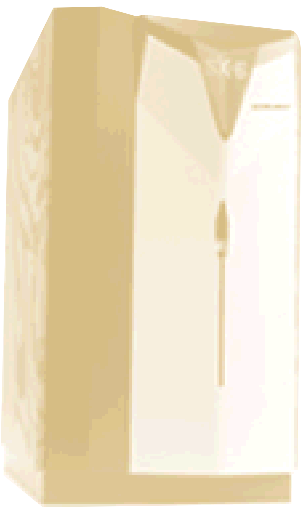
National Supercomputing Centres – Turning the Innovation Spiral

Scientific Supercomputing as a Key Technology

For the first time in computing history, in the 1990s we were able to establish a well balanced pyramid ranging from local-area and wide-area broadband networks, via the diversity of work-station and PC platforms in client-server structures supporting cooperative and even realtime computing, up to the layer of medium-sized innovative computer architectures capable to spread computational science and engineering as a key technology over science and industry and also to support methodologically and capacity-wise, finally, the apex of the pyramid, the infrastructure of top-level supercomputers with the mission of a nation-wide resource. Several national initiatives focused much attention and gave terrific technological and scientific impact to a research and development field which developed in parallel with the tremendous increase and ubiquitous distribution of computer capacity over the past five decades: Although born in the 1940s, it has been named Computational Science only in the mid-1980s by the Nobel Price Winner Kenneth Wilson and has been termed in the 1990s Computational Science & Engineering. Computer simulation has grown and established itself as the third category of scientific methodology. This ever-innovating discipline fundamentally supplements and complements theory and experiment, as the two traditional categories of scientific investigation, in a qualitative and quantitative manner while integrating these into the methodological tripod of science and engineering. Being comparable rather with an experimental discipline, Computational Science and Engineering wastly extends the analytical techniques provided by theory and mathematics; today, in a sense, it is synonymous with investigating complex systems. Its main instrument is the supercomputer; its primary technique is computer simulation. Unsolved complex problems in the areas of climate research and weather forecast, chemical reactions and combustion, biochemistry, biology, environment and ecological as well as economic and sociologic systems, order-disorder phenomena in condensed-matter physics, astrophysics and cosmology, quantum chromodynamics, and, in particular, aerodynamics have been identified as "Grand Challenges". The tripod of science and engineering, thus, has proved to provide scientific research and technology with the methodological basis and the instrumental laboratory to effectively approach the solutions of complex problems which are critical to the future of science, technology, and society. It will be a crucial factor for the industry in order to meet the requirements of international economic competition especially in the area of high-tech products. The various strategic position papers and the government technology programs in the USA, in Europe, and in Japan in the 1990s claimed that the timely provision of supercomputers to science and engineering and the ambitious development of innovative supercomputing hardware and software architectures as well as new algorithms and effective programming tools are an urgent research-strategic response to the grand challenges arising from these huge scientific and technological barriers. Their goals were also to enhance supercomputing by stimulating the technology transfer from universities and research institutions into industry and by increasing the fraction of the technical community which gets the opportunity to develop the skills required to efficiently access the high-performance computing resources.
Thus, scientific supercomputing as a discipline covering the fields of mathematical modeling, computer simulation, and visualization has become a strategic key technology. The growing complexity of the systems and processes under investigation in natural sciences and engineering results in simultaneously increasing requirements on the accuracy of mathematical modeling, the efficiency of numerical and non-numerical methods as well as on the performance of computer architectures and networks, and on the software systems, programming models, and programming techniques available for this purpose.
In industry, design optimization for improving products and accelerating development cycles is a major economic factor. Hence, competency in scientific computing has become an indispensable site factor of competitiveness. In the USA, strategic funding programmes push innovation: Apart from the programs and efforts under the NPACI initiative of the National Science Foundation, the US government has launched a big programmatic offensive for the methodical upgrade of scientific computing, i.e. the DoE's Accelerated Strategic Computing Initiative (ASCI), together with the national research laboratories of Los Alamos, Lawrence Livermore, and Sandia, universities, and industries. Despite or even challenged by the success of the Japanese Earth Simulator Project which conquered the top of the TOP500 list in spring 2002, ASCI research and development will considerably increase the scientific and technological lead of the USA and enhance the instrumental equipment of their centres with new parallel supercomputers in a nearly unrivaled manner for years. However, these developments will challenge not only system reliability, availability and serviceability to novel levels, but also algorithm design and, in particular, adaptivity, accuracy, and stability of parallel numerical methods. In the future, research and industry will fall behind where such supercomputers of highest class will not be available. Therefore, Germany as a traditionally strong site of science and industry requires long-lasting measures to maintain and enhance scientific supercomputing.



