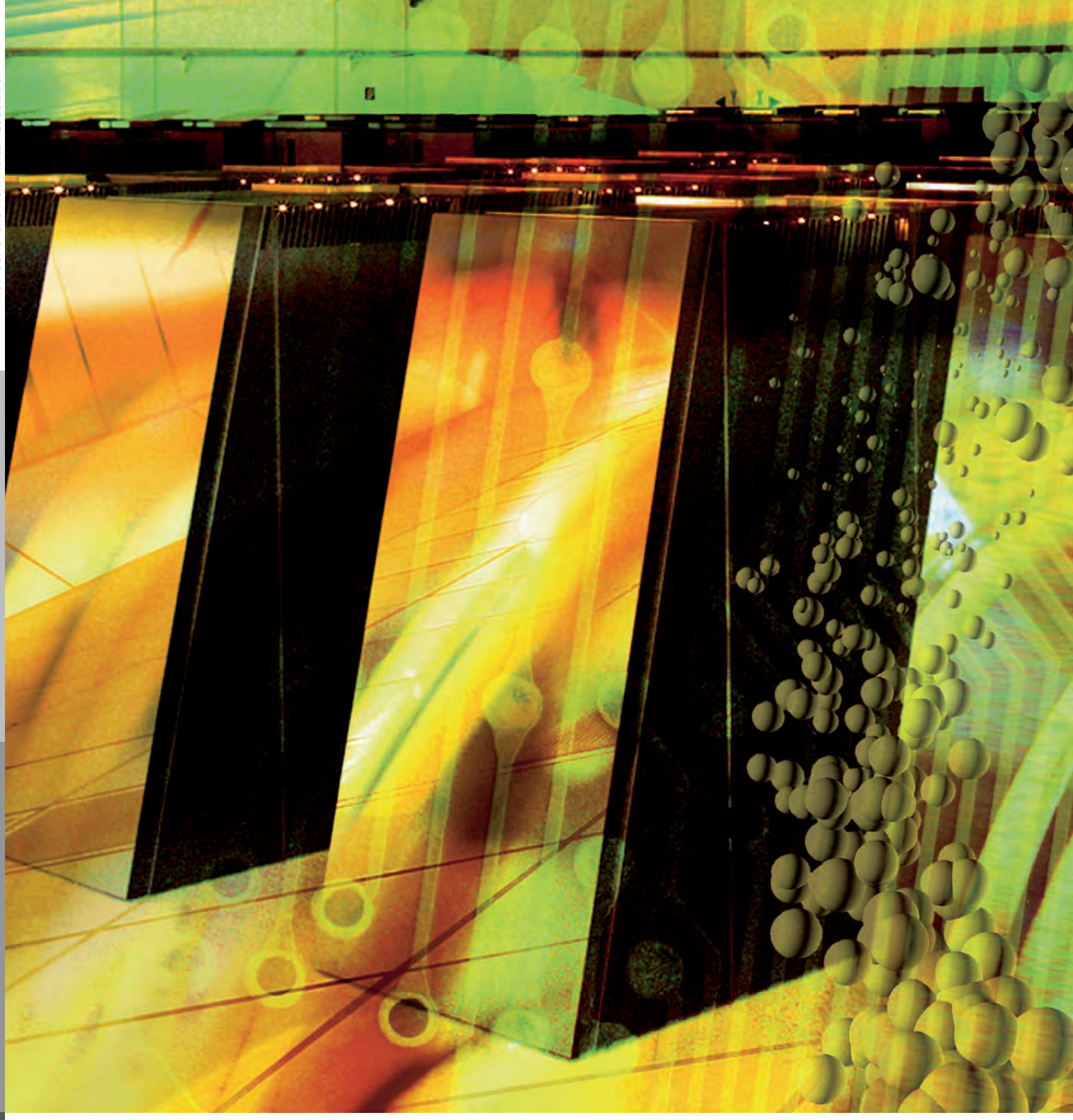
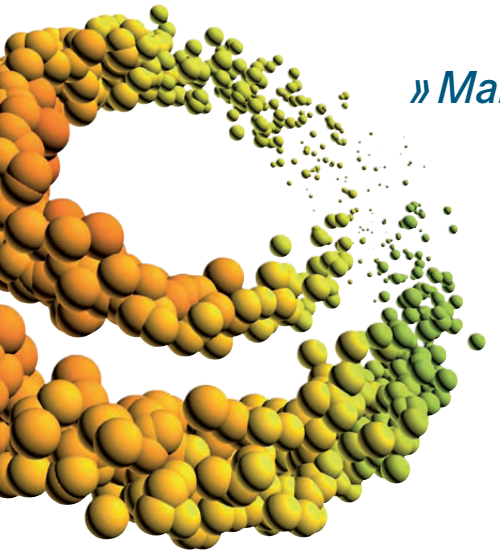
Member of the Helmholtz Association



