The John von Neumann Institute for Computing (NIC):
A survey of its supercomputer facilities and
its Europe-wide computational science activities

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The John von Neumann Institute for Computing (NIC) at the Research Centre Jülich, Germany, is one of
the leading supercomputing centres in Europe. Founded as a national centre in the mid-eighties it now provides
more and more resources to European scientists. This happens within EU-funded projects (I3HP, DEISA) or
Europe-wide scientific collaborations. Beyond these activities NIC started an initiative towards the new EU
member states in summer 2004. Outstanding research groups are offered to exploit the supercomputers at NIC
to accelerate their investigations on leading-edge technology.

The article gives an overview of the organisational structure of NIC, its current supercomputer systems, and
its user support. Transnational Access (TA) within I3HP is described as well as access by the initiative for new
EU member states. The volume of these offers and the procedure of how to apply for supercomputer resources is
introduced in detail.

1. NIC WITHIN THE GERMAN RESEARCH INFRASTRUCTURE

The John von Neumann Institute for Computing (NIC) is embedded in the German research infrastructure through the Helmholtz Association of National Research Centres, which is besides the Max Planck and the Fraunhofer Societies the leading extra-university research organisation in Germany. The member institutions of the Helmholtz Association perform application-oriented research in science and technology with large-scale facilities, e.g. particle accelerators. The biggest centre of the Helmholtz Association is the Research Centre Jülich, which has 4300 employees and is doing research in the fields of health, earth and environment, energy, structure of matter, and key technologies with a budget of 360 million Euro per year, funded to a large extent by the federal government of Germany.

Together with the German Electron Synchrotron Foundation DESY, also a Helmholtz centre, Research Centre Jülich founded NIC in 1987 as the first national high-performance computing centre in Germany. NIC’s mission is primarily the provision of supercomputer capacity for projects in science, research, and industry. Secondly, NIC conducts supercomputer-oriented research and development in selected fields of physics and other natural sciences by research groups of competence. These tasks are complemented by high-level training and education in the fields of supercomputing by symposia, workshops, summer schools, seminars and courses. This mission exactly corresponds to the general Helmholtz mission “to enable scientists to solve grand challenge problems by operating large-scale facilities”.

In 2004 an international Perspective Committee made an assessment of the future development of the Research Centre Jülich. Its major recommendations were i.) to focus on condensed matter physics as the basis for the investigation of functions and diseases of the human brain, bio and nanoelectronics, sustained energy supply, and networked environmental research and ii.) to expand the supercomputing centre NIC into a European centre for high-end computing. Since then NIC

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strengthened its European activities, which already existed partly since many years.

2. ORGANISATION OF NIC

NIC is managed by a board of directors. A scientific council gives recommendations with respect to the scientific programme of NIC and the allocation of supercomputing resources to the NIC projects. Within NIC the Central Institute for Applied Mathematics (ZAM) of the Research Centre Jülich provides the major production systems to the scientific community of NIC. The Centre for Parallel Computing at the DESY laboratory in Zeuthen makes available special-purpose computers to research groups in elementary particle physics. Research Groups are dedicated to supercomputer-oriented investigation in selected fields of physics and other natural sciences. Recently a research group on computational biology and biophysics in Jülich has been set up. Another group in Zeuthen works in the field of elementary particle physics.

Figure 1. NIC organisation chart.

3. SUPERCOMPUTING FACILITIES AT NIC

NIC/ZAM has a long tradition in providing IT services and in research and development in the area of scientific computing. Very early the potential of supercomputing-related research was recognised and the first multiprocessor Cray outside the U.S. was installed at the Research Centre Jülich in 1983. Since that time all major technologies which came up in supercomputing were immediately evaluated at NIC/ZAM and brought to production on large systems, ranking among the Top20 worldwide at a very early stage.

The current supercomputer in Jülich is an IBM p690 based system called JUMP, consisting of 1312 POWER4+ processors, reaching an overall peak performance of 8.9 Tflops and a LINPACK performance of 5.6 Tflops. It is complemented by an IBM Blue Gene/L, a highly scalable system with low power and floor space requirements. Its 2048 PowerPC 440 processors reach a peak performance of 5.7 Tflops (4.7 Tflops LINPACK performance) and are very well suited for applications which scale up to thousands of processors and have only limited memory requirements.

