Supercomputing

Made in Jülich

JÜLICH
FORSCHUNGSZENTRUM

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Forschungszentrum Jülich ...

... pursues cutting-edge interdisciplinary research addressing the pressing issues of the present. With its competence in materials science and simulation and its expertise in physics, nanotechnology and information technology, the biosciences and brain research, Jülich is developing the basis for the key technologies of tomorrow. Forschungszentrum Jülich helps to solve the grand challenges facing society in the fields of energy and the environment, health, and information technology. With more than 5,000 employees, Jülich – a member of the Helmholtz Association – is one of the large interdisciplinary research centres in Europe.

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Welcome to the Jülich Supercomputing Centre

The Jülich Supercomputing Centre (JSC) is all about simulations using supercomputers of the highest performance class. Not only do the experts at JSC operate leading computer systems around the clock, they also support scientific users in terms of methods and content. At the same time, they perform intensive research on solutions for the grand challenges facing modern society and are involved in the development of state-of-the-art computer architectures.

Scientific challenges are as diverse as the requirements on the computers used to address them. While simulations in brain research, such as the Human Brain Project, or from the area of climate research primarily require high main memory capacity, quantum calculations in nanoelectronics need extremely high computing power. Data analysis problems are best solved with cluster computers, some of which are accelerated with graphics chips. One example is the analysis at JSC of data from the Alpha Magnetic Spectrometer (AMS) experiment on the International Space Station, which is designed to detect antimatter in space.

Tailor-made solutions must be developed for use on all these systems. Only then is it possible to guarantee the most efficient exploitation of these expensive resources. This is made possible on site by the expertise of the simulation laboratories specializing in individual subject areas, and interdisciplinary teams focusing on methodology, algorithmics, optimization, analysis, and visualization. Outside of Forschungszentrum Jülich, JSC represents user needs in national and international committees and organizations, such as the Gauss Centre for Supercomputing (GCS) and the Partnership for Advanced Computing in Europe (PRACE). It is precisely this comprehensive user support and the simultaneous focus on thematic priorities that have earned the Jülich Supercomputing Centre its international reputation.

The ultimate challenge – simulating the human brain

The brain is the most complex organ in the human body. In order to treat diseases of the brain such as Parkinson's or Alzheimer's in a more targeted manner, a deeper understanding of its structure and functioning is necessary than is currently possible with existing methods. The problem can be solved by simulating the brain using supercomputers. Computing power of a quintillion (10^{18}) arithmetic operations per second (1 exaflop/s) and a working memory of around 100,000 terabytes envisaged for 2020 will ensure that neuroscientists will have a complete virtual brain with about a hundred billion neurons at their disposal for research.

Researchers from all over Europe are now working jointly on this project. As part of the European FET flagship programme, the Human Brain Project (HBP) was launched in 2013 with a budget of about € 1 billion. JSC is a major player in this endeavour. The supercomputer for the virtual brain to be developed in the HBP will be planned, installed and operated in Jülich. The declared aim is not only medical innovations. A detailed understanding of the brain can at the same time serve as a model for future IT systems.

Along the way, a queen will help to solve these highly complex problems. With almost six quadrillion arithmetic operations per second, Jülich's JUQUEEN supercomputer provides scientists with the top computing power that Europe currently has to offer for their research.

> "Understanding the human brain and learning from it – for this purpose, we combine neuroscience and supercomputing at Forschungszentrum Jülich."
>
> Dr. Boris Orth, head of High Performance Computing in Neuroscience division

JUQUEEN
Jülich Blue Gene/Q

Computing power:	5.9 petaflop/s
Processor cores:	458,752
Main memory:	448 terabytes
TOP500 (June 2013):	7th place

New concepts for shaping the future of computing

The objective for supercomputers of the future is clearly defined: reaching exaflop computing power by about 2020 – that's one quintillion arithmetic operations per second. However, numerous questions remain to be answered before this can become a reality: How can energy consumption be reduced? How can millions of processor cores be synchronized? How can the workload be efficiently allocated to the many processors?