Supercomputing

World-class performance for research

JÜLICH
FORSCHUNGSZENTRUM



» Man is still the most extraordinary computer of all. «

John F. Kennedy

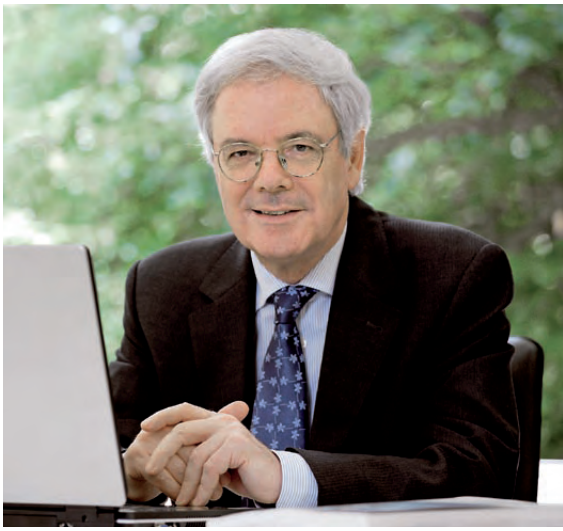
With its JUGENE supercomputer, Forschungzentrum Jülich has set a milestone on the road to tomorrow's research. The fastest computer in the world outside the USA provides insights and thus knowledge previously unavailable to us – for financial, ethical or physical reasons. This is why more and more scientists are now working with computer simulations - whether in order to explain how proteins are folded in the body, how semiconductors function, how water vapour rises into the stratosphere or how cars behave in road accidents.

However, we shouldn't rest too long on just one milestone. The race goes on. More and more research groups need more and more computing time to defend their leading place in international top-class research. Together with its German and European partners, Forschungszentrum Jülich is working on new concepts and computer prototypes in order to satisfy this rapidly growing demand. The challenge is to provide computing power beyond the petaflop/s* barrier and here in Jülich we are rising to this challenge with our partners and friends.

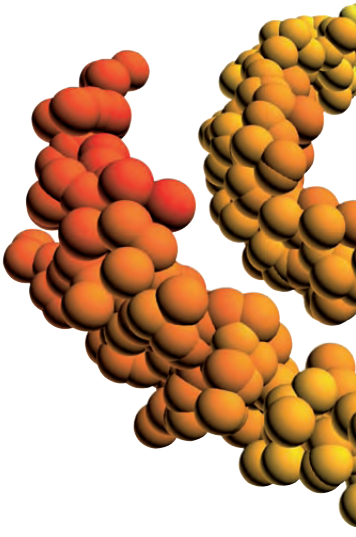
However, the race can't be won by greater computing capacity alone – you have to know how to use this capacity. This is why Forschungszentrum Jülich mainly depends on human brains and not on computer processors. The scientists at the *Jülich Supercomputing Centre (JSC)* do not just keep operations up and running and concentrate on developing future computer generations, but rather from computing time and numerical values they ultimately create new knowledge and solutions for the most complex problems ever to confront mankind. It is this expertise in the simulation sciences – combined with the multifaceted scientific environment – which leads to the considerable added value of the Jülich computer for research work. But even more important: this expertise enables us to guarantee independent access to the key technology of "supercomputing" for Germany and Europe. Only in this way will we keep the key to this significant element in the scientific and industrial value-added chain in our own hands.

In the 1960s, the USA's space flight programme was the lead technology that inspired a wide range of scientific innovations. Today, supercomputing is taking over this leading role and opening the door to new knowledge. Here in Jülich, we are not just keeping up this development, we are actively shaping it.