Furthermore, a CRAY XD1 system, which is based on Opteron processors and a very fast interconnect, has been provided for the NIC biophysics research group. Part of this machine is being equipped with FPGA co-processors in order to further speed up the basic algorithms of particle interactions in bio- and astrophysics.

4. ACCESS TO NIC RESOURCES

Being one of the leading supercomputing centres in Europe, NIC offers supercomputer capacity and capabilities to science, research and industry Europe-wide; resources are granted through an international peer review process for a one-year period, decision criterion is solely the scientific quality of the proposal. Details about the preparation of the proposal and guidelines for the submission can be found at www.fz-juelich.de/nic.

5. ORIGIN OF USERS

NIC currently serves more than 150 projects in computational science and engineering with more than 400 scientists at 45 sites in Germany, in particular at universities. But not only German institutions use the supercomputing facilities at NIC. An increasing number of European research groups of different origin are accessing NIC and take advantage of its facilities and its expertise in computational science.
5.1. Individual NIC projects in Europe

Individual NIC projects, which are located outside Germany have three different origins: One source are German researchers, who move to a position abroad and continue running their projects at the new location. Another source are foreign guest scientists who visit NIC for a certain time. They learn very quickly to exploit the supercomputers at NIC, which accelerate their research in many cases significantly. So they try to extend their projects and to profit from NIC even after their return. A third kind of individual projects has its origin in a scientific collaboration with computational scientists at NIC/ZAM. For example, common European projects which perform methodological development of software packages in theoretical chemistry make it necessary to access the supercomputers at NIC from different sites in Europe. Altogether NIC currently serves about ten projects of this kind in Europe.

5.2. EU project I3HP

Within the EU project Integrated Infrastructure Initiative on Hadron Physics (I3HP) NIC offers Transnational Access (TA) to its supercomputer facilities. Currently, four different user groups – DESY (Germany), University of Glasgow (UK), University of Edinburgh (UK), and University of Cyprus (Cyprus) – which are all integrated in the I3HP networking activity N2 Computational Hadron Physics (ComHP) make use of this offer.

The EU is funding 500,000 GFlops hours on JUMP at Jülich for the years 2004-2007 for non-German researchers. This number corresponds to 73,400 processor hours on the system which means less than 2,000 processor hours per month. Additionally, NIC agreed to spend another 4,000 processor hours per month for German I3HP users. However, even the aggregated number of processor hours is not sufficient for large-scale lattice QCD simulations. Nevertheless it should be used in an appropriate manner to demonstrate the value of leveraging supercomputing resources in the framework of the I3HP project. Researchers who are interested in requesting part of these resources should visit the web page www.fz-juelich.de/nic/i3hp-nic-ta, where a lot of information is given about the application procedure and the usage of the supercomputer facility. It is also advisable to coordinate any access plan with the management of the ComHP project. As for any other NIC project a scientific proposal has to be written and submitted to the chairman of the NIC scientific council. It will be reviewed by the NIC resource allocation committee taking into account the remaining resources.

5.3. EU project DEISA

DEISA (Distributed European Infrastructure for Supercomputing Applications) is like I3HP a European I3 project. The goal of its partners, mainly institutions which operate large supercomputer facilities, is to establish a distributed European infrastructure for supercomputing applications. After developing and implementing methods and software, which guarantee a transparent access to the different supercomputers and file systems, DEISA in April 2005 started its DEISA Extreme Computing Initiative (DECI) by selecting applications with extreme computing demands, which will benefit a lot from the established infrastructure. They are peer-reviewed and nominated by national scientific evaluation committees.

The DEISA partners spend up to 10% of their supercomputer resources for DECI applications, which really allows for large-scale projects. First DECI applications are running since October 2005 at the different DEISA sites. Applications proposed for DECI should be challenging projects which are tackled in international collaborations and which have either extreme computing demands or base on a workflow between at least two platforms or are coupled applications involving more than one system. Details can be found at www.deisa.org, the next deadline for further DECI proposals will be spring 2006.

