

Preface

It is a pleasure to announce that after the installation of the IBM Blue Gene/P at NIC/JSC in May 2009, as part of the Gauss Centre for Supercomputing (GCS) – linking together the three national supercomputing centres HLRS (Stuttgart), NIC/JSC (Jülich), and LRZ (Garching) – the next major step has been realized at HLRS with the installation of a new system, HERMIT, in October 2011. HERMIT is a large Cray XE-6 with a peak speed of more than 1 PFLOP/s. Based on the new AMD Interlagos chip, two sockets form a node, and HERMIT brings together 3,552 compute nodes with 113,664 cores, integrated into 38 water-cooled cabinets. Additionally, the system is tightly integrated with external servers for pre- and post-processing to support complex workflows. The new system entered the Top500 list in November 2011 and ranked number 12 on a worldwide level, achieving a Linpack value of 831,4 TFLOP/s. Having the new Petaflop system 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 2013, the second delivery phase will follow, and the final Cray system will then have a peak performance of roughly 5 PFLOP/s. Additionally, the LRZ will upgrade its own systems accordingly to a 3 PFLOP/s system in summer 2012. The plan is to have a Tier-0 HPC system within the GCS operating at any time within the five year period.

The HLRS also 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. Within the PRACE project, the GCS will provide access to high performance computing resources valued at 100 Million Euros. Moreover, the PRACE activities are well aligned with the HLRS activities in the European HPC support project, HPC-Europa2. 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 Centre, via a network of competence centres across Germany. This gap is addressed by the Gauß–Allianz (GA), in which regional and local centres 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 centres, the necessary ecosystem for computational science has been created. Strengthening the research and increasing the visibility to compete at the international level are further goals of the Gauß–Allianz. To disseminate information about its activities, the Gauß–Allianz has started to publish a flyer (GA-Infobrief, <http://www.gauss-allianz.de/infobrief>), issued several times a year.

A number of projects of the second BMBF HPC-call have started as early as April 2011. 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 will complete within the next 6 months, the follow-up call had been delayed 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 another 20 Million Euros, with a yearly follow-up call over the next three 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 five year period, the investment in software is still comparatively small, amounting to less than 20 per cent 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 at Exascale systems as well. 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 in October 2011, the German Research Foundation (DFG) has funded an additional Priority Program 1648 “Software for Exascale Computing (SPPEXA)” in the field of HPC. The funding is available for 6 years, starting January 2013 with 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 on October 4–5, 2011 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 one-year period between October 2010 and October 2011. Overall, a number of 47 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 13 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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