*(10^{15} arithmetic operations per second)



Prof. Dr. Achim Bachem, Chairman of the Board of Directors of Forschungszentrum Jülich



Supercomputers: More than the sum of their parts

Thousands of processors work together effectively in Jülich's supercomputers. They represent an indispensable research tool.

Supercomputers have become a permanent fixture in science. Computer simulations are part of the scientist's tools of the trade in the most varied fields. They explain how galaxies are formed, how proteins are folded, how aircraft wings behave and how semiconductors function. As a complement to theory and experiment, simulation science today forms a third pillar of research work. Scientists harness the concerted computing power of supercomputers in which a large number of processors work in parallel on one job.

With their codes, Jülich researchers weld together thousands of processors into one functional unit. Teamwork is the order of the day. Each individual processor can only solve a small part of the overall problem. Data are exchanged between the chips and are then used for the next step in the computation. As in a mosaic, the individual parts are pieced together and finally form a coherent overall picture. In order to achieve this, the data must arrive at their destination safely and in good time. Only by means of the high-performance data network between the processors and thanks to their know-how in algorithms and programming are the Jülich experts able to construct one supercomputer from a multitude of chips.

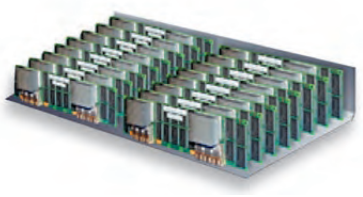
Specifications of the Jülich supercomputer JUGENE

Architecture:	IBM Blue Gene/P
Computing power:	223 teraflop/s
Processors :	65,536
Processor type:	Power PC 450
Frequency:	850 megahertz
Main memory:	32 terabyte
Storage bandwidth:	13.6 GB/s
Local network bandwidth:	5.1 GB/s
Network latency:	160 nanoseconds
Electric power:	560 kW

Rack = 4,096 CPUs

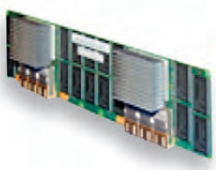
13.9 teraflop/s

Node Book = 128 CPUs



435.2 gigaflop/s

Card = 8 CPUs



27.2 gigaflop/s

Node = 4 CPUs

13.6 gigaflop/s

The Jülich supercomputer JUGENE (Jülich Blue GENE) has more than 65,000 processors. They are accommodated in 16 cabinets each as tall as a man and reach a processing speed of up to 223 teraflop/s, which corresponds to 223×10^{15} arithmetic operations per second. An arithmetic operation is, for example, the addition or multiplication of two 16-digit numbers. The following comparison shows how fast JUGENE works. If the entire world population of 6 billion people were each to perform more than 30,000 arithmetic operations per second and were then to exchange their results, this would roughly correspond to JUGENE's computing power.

JUGENE = 16 Racks = 65,536 CPUs

222.8 Teraflop/s

About 65,000 processors operate in Jülich's JUGENE supercomputer. Each processor works on a small part of the problem and passes its result on to other processors. This is how the overall solution to the problem in hand is found in single parallel steps.

"A commitment that pays dividends"

Interview with Martin Jetter, IBM

Is there a place for supercomputers outside research?

Absolutely. Research paves the way in many spheres and encourages innovations. A key word in industry is "virtual prototyping". But financial service providers now also make use of supercomputers. Other markets are still waiting to be discovered. Germany should therefore keep a supply of experts available for hardware, software and applications. And as students, they will be trained in exciting research projects on supercomputers. Jülich's commitment to supercomputing is therefore paying dividends for Germany in a number of ways.

Why is IBM backing the Blue Gene architecture?

Blue Gene architecture combines the best features of a supercomputer. It is fast, cheap, energy- and space-saving due to optimized communication between the processors. Only in this way are we able to set our sights on the next milestone: petaflop/s systems, that is to say supercomputer systems that execute 10^{15} arithmetic operations per second. They will make realistic and extremely detailed simulations possible thus giving rise to new knowledge in the field of science and technology.