5.4. NIC initiative

In summer 2004 the NIC directorate started an initiative towards the new EU member states implementing the recommendations of the Perspec-
tive Committee. Outstanding research groups are offered to exploit the supercomputers at NIC to accelerate their investigations on leading-edge computing technology. Resources in the range of 50,000 processor hours per month on the IBM JUMP system have been reserved. Interested researchers from universities or research laboratories in the corresponding countries are invited to submit scientific proposals. They will undergo a peer reviewing process like any other proposal and, after a positive evaluation, they will be granted an adequate amount of free supercomputer time. There are no further administrative requirements.

From this initiative NIC expects both a closer collaboration with researchers from the new EU member states who rely on supercomputing and an exchange of views on a future European high-end computing infrastructure for the computational sciences, which is to be established in the 7th Framework Programme of the European Commission. A platform to discuss this issue will be the workshop “Strengthening Computational Science in Europe” organised by NIC and renowned experts in the field of supercomputing from the new EU member states, to be held in Jülich in January 2006.

This initiative is also being promoted by presentations of NIC/ZAM at different research institutions of the new EU member states. Potential users could be attracted in Prague, Brno, Warsaw, Bratislava, Budapest, and Nicosia.

6. USER SUPPORT

It is obvious that this large number of different users requires an efficient and well-organised user support. At NIC users are supported by a three level structure: A user help desk is the first level to be contacted for all questions and problems that may arise. If necessary the problem is forwarded to a ZAM specialist who may help with more specific questions, concerning in particular methodological and optimisation aspects. Furthermore, each of the projects is assigned a special advisor, a staff member of ZAM, who has a corresponding scientific education, can discuss scientific questions with the project members, and form long-term partnerships.

7. RESEARCH AT NIC

Research being done by NIC itself is separated into two parts. On one hand NIC operates research groups of competence, as can be seen in Figure 1. Currently there is one group on computational biology and biophysics (see www.fz-juelich.de/nic/cbb for details) and another one on elementary particles (see www-zeuthen.desy.de/nic). Both groups are doing research like groups at universities with the advantage of a very easy access to supercomputing facilities and to computer scientists at NIC.

On the other hand, there is a variety of research done by scientists at NIC/ZAM, which is motivated primarily by the scientific interests of the NIC user community and aims to improve the methods and techniques applied by researchers of the NIC projects. In the Computational Sciences, NIC/ZAM is active in modelling and simulating complex atomistic models, Quantum Chromodynamics simulations, and quantum computer simulations [1,2,3,4]. In Applied Mathematics, fast parallel algorithms for the efficient calculation of long-range interactions are developed [5,6], as well as fast linear algebra algorithms, stochastic models, and data mining techniques [7,8,9]. In Computer Science, the focus is on performance tools, virtual reality and computational steering techniques [10,11,12,13], and middleware for cluster computing [14]. A very active research field is Grid Computing, where an easy and secure access to computing resources and data has to be ensured by developing the corresponding Grid middleware [15,16,17,18,19,20] as well as the underlying high-speed data communication [21].

This research is complemented by a rich offer of high-level education and training activities, like conferences [22], symposia [23], schools, workshops, student programs, seminars and advanced courses. For the schools, lecture notes are published, whose review style makes them a highly valuable source of knowledge for every scientist, who wants to work in the area [24,25].
8. SUMMARY AND OUTLOOK

With all these activities NIC works towards becoming a leading site in a future European supercomputing network and towards remaining among the Top 10 supercomputing centres worldwide with respect to compute power, service and research.

Besides continually enhancing its supercomputing facilities, NIC will further improve its research relations to European computational science communities like e.g. PSI-k, ILDG, and Ce- cam. Together with the user communities, Simulation Laboratories will be founded around the computing facilities, e.g. for nanoscience, atomistic simulation of materials, astrophysics, ab initio molecular dynamics, biology, etc. Within the Simulation Laboratories, jointly with NIC support-teams, representatives from the various scientific communities will provide specific user support such as provision of complex computer codes, maintenance and optimization of software and algorithms, as well as specific in-depth education in order to guarantee the most effective exploitation of the computer resources and to ensure the utmost scientific impact.

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