

Preface

The Leibniz Supercomputing Centre (LRZ) and the Bavarian Competence Network for Technical and Scientific High Performance Computing (KONWIHR) publish in the present book results of numerical simulations facilitated by the High Performance Computer System in Bavaria (HLRB II) within the last two years. The papers were presented at the Fourth Joint HLRB and KONWIHR Review and Result Workshop in Garching on 8th and 9th December 2009, and were selected from all progress reports of projects that use the HLRB II. Similar to the workshop two years ago, the majority of the contributed papers belong to the area of computational fluid dynamics (CFD), condensed matter physics, astrophysics, chemistry, computer sciences and high-energy physics. We note a considerable increase of the user community in some areas: Compared to 2007, the number of papers increased from 6 to 12 in condensed matter physics and from 2 to 5 in high-energy physics. Bio sciences contributed only one paper in 2007, but four papers in 2009. This indicates that the area of application of supercomputers is continuously growing and entering new fields of research.

The year 2007 saw two major events of particular importance for the LRZ. First, after a substantial upgrade with dual-core processors the SGI Altix 4700 supercomputer reached a peak performance of more than 62 Teraflop/s. And second, the non-profit organization *Gauss Centre for Supercomputing e. V. (GCS)* was founded on April 13th. Its founding members were four representatives of the Jülich Research Centre, the Bavarian Academy of Sciences, and the University of Stuttgart, the heads of the three national supercomputing centres in Germany, namely the John von Neumann Institute for Computing/Jülich Supercomputing Centre (NIC/JSC), the LRZ (Munich), and the High Performance Computing Centre Stuttgart (HLRS), and the chairpersons of their respective steering committees. The foundation of the GCS marks an important strategic step towards creating a powerful HPC infrastructure at the Tier-0 level in Germany. Furthermore, on 17th April 2007 a European Tier-0 High Performance Computing Service was established at a meeting chaired by the German Federal Ministry of Education and Research in Berlin involving 14 partner nations in Europe. Today, 21 European nations form the Partnership for Advanced Computing in Europe (PRACE) with the goal to implement a Tier-0 HPC system

infrastructure. Six nations plan to offer HPC cycles with a value of EUR 100 million each over a period of 5 years. These nations are called ‘hosting members’ of PRACE, one of which is Germany. Via the GCS the LRZ will thus be one of the PRACE Tier-0 centres in the future.

It is of utmost importance that users of the HLRB II gain further experience in the development of sophisticated numerical methods and advanced algorithms. The workshop in December 2009 has demonstrated remarkable progress in this respect over the past two years: The number of cores that were employed in several applications has increased remarkably, though it is still fairly below the approximately 10,000 cores available at the HLRB II. The next generation of supercomputers will have a number of cores that is an order of magnitude larger in order to allow for computations in the Petaflop/s range. Scaling applications to such a high number of cores will be a formidable challenge for the near future and will require major revisions in the simulation software, with a special emphasize on new parallelization techniques.

Besides the aforementioned founding role in PRACE, the LRZ is an active partner in the European HPC infrastructure project DEISA (Distributed European Infrastructure for Supercomputing Applications). Customers of the HLRB II thus also have access to other European High Performance Computers and can choose whatever architecture is best suited for their specific project. Analogously, HLRB II serves customers from other European countries for the same reason.

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