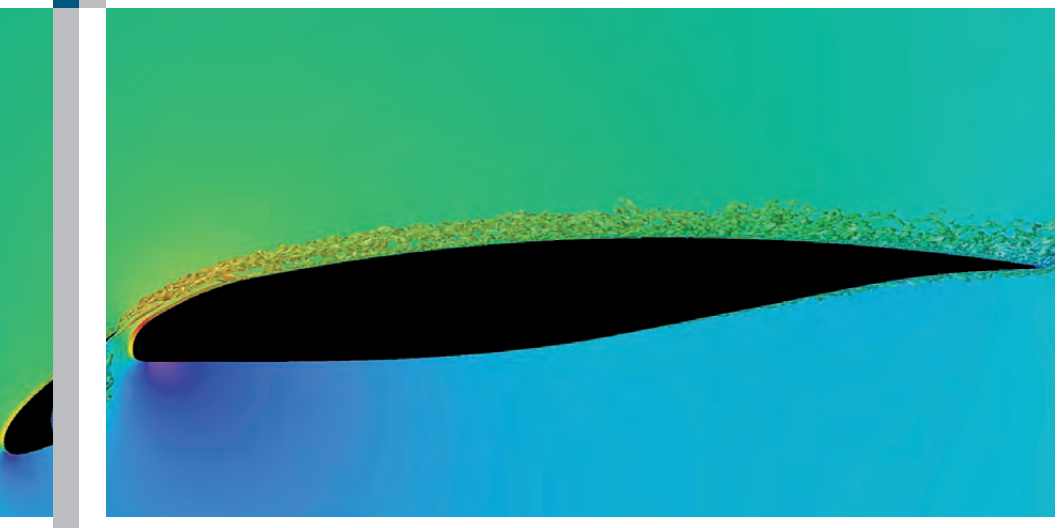
Why are you cooperating with Forschungszentrum Jülich?

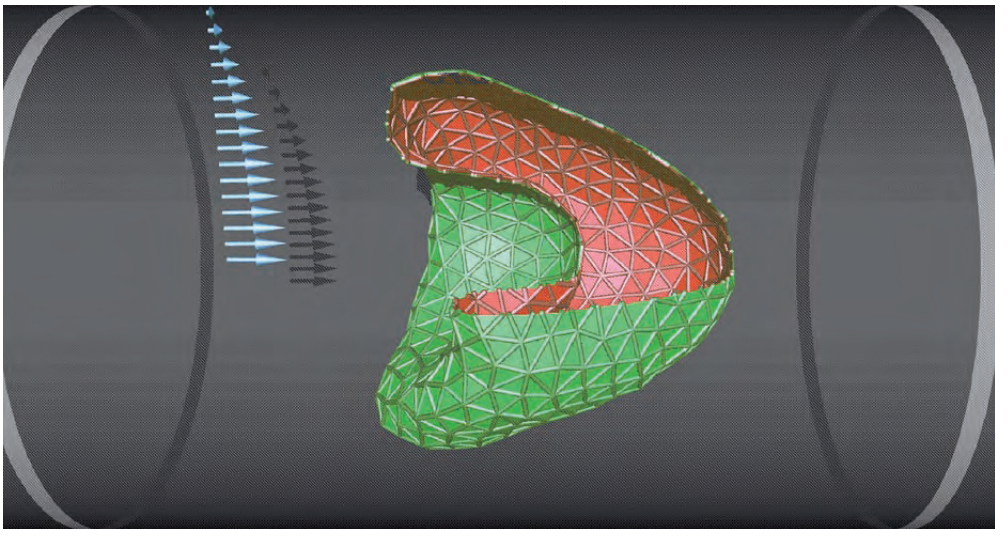
Forschungszentrum Jülich is an important partner for us and not just a client. Jülich sets high standards, above all in the fields of communications infrastructure and algorithm development, which are of great benefit for our joint development of the next generation of supercomputers. Thanks to our complementary perspectives in the field of supercomputing we represent the perfect team for developing effective, compact, top-performance computers for large research projects involving huge volumes of data.

Martin Jetter is the General Manager and Chairman of the Board of IBM Deutschland GmbH. With its Blue Gene architecture, IBM regularly occupies the top place in the rankings of the fastest computers in the world. Among the TOP500 supercomputers, more than 200 systems are from IBM.