In the 'Dynamical Exascale Entry Platform' (DEEP) project funded by the European Union, JSC and 15 other partners from industry and research institutions are attending to these issues. The goal is to develop a computer that represents a leap into the next generation of computers. To this end, Jülich scientists have conceptualized a novel cluster booster architecture. The cluster of the computer consists of conventional multi-core processors. For the booster, novel processors with up to 50 cores referred to as many-core processors will be used – a development of the last five years. This architecture concept takes account of the fact that simulations usually comprise several tasks of different nature, with both complex communication patterns between the processors as well as simple regular patterns.

The basic idea behind DEEP is an ingenious division of these tasks: those parts of a program that require complex processors will be executed on the cluster. Simple, highly parallel parts of a program that do not require such CPUs will be delegated to the booster modules consisting of a large number of processor cores with a simple structure (many-core processors). A special software system will facilitate the allocation of program parts across cluster and booster and control their communication with each other.

The DEEP computer will even be particularly energy-efficient. Using the accelerating components for the compute-intensive parts of a program already constitutes a way of saving power. System cooling will also require little energy: the water in the computer's cooling system will not be cooled down to room temperature, but can be reused for cooling at a temperature of 40 °C. The new system will be tested using six applications from different subject areas, and its development will be completed by early 2015. If all goes according to plan, this will be an important step towards exascale systems.

> "By being involved in DEEP, we are pushing the development of exascale computing in Europe."
>
> Dr. Estela Suarez, DEEP project manager

DEEP
Dynamical Exascale Entry Platform

DEEP Cluster

Computing power:	44 teraflop/s
Processor cores:	2,048

DEEP Booster

Computing power:	500 teraflop/s
Processor cores (Intel Xeon Phi):	31,232

The supercomputer as a crystal ball

Taking a peep into the future is no longer just an esoteric daydream: today it is also a necessity in science for predicting climate change and getting to grips with the consequences. Numerical simulations on supercomputers can help us get one step closer to fulfilling this dream. Scientists at JSC's Simulation Laboratory Climate Science are helping researchers to predict the impacts of climate change.

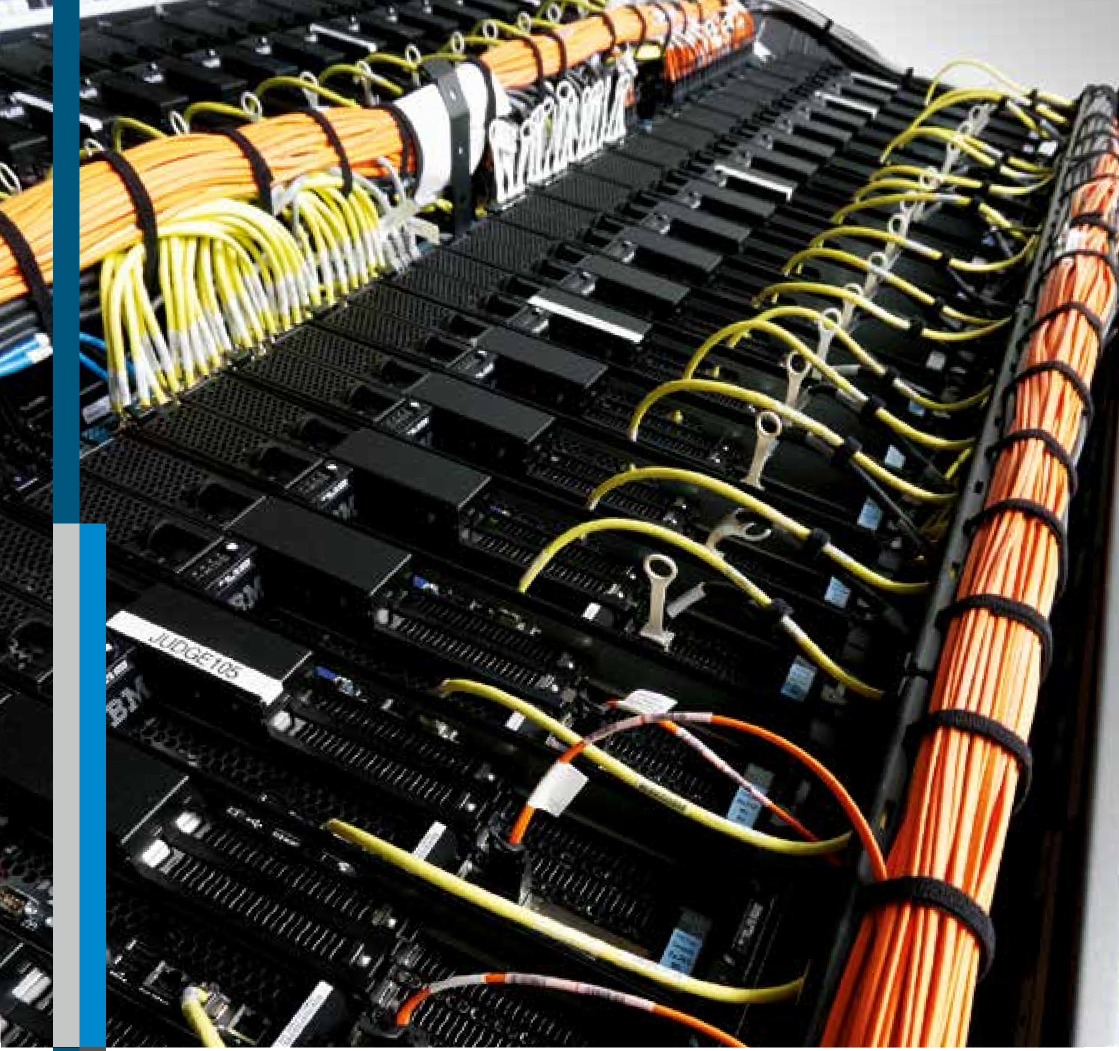
Only the computing power of supercomputers makes it possible to fully exploit the potential of these ensemble simulations. In this approach, the same simulation is started over and over again but with slightly different parameters in order to determine the uncertainties of the simulations. This is necessary because the boundary conditions, such as the emission rates of greenhouse gases, frequently change during test periods. Climate simulations are becoming an important tool for analysing 'what would happen if' questions and can, for example, serve as a vital aid for policy-making.