Recommendations of the German Science Council

In 1995 and 2000, the Science Council made recommendations with regard to the role of supercomputing for German science and technology. These recommendations clearly underline the significance of supercomputing in order to gain scientific know-how as well as to establish an efficient research infrastructure. At the top of the pyramid, sufficient supercomputing capacity is to be supplied by several national centres.

Access to these centres via efficient data networks must be ensured. Furthermore, the centres have to be embedded in a competence network in order to promote the development of methods, tools, and applications, and the education and training of young scientists and engineers.
In the Year 2000 Recommendation, the German Science Council stated that high performance computing (HPC) is indispensable for top research in the global competition of science, research, and engineering while the demand on HPC capacity tends to become unlimited due to the increasing problem complexity. Therefore, continuous investments are necessary on all levels of the performance pyramid for scientific computing. In addition, networks of competence must support the efficient usage of supercomputers, and HPC education and training must be enhanced, since so far HPC is yet insufficiently integrated into curricula; education must not be limited to PCs and workstations. In particular, efforts in HPC software development need to be enforced. Finally, strategic coordination of investments and procurements is necessary. Therefore, a National Coordination Committee was founded to develop strategies for continuous funding and upgrade scheduling of the HPC centres' resources (and balance potential regional ambitions according to national goals). This Coordination Committee started working in May 2001.
Its tasks and responsibilities are:

- Decisions on investments supported by prospective exploration of HPC demands, strategic advice for federal and "Länder" HPC plans and decisions as well as recommendations for upgrades in infrastructure and staffing.
- Orientational support by position papers and hearings on HPC issues and advice to the Science Council's HBFG Committee.
- Evolution of control and steering models by development and testing of demand-driven self-control mechanisms and investigations of differing accounting models for suitable user profiles.
- Develop a nation-wide concept for HPC provision including all centres independent of funding and institutional type and keeping the list of centres open for change and innovation.

The German Science Council favours in the Recommendation on the establishment and enhancement of national supercomputing centres a significant increase of the innovation frequency of the supercomputer hardware, however, without eliminating the financial and administrative barriers which force the individual centres to stick much too long with the systems. Therefore it is important to guarantee innovation also and primarily via other ways. The Recommendation proposes up to four national supercomputing centres which should be equipped to compete internationally at the apex of the performance pyramid. In the past, already four centres had qualified themselves with internationally outstanding profiles: HLRS in Stuttgart, LRZ in Munich, NIC at the Research Centre Jülich, and ZIB in Berlin. A single centre, which is either carried budget-wise by the Federal Government – like NIC – or according to the so-called HBFG Law by the corresponding federal country and the federal government with equal portions – like HLRS, LRZ, and ZIB – is not in the position today to place itself by its own financial power permanently in the pyramid apex, because in comparison to the long individual installation periods the decay of the once installed supercomputer power relative to the worldwide progress of supercomputer technology is extremely fast.
With respect to the dynamics of the supercomputer technology, effective concepts and procedures had to be developed to increase the flexibility in order to permanently provide science, research and engineering with access to the highest level of computing power. Thus, the intention of the Science Council to place Germany continuously at the apex of the performance pyramid must ground on a spiral of innovation which is steadily turned, with adequate phase shifts, by the three approved national supercomputing centres: HLRS, NIC, and LRZ, by coordinating and timely adapting their supercomputer procurements. In this way, it can be warrented that at any time the utmost novelty of supercomputer architecture and highest performance are available for science and research in Germany. This comprehensive strategy, of course, needs as necessary and sufficient condition and prerequisite a long-term guarantee and stabilization of the required budget frameworks by the federal as well as the local governments – which definitely has not yet been achieved, thus making every new procurement an ever challenging adventure.
In the same sense, as the Science Council outlined in corresponding recommendations, the demand of powerful data networks to support the interconnection of the supercomputing centres requests also the long-term government responsibility to maintain and enhance broadband communications in ever innovative steps in order to promote the key technology of scientific computing in science and industry. A corresponding long-range research program would be beneficial to improve the perspectives and the position of German science and technology as well as industry in the process of establishing enhanced broadband interconnections of supercomputing centres and competence centres to keep scientific computing in this country competitive within the EU and in interaction with the corresponding activity centres in USA and Japan.

