Preface

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In 2006 the NIC Symposium again brings together scientists from a variety of scientific fields, who have used the facilities of the John von Neumann-Institute for Computing (NIC) for their high performance computing applications. For the present proceedings of the NIC Symposium a referee panel selected 45 contributions which illustrate the progress in computer based science at NIC. Out of these, 15 projects were selected to be presented in talks at the NIC Symposium. Before turning to the projects let us focus on recent developments at NIC.

Since the last NIC Symposium in 2004 the IBM p690 supercomputer JuMP (Jülich Multiprocessor) with its peak performance of 8.9 TFlop/s has been the main working horse. This year a new era of supercomputing at NIC has begun with the installation of an IBM Blue Gene/L system. Its peak performance of 45 TFlop/s makes it presently the most powerful supercomputer in Europe. It will be available primarily for flagship projects which are particularly suited for such a machine and can use the very large numbers of processors in parallel, which this system offers. The majority of applications at NIC will, however, still be carried out on the JuMP system. At the same time the computer installation at DESY Zeuthen has been augmented with the newest generation of APE machines, the apeNEXT special purpose high-performance computers.

Some further developments at NIC can also be reported. So far NIC has been supported by its founding organizations, the Forschungszentrum Jülich (FZJ) and the Deutsches Elektronen-Synchrotron DESY. In 2006 the Gesellschaft für Schwerionenforschung (GSI) in Darmstadt will join the party as a third member, based on its efforts in the area of computational nuclear and particle physics. In line with this decision GSI intends to create a new research group focussing on topics relevant for GSI. In July 2005 the former NIC research group on “Complex Systems” changed into the research group on “Computational Biology and Biophysics”, headed by Prof. U. Hansmann.

NIC has participated in a number of European projects. Among them is the Distributed European Infrastructure for Supercomputing (DEISA) with 11 partner institutions. The main objectives of the DEISA consortium are to deploy and operate a persistent distributed supercomputing environment with continental scope and to enable scientific discovery across a broad spectrum of science and technology. In 2005 the DEISA Extreme Computing Initiative (DECI) has been launched with the purpose to enable a number of grand challenge applications in all areas of science and technology. Out of 52 applications 29 have been approved, including the 3 ones handed in via NIC, which can now benefit from the DEISA infrastructure. Another example, where NIC plays a central role, is the second stage of "Enabling Grids for E-Science in Europe" (EGEE2), a CERN-led, EU-sponsored collaboration of more than 100 institutes from Europe and beyond, aimed at providing the infrastructure to be used by the LHC Computing Grid (LCG) project and subsequently by other sciences.

An initiative directed towards the new member states of the European Union was started in 2005 with the aim to trigger and advance the collaboration with computational scientists from those countries. The related NIC Workshop "Strengthening Computational Science in Europe" in January 2006 also served this goal.

Altogether NIC has further consolidated its role as a leading European supercomputer centre. If supercomputing in Europe is not to fall behind the international development, substantial efforts have to be made. NIC is well prepared to contribute its part.

The research done with the computers at NIC mirrors the diversity of science. Most of the projects carried out at NIC come from universities. They cover a wide range of scientific activities from basic to applied research. Basic research, which is oriented towards the acquisition of scientific knowledge, includes the physics of elementary particles, which is strongly represented at NIC. Involved Monte Carlo calculations lead to a better understanding of the fundamental constituents of matter and their interactions. Another example is astrophysics, which attempts with the help of computer simulations to find out how structures in the universe formed and how objects like stars end in supernova explosions.

On the other hand projects are carried out at NIC which are closer to applications, from materials science and chemistry to earth and environmental sciences. Properties of materials like liquid crystals and nanostructured solids as well as the transport of contaminants in the soil and nonlinear EEG analysis of epilepsy patients are research topics which can nowadays not be pursued successfully without the use of powerful supercomputers.

The NIC symposium and its proceedings provide an overview over the fascinating field of computer based modern science. Essential for the prosperity of fields like those mentioned above are not only centres like NIC, but beyond it the presence of a pyramidal structure of computational resources, from local workstations and smaller clusters, very high performance computers at universities, up to national and international supercomputer centres.

We thank the referees for selecting the contributions for his book. Most of them are also members of the NIC peer review board. We also thank the authors for representing the NIC by their contributions in this book. Special thanks go to the Institute for Applied Mathematics (ZAM) at FZJ and to DESY for providing the high quality computing environments

and user service, which are crucial for the successful realisation of the projects presented in this book and the talks at the symposium. Thanks go also to Fabian Fredel and Ms. Beate Herrmann for their efforts to compile all the contributions and to create a high quality book from them. Last, but not least we thank Ms. Helga Frank and Ms. Erika Wittig for their help in organizing the 3rd NIC-Symposium.

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