The Jülich cluster system JUROPA is particularly well-suited for these types of calculations since this computer's large memory enables it to work with enormous volumes of data. This mainly comprises the data-intensive evaluation of long time series of satellite measurements and also the large volumes of input data for atmospheric chemistry and climate simulations. JUROPA and cluster computing already have a long tradition at Jülich since JSC was also involved in developing components for JUROPA and its predecessors. The prototype of an even more powerful successor is already waiting in the wings and it will soon be helping researchers to perform even more data-intensive calculations.

> "We are using atmospheric simulations to develop new detection methods for volcanic emissions."
>
> Dr. Sabine Grießbach, Simulation Laboratory Climate Science

JUROPA
Jülich Research on Petaflop Architectures

Computing power:	308 teraflop/s
Processor cores:	26,304
Main memory:	79 terabytes



A turbo engine for supercomputing

Fast results – that's what scientists want from their simulations. The use of graphics processing units (GPUs) for compute-intensive applications is a particularly promising approach. Not only do they speed up calculations, they also achieve this in an exceptionally energy-efficient manner. JSC has been employing GPUs for several years. Its supercomputer JUDGE is a high-performance computer with graphics processing units.

However, not all applications benefit from the higher speed of these special processors. They are particularly suitable for programs in which a large number of small, identical subtasks can be calculated in parallel and only depend on each other to a minor extent. JSC cooperates closely with GPU manufacturer NVIDIA to increase the number of applications that are able to use GPUs efficiently. In the NVIDIA Application Lab, the two partners and application developers are pursuing a number of strategies to optimize simulation programs and port them to GPU-based computers. Simulations from the areas of computer-assisted neuroscience, high-energy physics, and radioastronomy have proven to be particularly suitable. The analysis of the large amounts of data produced in many large-scale scientific experiments can also be hastened with graphics processors.