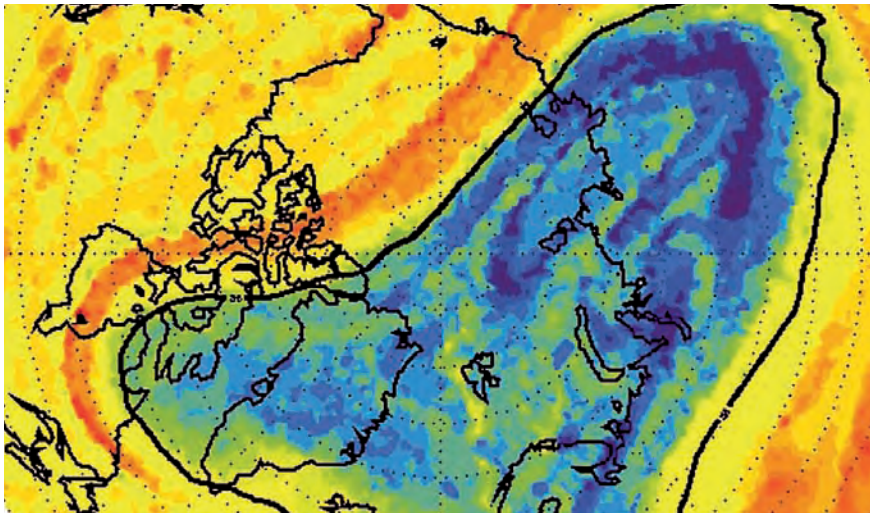
Simulation sciences: Solving complex problems

Virtual laboratory, telescope, time machine: Simulations with supercomputers serve research and industry.





Supercomputers provide insights into complex systems. Simulations are used wherever experiments are impossible for financial and ethical reasons, due to the risks involved or for basic physical and technical reasons, as is frequently the case in medicine or astronomy. In science such simulations help to provide new knowledge and in industry they cut the time to production. In Jülich, simulations on supercomputers enable theoretical models to be verified and virtual experiments to be performed with otherwise unattainable precision. As a complement to theory and experiment, simulation science forms the third pillar of research work and will become an indispensable prerequisite for great leaps in knowledge in the future. Supercomputers are flexible. Apart from the possibility of using them as virtual laboratories, microscopes or telescopes, they also serve as a virtual window into the future. More detailed simulations enable the consequences of human actions to be



Weather, medicine and aircraft: Supercomputers like JUGENE can be used in almost all conceivable fields of research to contribute to achieving new knowledge. Simulations enable complex systems and interactions to be determined and their behaviour estimated. These findings lead to early warning systems, customized drugs or improved technology.

Research topics on the Jülich supercomputer:

