High Performance Computing in Science and Engineering ’08

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Editors

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Preface

The discussions and plans on all scientific, advisory, and political levels to realize an even larger "European Supercomputer" in Germany, where the hardware costs alone will be hundreds of millions Euro – much more than in the past – are getting closer to realization. As part of the strategy, the three national supercomputing centres HLRS (Stuttgart), NIC/JSC (Jülich) and LRZ (Munich) have formed the Gauss Centre for Supercomputing (GCS) as a new virtual organization enabled by an agreement between the Federal Ministry of Education and Research (BMBF) and the state ministries for research of Baden-Württemberg, Bayern, and Nordrhein-Westfalen. Already today, the GCS provides the most powerful high-performance computing infrastructure in Europe. Through GCS, HLRS participates in the European project PRACE (Partnership for Advances Computing in Europe) and extends its reach to all European member countries. These activities aligns well with the activities of HLRS in the European HPC infrastructure project DEISA (Distributed European Infrastructure for Supercomputing Applications) and in the European HPC support project HPC-Europa. Beyond that, HLRS and its partners in the GCS have agreed on a common strategy for the installation of the next generation of leading edge HPC hardware over the next five years.

The University of Stuttgart and the University of Karlsruhe have furthermore agreed to bundle their competences and resources. Stuttgart will take a leading role in HPC being responsible for the operation and support for the national HPC facilities. Karlsruhe – with the newly created Karlsruhe Institute of Technology – will integrate its activities in Grid computing to take a lead in the state of Baden-Württemberg in the field of distributed systems and data management. The two centers will collaborate under the umbrella of a common organization.

Moreover, it is expected that in the next few months – following the proposal of the German HPC community, guided by Professor Andreas Reuter (EML) – the reshape of the High Performance Computing in Germany will

proceed to form the German HPC "Gauß-Allianz", with the goal to improve and establish competitiveness for the coming years.

Beyond stabilization and strengthening of the existing German infrastructures – including the necessary hardware at a worldwide competitive level – a major software research and support program to enable Computational Science and Engineering on the required level of expertise and performance – which means: running Petascale applications on more than 100.000 processors – has been established by the BMBF. The projects of the first funding round are about to start at the end of 2008. It is expected that – after this first funding round – the next four years another 20 Million Euro will be spend – on a yearly basis – for projects to develop scalable algorithms, methods, and tools to support massively parallel systems. As we all know, we do not only need competitive hardware but also excellent software and methods to approach – and solve – the most demanding problems in science and engineering. The success of this approach is of utmost importance for our community and also will strongly influence the development of new technologies and industrial products; beyond that, this will finally determine if Germany will be an accepted partner among the leading technology and research nations.

Having been awarded funding as part of the German national initiative of excellence in the Cluster of Excellence for Simulation Technology, HLRS has started to further integrate its research with application scientists, computer scientists and mathematicians over the last year. With a focus on workflow management and the programming of large scale systems, HLRS is pursuing a strategy that will improve support for user with the demand to run thousands of jobs in the next years.

In addition, HLRS has significantly strengthened its collaboration within Germany. On March 7th 2008, the Automotive Simulation Center Stuttgart (ASCS) was founded. The focus of the center is on the development for simulation software for research in automotive engineering. Bringing together automotive manufactures and independent software vendors as well as researchers and hardware vendors the center is excellently positioned to not only strongly drive application research for automotive HPC simulation but will also significantly accelerate the know-how transfer from research into industrial development.

Since 1996, HLRS is supporting the scientific community as part of its official mission. Like in the years before, the major results of the last 12 months were reported at the Eleventh Results and Review Workshop on High Performance Computing in Science and Engineering, which was held September 29-30, 2008 at Stuttgart University. This volume contains the written versions of the research work presented. The papers have been selected from all projects running at HLRS and at SSC Karlsruhe during the one year period beginning October 2007. Overall, about 40 papers have been chosen from Physics, Solid State Physics, Computational Fluid Dynamics, Chemistry, and other topics. The largest number of contributions, as in many other years, came from CFD with 18 papers. Although such a small collection cannot represent a large area

in total, the selected papers demonstrate the state of the art in high performance computing in Germany. The authors were encouraged to emphasize computational techniques used in solving the problems examined. This often forgotten aspect was the major focus of these proceedings, nevertheless this should not disregard the importance of the newly computed scientific results for the specific disciplines.

We gratefully acknowledge the continued support of the Land Baden-Württemberg in promoting and supporting high performance computing. Grateful acknowledgement is also due to the Deutsche Forschungsgemeinschaft (DFG): many projects processed on the machines of HLRS and SSC could not have been carried out without the support of the DFG. Also, we thank the Springer Verlag for publishing this volume and, thus, helping to position the local activities into an international frame. We hope that this series of publications is contributing to the global promotion of high performance scientific computing.

Stuttgart, October 2008

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