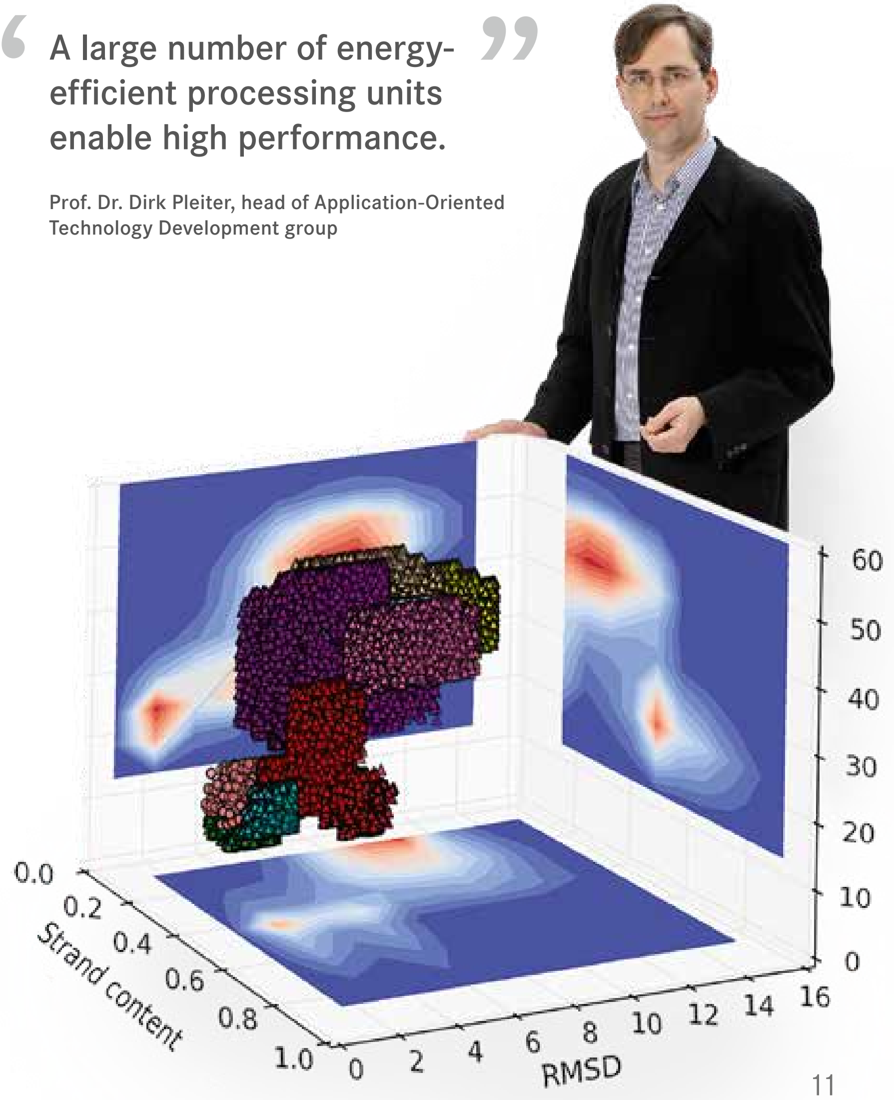
The lab not only supports developers of faster applications, but it is also developing improved architectures for future computers. To this end, the researchers are investigating how certain characteristics of a computer architecture impact on the speed at which applications are executed. What happens, for example, when computing power increases significantly while access time is only improved very little? Many questions remain to be answered by research – JSC and NVIDIA are facing this challenge head-on.

JUDGE
Jülich Dedicated GPU Environment

Computing power:	239 teraflop/s
Graphics processing units:	412
Processor cores:	2,472
Main memory:	19.8 terabytes

“A large number of energy-efficient processing units enable high performance.”

Prof. Dr. Dirk Pleiter, head of Application-Oriented Technology Development group



Big computers, masses of data

Big projects leave their mark. Projects on JUQUEEN requiring more than 10 million processor hours of computing time rapidly generate dozens of petabytes of data (big data). These vast volumes of data are difficult to handle for three reasons known as the three Vs: volume – the data volume is too big for conventional processing methods, variety – the different types of data make standardized processing difficult, and velocity – data are generated too fast to be saved in their entirety.

The great complexity of research issues from areas such as astrophysics or brain research inevitably leads to the analysis of complex data volumes. JSC provides three types of assistance: Firstly, software tools for data management are developed; secondly, scientists adapt their programs for analysing the data; thirdly, JSC makes web portals available, providing the international science community with access to these data.

