing a flyer (GA-Infobrief, <http://www.gauss-allianz.de/infobrief>), issued several times a year.

A number of projects of the third BMBF HPC-call have started as early as October 2013. This call was directed towards proposals that enable and support petascale applications on more than 100,000 processors, as they are also currently available at HLRS. While the projects of the first funding round started in early 2009 and the second one in April 2011, the follow-up call had been delayed again by more than 18 months. Nevertheless, all experts and administration authorities continue to acknowledge the strong need for such a funding program, given that the main issue identified in nearly all applications is that of *scalability*. The strategic funding plan involves more than 10 million Euros, with the hope of follow-up calls over the next 5 years, for projects that develop scalable algorithms, methods, and tools to support massively parallel systems. This can be seen as a very large investment. Nevertheless, in relation to the investment in computing hardware within Germany over this 5-year period, the investment in software is still comparatively small amounting to less than 20 % of the hardware investment. Furthermore, the investment in software will produce the “brains” that will be needed to use the newly developed innovative methods and tools, to accomplish technological breakthroughs in scientific as well as industrial fields of applications.

It is widely known that the long-term target is aimed not only at Petascale but also at Exascale systems. We do not only need competitive hardware but also excellent software and methods to address—and solve—the most demanding problems in science and engineering. The success of this approach is of significant importance for our community and will also greatly influence the development of new technologies and industrial products. Beyond being important, the success of this approach will finally determine whether Germany will be an accepted partner alongside the leading technology and research nations.

It is, therefore, a pleasure to announce that the German Research Foundation (DFG) has started the additional Priority Program 1648 “Software for Exascale Computing (SPPEXA)” in the field of HPC in January 2013. The funding is available for 6 years, with about 4 million Euros per year, to support fundamental and basic research questions in several specific areas related to HPC.

Since 1996, the HLRS has supported the scientific community as part of its official mission. Just as in the past years, the major results of the last 12 months were presented at the 15th annual Results and Review Workshop on High Performance Computing in Science and Engineering, which was held from September 30 to October 1, 2013, at the Universität Stuttgart. The workshop proceedings contain the written versions of the research work presented. The papers were selected from all projects running at the HLRS and the SSC Karlsruhe during a 1-year period between October 2012 and September 2013. Overall, a number of 48 papers were chosen from Physics, Solid State Physics, Chemistry, Reactive Flow, Computational Fluid Dynamics (CFD), Transport, Climate, and numerous other fields. The largest number of contributions originated from the CFD field, just as in many previous

years, with 15 papers. Even though such a small collection cannot entirely represent an area this vast, the selected papers demonstrate the state of the art in high performance computing in Germany. The authors were encouraged to emphasize the computational techniques used in solving the problems examined. This is an often forgotten aspect and was the major focus of the workshop proceedings. Nevertheless, the importance of the newly computed scientific results for the specific disciplines is impressive.

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