Supercomputing Centres as Attractors of Competence

Definitely, at least in Germany, missing (super)computer hardware industry demands supercomputer centres to play the role of crystallization kernels and attractors of competence in scientific computing and in computational science and engineering. Also with respect to the developments in the USA it must be stated, that supercomputer centres are indispensable creators of competence structures as well as attractors of scientific computing. The John von Neumann Institute for Computing (NIC) – whose primary supercomputing resources are provided by the Central Institute for Applied Mathematics (ZAM) at the Research Centre Jülich –, the Supercomputer Centre (HLRS) at the University of Stuttgart, and the Leibniz Computer Centre (LRZ) act as National Supercomputer Centres along the strategic lines of the German Science Council by offering

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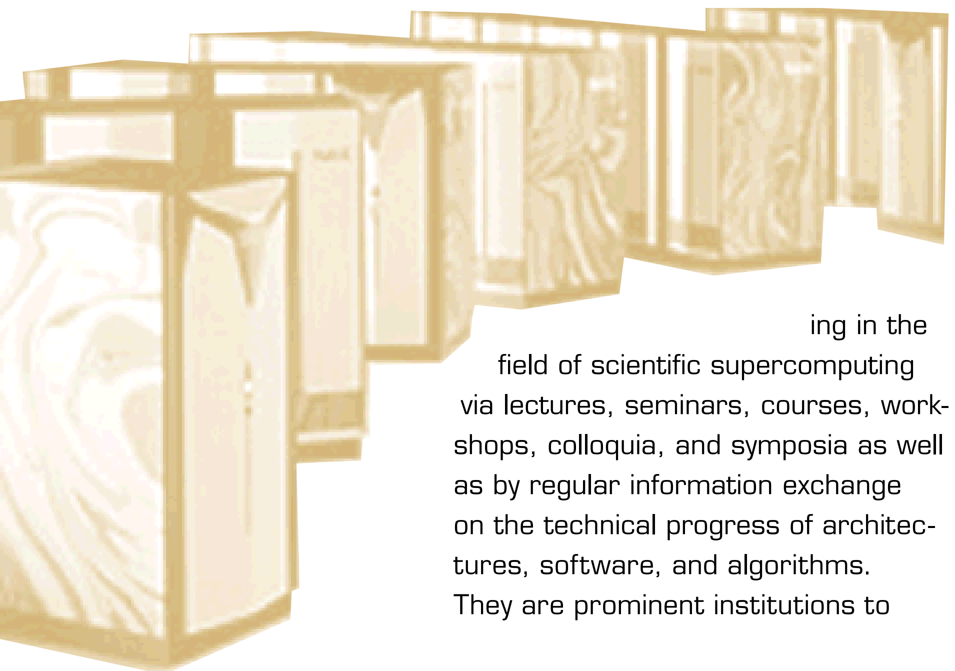
computing capabilities to scientists and engineers in universities, research institutes, and industry all over Germany, and by promoting competence and skills in scientific applications, mathematical algorithms, and visualization methods through research projects and educational programs. Since the very beginning of their operation, the utilization by science and research of the resources in these supercomputer centres is steered via peer reviewing and controlling procedures certifying the quality and scientific relevance of the projects which get approved access to these supercomputer resources. Steering Committees and Scientific Councils associated with the individual centres play an eminent role. The exchange of computer resources between the centres needs, of course, mutual aggreements on the votes of these committees which must guarantee the necessary exchange of information on the project applications and research proposals. The usage of these resources by the industry is ruled via different special regulations.
It is extremely important that the cooperating centres increase their joint efforts to foster education and train-



ing in the field of scientific supercomputing via lectures, seminars, courses, workshops, colloquia, and symposia as well as by regular information exchange on the technical progress of architectures, software, and algorithms.
They are prominent institutions to provide an efficient national scientific forum for the research groups in the competence centres and the project partners in science and industry in order to promote joint projects, to stimulate innovative research topics and facilitate interdisciplinary cooperations. Therefore, the question is becoming urgent whether and how the national supercomputing centres can be effectively integrated, together with the various competence centres of scientific computing, into a cooperative compound to further push innovative supercomputing methods and applications. The compound will act as a common turntable to strengthen and accelerate the transfer of the capabilities, techniques, and skills in scientific supercomputing into the applications in industry. This will increase mutual benefits and added values, which, finally, protect and perpetuate the high level of supercomputing in Germany in the international competition of science and economy, while the modern concepts and requirements of process modelling and product design, the "virtual laboratory" and "virtual product", are based on the potential of visualization and multimedia technologies, communication techniques, and cooperative work distribution.