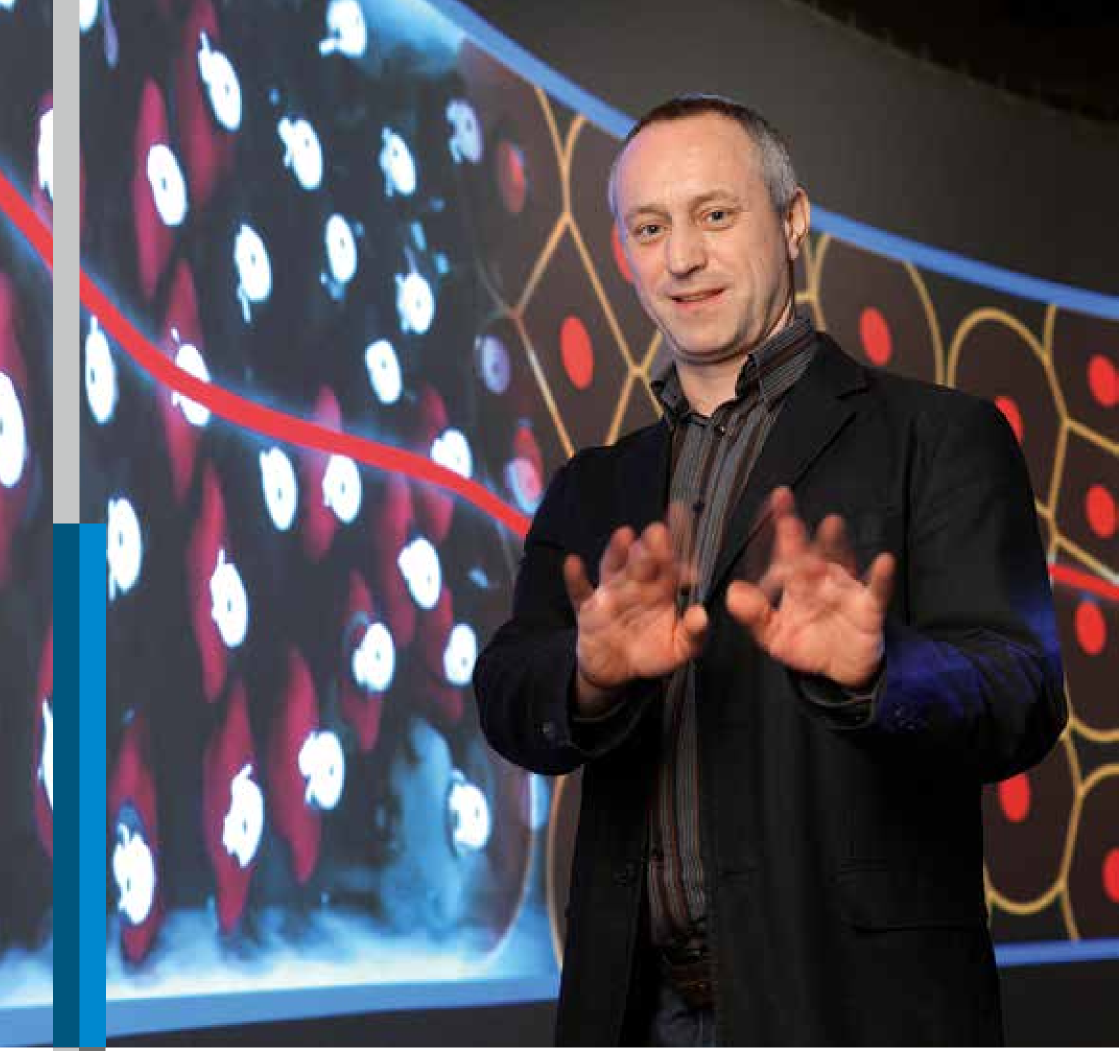
An example of such massive demands for data evaluation is the Alpha Magnetic Spectrometer (AMS) experiment. Forschungszentrum Jülich is involved in this international project on basic physical research as part of the Jülich Aachen Research Alliance (JARA). On the International Space Station, scientists intend to use the AMS experiment to verify hypotheses on the unexplained matter/antimatter asymmetry in the universe by investigating charged cosmic rays with previously unachievable precision.

Since JSC is envisaged as the future site of the human brain supercomputer, another important big data task is already in sight. The simulations to be performed as part of the Human Brain Project, which require exascale performance, will integrate data from hospitals and institutes all over Europe and can generate petabytes of data in just a few seconds that will be visualized and analysed in real time.