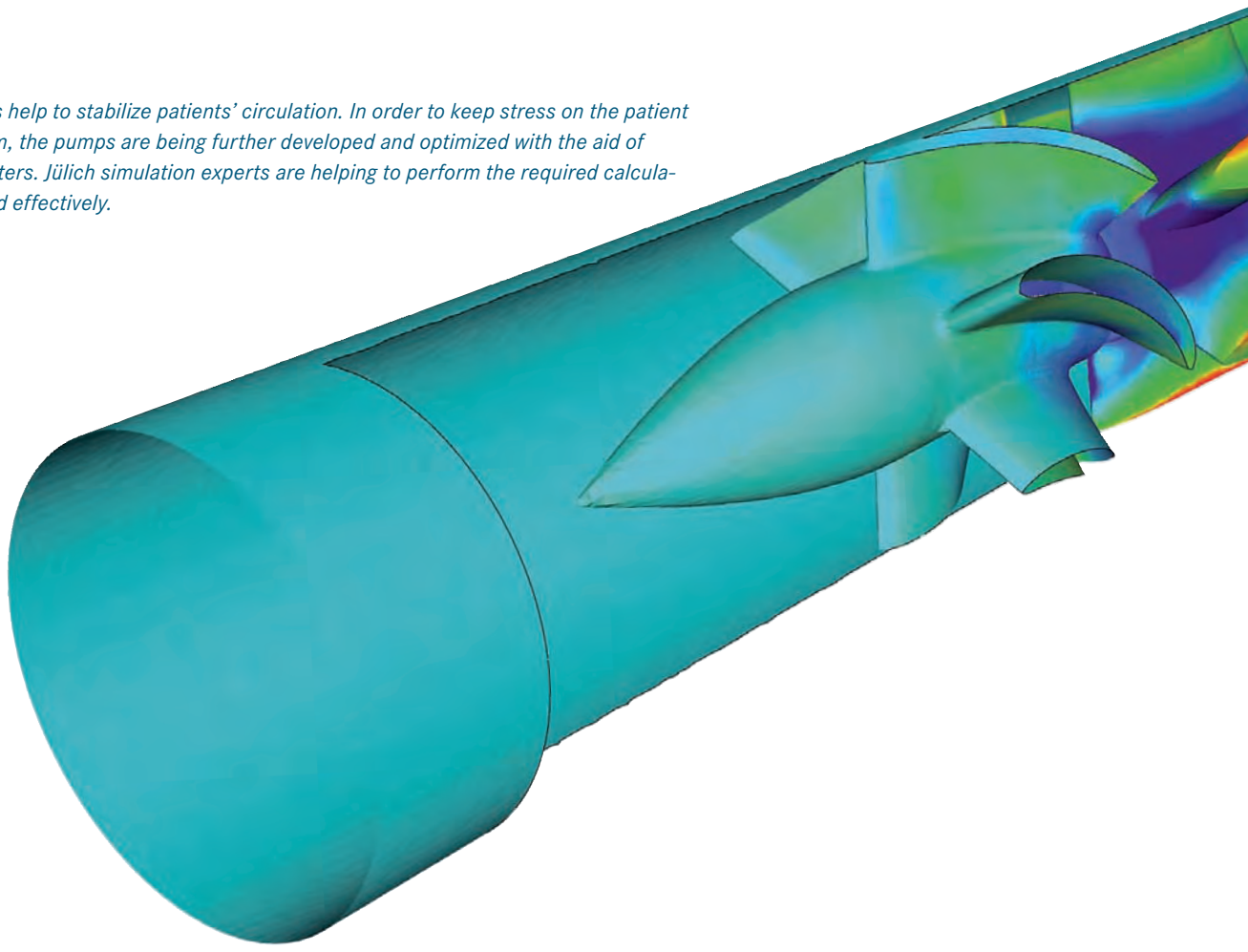
- **Pollutants in the soil**
- **Magma below the Earth's surface**
- **Chemical reactions in the atmosphere**
- **Galaxies and the formation of stars**
- **Polymers in solutions**
- **Lasers and particle physics**
- **Protein folding in cells**
- **Biological membranes**
- **Aviation and automotive engineering**
- **Fire protection and evacuation scenarios**

estimated and recommendations to be made. Climate predictions already enable us to estimate which regions will have to prepare for future climate change. Weather forecasts help us to protect houses and save human lives in the case of hurricanes like "Katrina" or storms like "Kyrill".

Prospects: Key technology for the 21st century

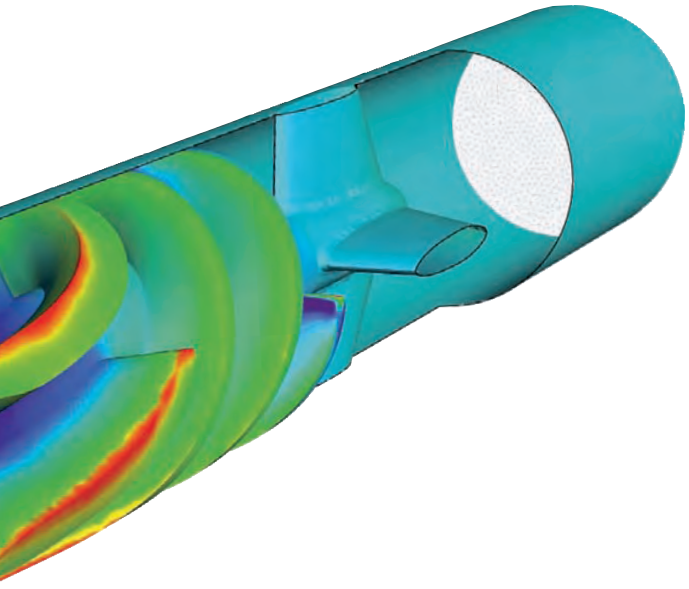
Demand for computing services is increasing because everybody wants to ensure they have the competitive edge. This is where Jülich's know-how comes into play.