Therefore, scientific computing is basically interdisciplinary. This innovative technology requires, in addition to solid knowledge and systematic know-how of the individual scientific and technical disciplines, the complete information-technological instruments of supercomputing and communications. The technology requests large performance steps in the computer architectures and algorithms. There is no doubt that the interaction of modelling, computer simulation and visualization with mathematical methodology and computer science has made the strategic interdiscipline of scientific supercomputing a key technology which definitely contributes to the strength of the international competitiveness of science and economy.
A major step in the support of science and research including industrial research projects by supercomputing capability and capacity was made in 1987 when the so-called HLRZ ("Höchstleistungsrechenzentrum") was founded by the Research Centre Jülich, DESY, and GMD. The Central Institute for Applied Mathematics in Jülich was and is the main carrier of this supercomputing centre which since 1998 is operated as the John von Neumann Institute for Computing (NIC) primarily by the Jülich Research Centre with DESY as partner who provides special purpose computers (of APE type) to the QCD community.
It definitely was a novelty in this country that supercomputer capacity could be provided to scientists all over Germany, based on the approval of peer-reviewed project proposals according to the DFG rules and regulations – a model which then was applied also to the foundation of the other two National Supercomputing Centres in Stuttgart and Munich in the 90-s. The establishment of the Stuttgart supercomputer centre HLRS in tight connection with the local industry Daimler and Porsche and the University of Karlsruhe via the joint venture "hww" with the debis company, now as T-Systems a daughter of the German Telekom, and DLR again represents a novel model of cooperation between science and industry on the strategic field of scientific supercomputing.

Synergy through Grid Technologies

In the past, technical and administrative conditions as well as the federal structure in Germany did not appear to ease the Germany-wide interconnection of computer centres as a natural instrument of scientific cooperation nor of economic exploitation of computer resources. Exceptions have been, on the one hand, the so-called North-German Vectorcomputer Compound (NVV) which, based on a state treatise of three federal countries, managed the joint usage and exchange of high-performance computer resources between ZIB in Berlin, the Regional Computer Centre (RRZN) in Hannover and the University Computer Centre in Kiel in the same manner as nowadays practiced with the two supercomputer subsystems at ZIB and RRZN extending the compound to six federal countries in Northern Germany; on the other hand, NIC in Jülich was able, according to the regulations within the Helmholtz Association of German Research Centres (HGF), to act beyond federal boundaries as a first national supercomputing centre until in the 90-s the two national supercomputing centres in Stuttgart and Munich got approved by the Science Council to offer their resources Germany-wide.
Today, a comprehensive competence structure provides beneficial conditions for the connection of supercomputing centres to exploit new concepts and paradigms of computing like grid computing on broadband communication

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networks. Thus, these supercomputing centres can