> “To harness the flood of data, we need clever algorithms and methods for data analysis.”
>
> Dr. Morris Riedel,
> Federated Systems and Data division

Storage

Number of hard disks:	6,868
Total data capacity:	15 petabytes
Bandwidth:	200 gigabit/s
Storage servers:	74

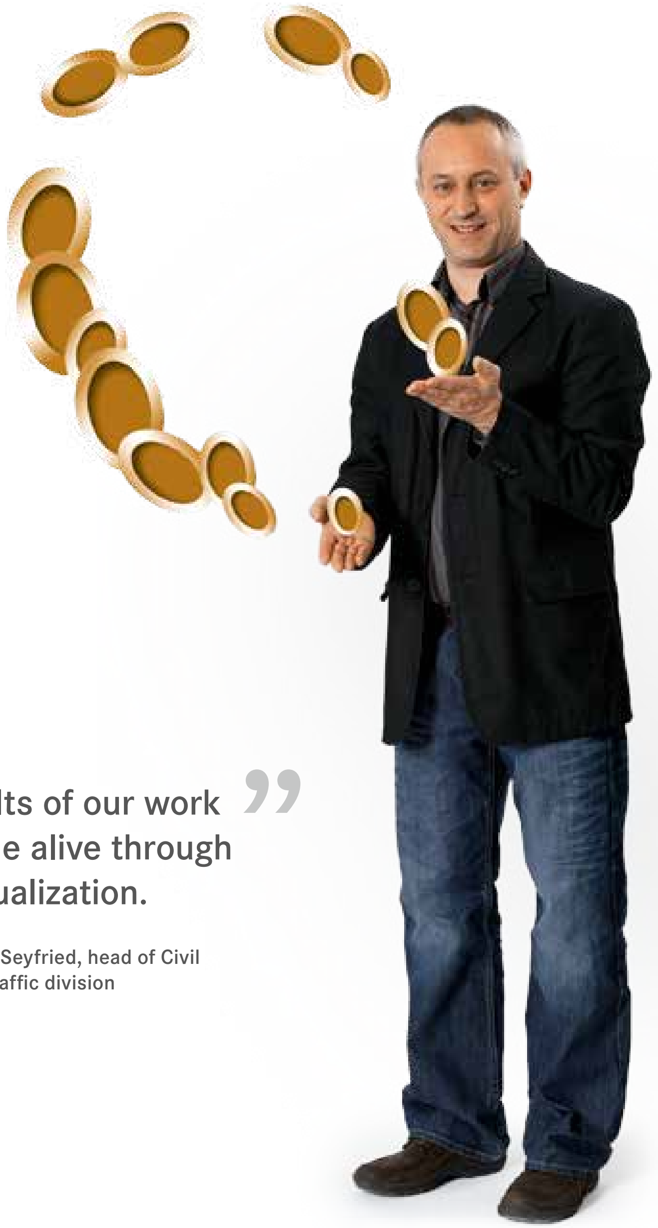


A picture paints a thousand words

Data from simulations are often very complex, making it difficult to keep a clear perspective. Many researchers therefore rely on visualizing their results in the form of images or videos. At JSC, they receive the support they need to transfer their simulation data into graphic representations. They have access to the required software tools and a dedicated computer for graphic applications. The scientists can choose between different projection systems, including 3D screens and a spherical projector, which is able to project data from climate research onto a globe. The special projectors in this room can be used to display visualizations in 3D on a huge screen, immersing observers completely in the simulations.

Jülich scientist Prof. Armin Seyfried even uses graphic tools in two ways: to gather experimental data and to visualize the corresponding simulations. Seyfried performs research in the field of traffic and civil security: he carries out experiments with pedestrians in order to learn more about the formation of jams and dangerous crushes. For this purpose, he records the routes taken by each individual using video technology developed for this purpose.

The analysis of the video data is the basis for his subsequent simulations. The results are then processed into striking video sequences. Seyfried’s research will lead to a better understanding of pedestrian traffic and the dynamics of large crowds of people. With the findings, he and his colleagues intend to contribute to optimizing escape routes in buildings and security at large public events.