Blood pumps help to stabilize patients' circulation. In order to keep stress on the patient to a minimum, the pumps are being further developed and optimized with the aid of supercomputers. Jülich simulation experts are helping to perform the required calculations fast and effectively.



Whether medicine or information technology, environment or energy research – scientists from the most varied fields are convinced that in future significant gains in knowledge are to be expected if supercomputer simulation methods are employed. In Jülich, scientists find both the necessary hardware and also competent local contacts for methodology and algorithms. Only with this combination can scientists be assured of achieving a leading research ranking.

The number of research groups and the complexity of the research issues means that there is an increasing demand for computing resources. In the next five years, more than 1,000 times as much computing time will be available in Germany than is provided by current resources. The supercomputer is becoming a central key technology when it comes to ensuring priority for scientific publications or industrial patents. The efficient and productive application of supercomputers – as demonstrated every day in Jülich – will become a key competency for researchers in the 21st century.



Demand for supercomputing capacity in Germany

Research topic	2005-07	2007-09	2010
Climate and environment	20	50-100	>500
Geophysics	1	10-100	>1,000
Nanoscale materials	1	10-50	>200
Solid-state physics	1	50-100	>1,000
Fluid mechanics	2.5-10	25-100	>1,000
Astrophysics	10	50-100	>500
Particle physics	30	100	>1,000
Materials research	10	50-100	>500
Theoretical chemistry	3	25-125	>300
Soft matter	3	30	>200
Biophysics and bioinformatics	3-15	18-80	>100
Plasma physics	10	50	>500

All figures in teraflop/s, Hillebrandt et al., 2005

JARA|SIM

"Research speeded up enormously"

Interview with Marek Behr, RWTH Aachen University

What is the aim of your research?

Heart disease is very widespread in Europe and is a frequent cause of death. It is possible to help some patients by implanting blood pumps to support the activity of their heart. My team is composed of engineers and computer scientists. They simulate the complex flow behaviour in the pumps and develop them further so that, on the one hand, the pumps effectively support the patients' circulation and, on the other hand, they do not destroy the sensitive cells in the blood. The high speed of the pumps used at the moment causes turbulences, which exert a high shear force on the blood cells thus crushing large numbers of them.

What part does the supercomputer play in your work?

The supercomputer is one of our tools of the trade. The simulation of our blood pump requires a computing power that cannot be achieved with a few networked computers. We use thousands of processors on the Jülich computers to simulate real pumps and blood flows. We also develop our own software. On the one hand, the software must realistically describe the physical model and, on the other hand, optimally exploit the architecture of the supercomputer.

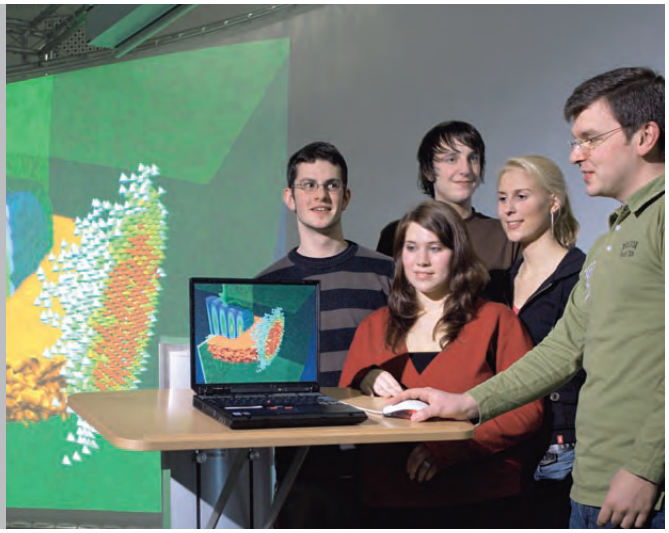
Why are you cooperating with Forschungszentrum Jülich?

