Preface

The new Cray XC40 supercomputer Hornet – completion of installation in November 2014 – is the new flagship computer at HLRS replacing the previous supercomputer Hermit after approximately 3 years in service. With a peak performance of 3.8 PFLOP/s it almost quadruples the performance of its predecessor. The system is based on the new Intel Xeon processors, formerly code-named 'Haswell', and the Cray Aries system interconnect. In its current configuration state, Hornet consists of 21 cabinets hosting 3,944 compute nodes, which sum up to a total of 94,656 compute cores. The system's main memory capacity is 493 terabytes. Users will benefit in particular from the quadrupled storage space the HLRS supercomputing infrastructure provides: 5.4 petabytes of file storage with an input/output speed in the range of 150 gigabyte/s is available to meet the performance challenges of today's most demanding users of HPC (high-performance computing) systems. The Cray XC40 system Hornet ranks as number 16 in the current Top500 list and achieved a Linpack value of 2,763 TFLOP/s. As part of the GCS, HLRS participates in the European project PRACE (Partnership for Advanced Computing in Europe), extending its reach to all European member countries, and has already provided hundreds of millions of cpu hours to the European user community. Additionally, HLRS participates with partners in Germany in two Exascale Software Initiatives at European Level, namely CRESTA (http://cresta.epcc.ed.ac.uk/) and Mont-Blanc 2 (http://www.montblanc-project.eu/), 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 GA 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. In October 2014, a new project has been started to strengthen the governance of the GA over the next 3 years.

Most of the projects from the second BMBF HPC-call have ended in mid-2014, while the projects from the third BMBF HPC-call will run for approximately one more year. This call was directed towards proposals that enable and support the execution of petascale applications on more than 100,000 processors. While the projects of the first funding round started in early 2009 and those of the second round in April 2011, the third (and thus far last) 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*. There is still the strong hope – and need – 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 very small amounting to less than 10 % 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 highly important for our community and will also greatly influence the development of new technologies and industrial products. Beyond being highly significant, the success of this approach will finally determine whether Germany will be an accepted partner alongside the leading technology and research nations worldwide.

With the support of the German Research Foundation (DFG), in January 2013 we have started the additional Priority Program 1648 'Software for Exascale Computing (SPPEXA)' in the field of HPC. As time is passing by so fast, a new round of proposals are already expected to be submitted on January 15, 2015, in response to the second phase of this Priority Program. This present call invites proposals for the second 3-year funding period from 2016 to 2018 and is now opening up to foster international collaboration. The call is intended to support collaborative projects of bilateral or trilateral research teams, bringing together researchers from France (ANR), Germany (DFG), and Japan (JST).

Since 1996, the HLRS has supported the scientific community as part of its official mission. As in the previous years, the major results of the last 12 months were presented at the 16th Annual Results and Review Workshop on High Performance Computing in Science and Engineering, held on September 29–30, 2014, 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 2013 and September 2014. Overall, a number of 45 papers were chosen from Physics; Molecules, Surfaces, and Solids; Reactive Flow; Computational Fluid Dynamics (CFD); Transport and Climate; and Miscellaneous Topics. The largest

number of contributions originated from the CFD field, as in many previous years, with 18 papers. Even though such a small collection cannot entirely represent an area this vast, the selected papers demonstrate the state-of-the-art use of high-performance computing in Germany. The authors were encouraged to emphasize the computational techniques used in solving the scientific or engineering problems examined. This is an often forgotten aspect and was the major focus of the workshop. Nevertheless, the importance of the newly computed scientific results for the specific disciplines is impressive.

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