> “The results of our work only come alive through good visualization.”
>
> Prof. Dr. Armin Seyfried, head of Civil Security and Traffic division

Careers at JSC – from vocational training to PhD project

Are you good at maths? Interested in computer science? JSC is the place to be for young people enthusiastic about these subjects. Here, you can receive vocational training, study for a bachelor's or master's degree, and complete your dissertation, or even pursue a PhD.

Highly qualified employees are vital for a supercomputing centre. That is why JSC has been committed to training in mathematical and technical occupations for its own requirements and beyond for more than 50 years. In cooperation with FH Aachen University of Applied Sciences at Jülich, it offers dual study programmes for those with a school leaving certificate – a combination of on-the-job vocational training and university studies. Those participating qualify as mathematical and technical software developers (MATSEs for short) at Forschungszentrum Jülich and simultaneously study for a bachelor's degree in Scientific Programming at FH Aachen. This programme closely dovetails theory and practice: apart from lectures in the fundamentals of mathematics and computer science, it also includes programming in small independent projects.

After completing the bachelor's degree, graduates can continue to delve deeper into their studies by pursuing a master's in technomathematics.

JSC also offers further training opportunities for students in other subject areas, for example during its annual visiting students' programme. It allows students specializing in the natural sciences and engineering to familiarize themselves with different aspects of scientific computing and supercomputing on systems that are among the most powerful in the world. The programme takes ten weeks, during which the students work on current research topics and are closely supervised by JSC employees. This often results in long-term cooperation: quite a few visiting students return to JSC to pursue a PhD.

> "Studying maths and computer science in an excellent environment and getting practical experience at the same time – it's perfect!"
>
> Anna Jakobs, postgraduate in technomathematics

www.fz-juelich.de/matse
www.fz-juelich.de/ias/jsc/gsp

Complex systems for addressing complex challenges

Increasingly faster processors, more and more of which are working in parallel – but in supercomputing, size is not an end in itself. Instead, the enhanced performance of the computers helps to account for the enormous complexity of current scientific challenges and to keep pace with the continuously increasing computing time requirements that go hand in hand with scientific progress.

A peak performance of one quintillion arithmetic operations per second will be necessary to simulate the entire human brain, for example, which is the goal that the European Human Brain Project has set itself. Along the way, however, it is not only the number or clock rate of processors that has to increase. Many million processor cores must be synchronized, the reliability of the components must be guaranteed, and innovative memory technologies are also required. The scalability of the user codes presents JSC with increasingly large challenges, and enhancing energy efficiency has also become an important issue.

But the effort is worth it: research on the brain promises greater success in the search for new methods of diagnosis and treatment for neurological disorders – one of the grand challenges to be overcome by our society.

JSC addresses the technical challenges in three 'exascale laboratories' that are developing and testing innovative concepts for the computers of the future. The name speaks for itself: in cooperation with the leading manufactures IBM, Intel, and NVIDIA, they are applying the kind of creative thinking that is necessary to climb the remaining steps to exascale computing.

In addition to these industry cooperations established by JSC, the institute is also an important partner and driving force for innovation in scientific institutions and political structures on a national and international level. JSC makes available its expertise in high-performance computing (HPC), which it has built up over decades, to meet the special requirements of the institutes at Forschungszentrum Jülich and the John von Neumann Institute for Computing. It operates the Supercomputing Facility and offers relevant expert support. This support offered by Forschungszentrum Jülich ranges from regional networking through the HPC section of the Jülich Aachen Research Alliance (JARA) to initiatives under the umbrella of the Helmholtz Association – the 18 centres in the Association have created a joint computing concept coordinated by JSC. In the Gauss Centre for Supercomputing (GCS), JSC helps to pool the strengths of the three large HPC centres in Germany. In addition, JSC coordinates European development projects. This enabled decisive impetus that established GCS as a pacemaker in the European infrastructure PRACE. All of these activities contribute to the high national and international visibility of simulation science at Jülich.

