The John von Neumann Institute for Computing (NIC): High-end computers for studying and promoting computational sciences in Europe

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Abstract

The John von Neumann Institute for Computing (NIC) at the Research Centre Jülich, Germany, is one of the leading supercomputing centres in Europe. Besides providing state-of-the-art hardware and software facilities, NIC focuses on research in scientific high-performance computing. In order to deliver excellent support to its users, it aims to gather and maintain competence in key areas of computational science. It stimulates interdisciplinary cooperation and promotes the knowledge transfer between the centre and the computational science communities (1).

This article covers the embedding of NIC in the German and European research structure, its organisation, its current supercomputer systems, its research activities in computational and computer science, its training and education, and its user support. It will be discussed how the different pieces fit together and how they enable scientists from Germany and Europe to perform state-of-the-art simulations of systems with highest complexity and to successfully compete with colleagues in the US and Japan. Furthermore, the status of European activities to establish a European supercomputing infrastructure will be presented.

1. NIC in Germany and in Europe

In Germany, the Helmholtz Association of National Research Centres is besides the Max-Planck and the Fraunhofer Society the leading extra-university research organisation. Its member institutions perform application-oriented research in science and technology with large-scale facilities, e.g. particle accelerators. NIC is a common institute of three major Helmholtz centres, acting since 1987 as the first national high-performance computing centre in Germany.

In Europe, NIC is well recognised for its activities in Grid Computing and its participation in European infrastructure projects like DEISA *(Distributed European Infrastructure for Supercomputing Applications)* or I3HP *(Integrated Infrastructure Initiative on Hadron Physics)*. Furthermore, NIC provides resources to an increasing number of European research projects of different origin.

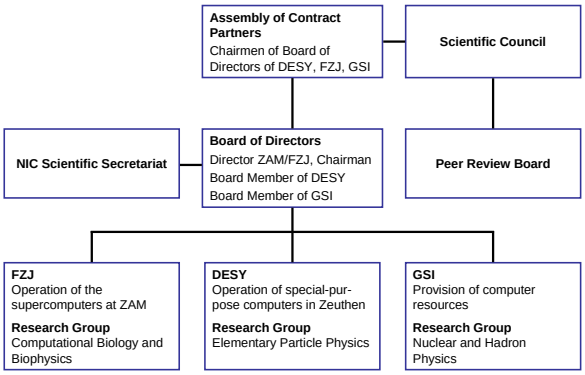

Fig. 1. NIC organisation chart.

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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 (see Figure 1).

3. Supercomputers at NIC

Currently, two big IBM systems are operated to meet the needs of our users: A Blue Gene/L system with 16,384 Power PC 440 processors reaches a peak performance of 46.8 Tflops and is very well suited for highly scalable applications with moderate memory requirements. A p690-based system with 1,312 POWER4+ processors reaching 8.9 Tflops serves as a general purpose supercomputer and is best for memory intensive applications.

4. Research Activities 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. All groups are doing research like university groups with the advantage of an 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 (2), and quantum computer simulations. In Applied Mathematics, fast parallel algorithms for the efficient calculation of long-range interactions are developed, as well as fast linear algebra algorithms, stochastic models, and data mining techniques. In Computer Science, the focus is on performance tools, virtual reality and computational steering techniques, and middleware for cluster computing. 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 as well as the underlying high-speed data communication.

This research is complemented by a rich offer of high-level education and training activities, like conferences, symposia, schools, workshops, student programs, and advanced courses. For the schools, lecture notes are published (3), whose review style makes them a valuable source of knowledge for every scientist, who wants to work in the area.

5. 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.

6. European Supercomputing Centre

The EU is currently investigating the options of setting up a powerful European HPC research infrastructure. In this process different policy-making groups are involved, like the European Strategy Forum on Research Infrastructures (ESFRI), the e-Infrastructure Reflection Group (e-IRG), and the HPC European Task Force (HET). Embedded in the Gauss Centre for Supercomputing, which is the recently founded network of the three German HPC centres and also comprises LRZ (Leibniz Computing Centre) and HLRS (High-performance Computing Centre Stuttgart), NIC aims to play a leading part in the future European HPC infrastructure.

References

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