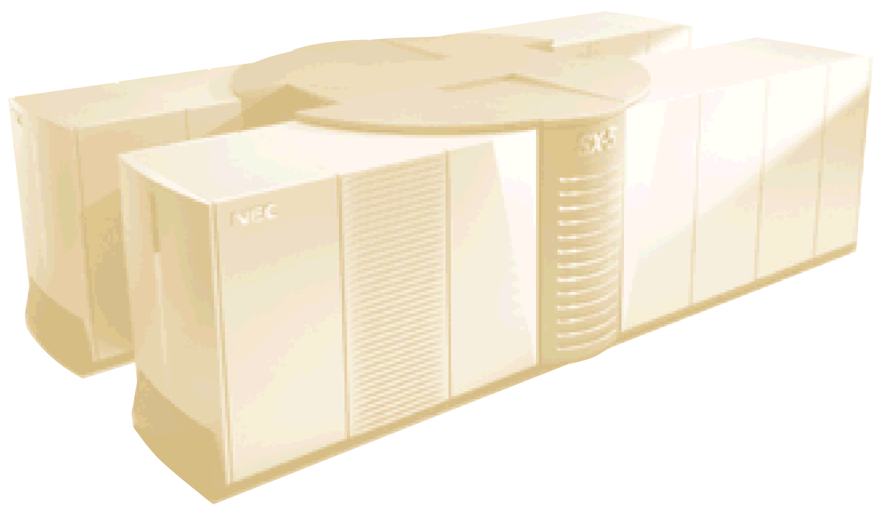
- promote supercomputing and its applications through interaction with other competence centres for scientific computing and their tight integration;
- enter more efficient cooperations through joint projects in scientific supercomputing, mathematical modelling, simulation methodology, and visualization;
- even better support and accelerate, with the compound of the centres as a turntable, the transfer of methods and technologies of this key technology into the application areas and product development in economy and industry;
- increase the efficient usage and, hence, the added value of their diverse and heterogeneous computer architectures through the tight connection via broadband networks and by the development of adequate interfaces and operations concepts;
- create and provide the scientific and technical platform, through the tight cooperation and communication compound of the centres, for future evolutionary steps of broadband communications, as offered by the DFN through G-WiN, and innovations via pilot testbed projects exploring, for instance, optical technology;
- can assure, through adequate financing strategies, mutual agreements, and coordination procedures, the permanent international top position of the supercomputing centres in Germany, thus contributing strongly to the international competetiveness of science and engineering.

The idea of a compound of the supercomputing-centres does not assume that in this way, as has been stated sometimes elsewhere in the past, the large computers in the centres, finally, could be ultimately efficiently utilized by a Germany-wide load-balancing model and, hence, the supposedly misguided local resource allocations get solved. The idea is rather the functional compound which exploits the diversity of supercomputer architectures and the broad and heterogeneous spectrum of large software systems. Technical and architectural reasons as well as licencing and economic criteria and aspects of competence, capability, and technical support make it sensible that the individual centres gradually specialize in (commercial) application software focussing on certain application fields. Such a functional compound of supercomputing centres will overcome the regional barriers which made it difficult in the past to provide resources on a reasonal mutual exchange basis to nonlocal users beyond those boundaries. In the future, one can guarantee such resource exchange via equivalent shares which can be dynamically controlled with respect to their mutual currencies through the already now installed sophisticated accounting systems

One of the major and most decisive factors of success of top research and, as a consequence, of industry and society in the future will be rapid and location-independent access to worldwide distributed data and other information technological (IT) resources and their sensible usage. The basis will be a highly complex, globally interlinked information infrastructure with complex access and administration mechanisms, which is commonly referred to as "grid computing" and, in UK, as "E-science". Grid computing or grid means the distributed IT infrastructure, including its access mechanisms. The structural concept of grid computing results from the necessity of combining supercomputers in a global functional system network of supercomputing centres and the integration of competence centres as well as from the worldwide linking of clusters of thousands of commodity processors.

Grid computing does not only set extreme requirements on broadband communications, but also needs the development of novel software systems for the "seamless access" to the distributed resources. In Germany, interconnection of supercomputers via grid technology was started with the UNICORE system already in 1996. For the global networks also other so-called open systems are being developed worldwide, e. g. Globus Toolkit. The grid or E-science concept additionally comprises application of grid technology to various disciplines, such as high-energy physics and astrophysics, biological sciences and medicine, or geo-research and environmental research, with the integration of large experimental devices (accelerators, satellites, tomographs, telescopes, and others) on the one hand and the setup of regionally distributed mass data archives and their supply for sophisticated information analysis (e.g. of accelerator data – from CERN – or satellite measurements) on the other hand. The initiative for the development of the UNICORE software system was launched in 1996 at ZAM in Jülich and funded by the BMBF through the UNICORE and the UNICORE Plus projects from 1997 to 1999 and from 2000 to 2002, respectively. With this software system, the concept of grid computing is provided with an effective "seamless interface". The software is also serving as a technical basis of several EU-funded grid projects like EUROGRID (European network of supercomputing centres), OpenMolGrid (Molecular Biology), and GRIP, ZAM being an important partner in these projects.

Recently, an initiative has been launched by the Helmholtz Association, in coordination with the other German science and research institutions and universities, in order to create and promote a new infrastructure which, as in other countries, is apt to revolutionize scientific research and development in Germany: the D-Grid. The tight interconnection of the National Supercomputer Centres and the integration of competence centres of scientific computing will definitely be one of the important missions of D-Grid.



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