Prof. Dr. Dr. Thomas Lippert
Director of the Jülich Supercomputing Centre

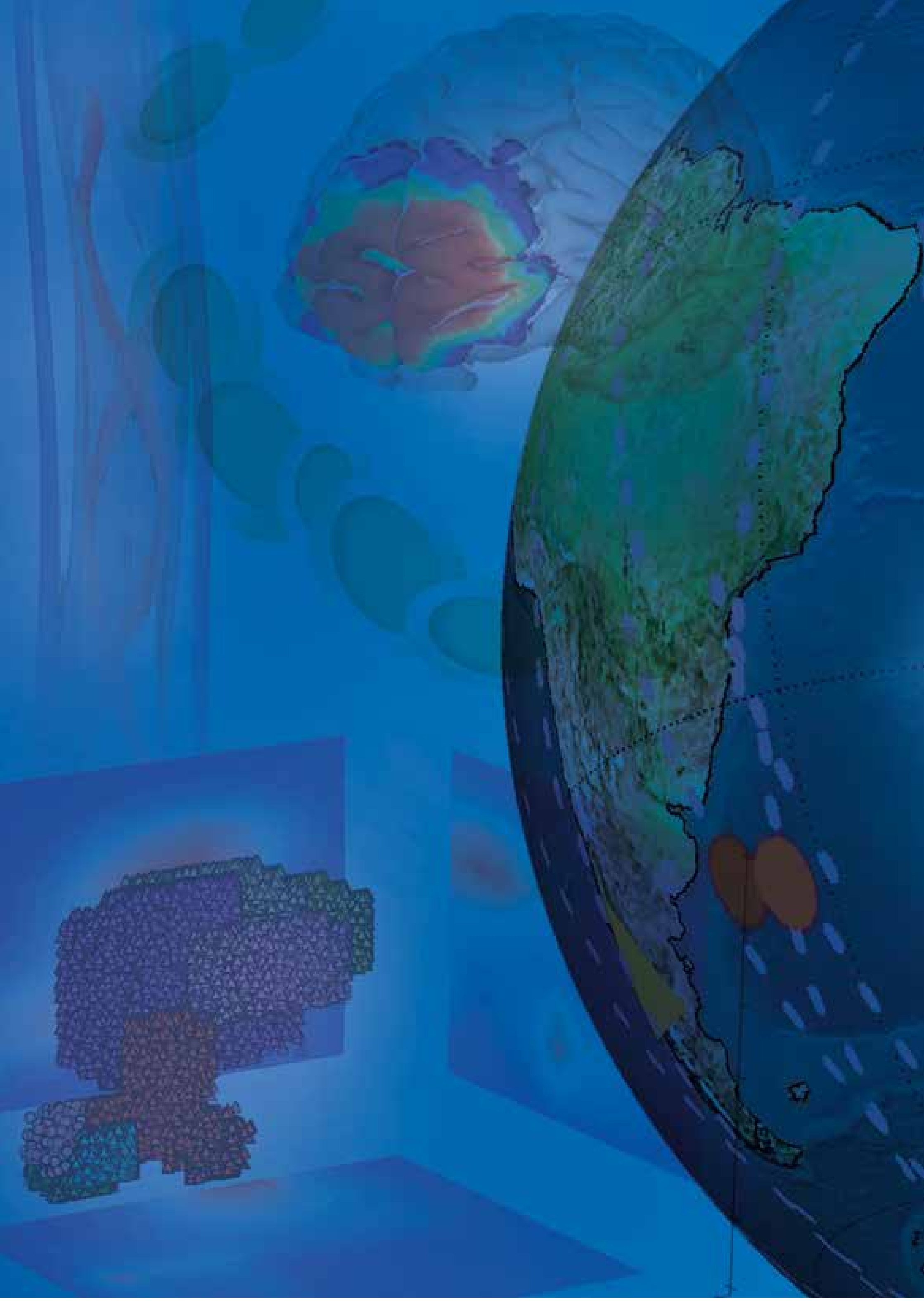
Photo (from left to right): Prof. Dr. Dr. Thomas Lippert, Director of the Jülich Supercomputing Centre, Prof. Dr. Sebastian M. Schmidt, Member of the Board of Directors of Forschungszentrum Jülich, Prof. Dr. Achim Bachem, Chairman of the Board of Directors of Forschungszentrum Jülich

Important international cooperation partners:

USA:
NCSA – National Center for Supercomputing Applications, Urbana-Champaign
ORNL – Oak Ridge National Laboratory, Oak Ridge

Japan:
RIKEN, Tokyo

China:
CNIC – Computer Network Information Center, Beijing
NSCC – National Supercomputing Center, Tianjin



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