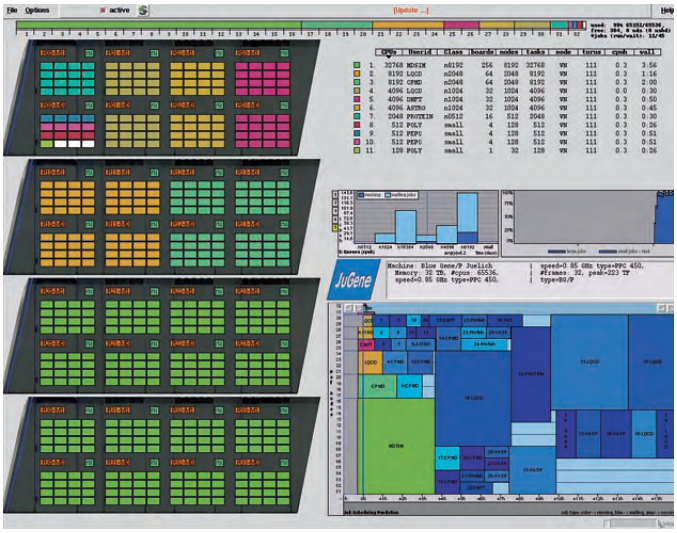
The expertise available at Jülich has speeded up our research enormously. And I am not just talking about computing power. Together with the team of experts at Jülich, we specifically analysed the performance of our software and eliminated a number of bottlenecks. We can now use more processors in parallel and reduce the computing time. Instead of computing just one configuration in several weeks we are now able to do it in a few days. In this way, we can rapidly convert specific improvements into practical applications and thus help patients.

Prof. Dr. Marek Behr holds the Chair of Computational Analysis of Technical Systems at RWTH Aachen University and is the scientific director of the graduate school "Aachen Institute for Advanced Study in Computational Engineering Science (AICES)". He cooperates with Jülich scientists as part of JARA-SIM, the Jülich Aachen Research Alliance – Section Simulation Science. Behr has been developing blood pumps since 2000 and he is currently working on a customized model for children.

Jülich: One-stop expertise

Hardware, software and training are linked at the *Jülich Supercomputing Centre.*





The *Jülich Supercomputing Centre (JSC)* makes its expertise available to more than 200 research groups throughout Europe. A staff of about 120 work on all aspects of supercomputing and are available as contacts for simulation scientists. JSC is characterized by three fields of activity:

- **Operation and further development of the most powerful supercomputers**
  Jülich's dual concept means that users have the most appropriate computer resources at their disposal. JUGENE, one of the fastest computers in the world, is used for problems requiring vast amounts of computing power, whereas JUMP, equipped with an enormous working memory, is designed for data-intensive applications. The background infrastructure operates with, for example, 10 petabytes of hard disc and tape memory. Developments in the computer industry are evaluated in Jülich in order to continue to provide innovative and efficient technology for the ever increasing demand for computing power. Concepts are continually improved and prototypes developed in cooperation with industrial partners.

- **Professional support for external scientists**
  The effective application of supercomputers requires technical support as well as scientific exchange. Jülich experts develop software for analysing the performance of applications, for mathematical modelling and for fast, seamless access to various resources in networks. They use their know-how and experience to make the applications more effective and faster. Simulation scientists also perform research at the *Jülich Supercomputing Centre*, for example on topics from plasma physics, materials science and the biosciences. In "simulation laboratories", activities are focused according to research field and contribute to cooperations with external colleagues.

- **Training young scientists**
  Simulation science is a new and innovative discipline. The resources of this still young science expand enormously with each computer generation. This is why the *Jülich Supercomputing Centre* attaches great importance to regularly communicating the latest developments in workshops and seminars. Undergraduates, PhD students and scientists from all over Europe take part in these events.
  From 2008, the *German Research School for Simulation Sciences* will also open its doors on the Jülich campus. It will provide masters and PhD courses for outstanding students.

Training and teaching are well established at Jülich. The students come into contact with the latest methods and technology (left). The modern computer room at the Jülich Supercomputing Centre is capable of accommodating large supercomputers such as JUGENE, which is used for simulations and models (right). It is important to keep control of computing and technology. This is made easier by software tools developed at Jülich (centre).

"On the way to the exaflop/s era"

By Thomas Lippert

Supercomputing is regarded as a strategic key technology both for theoretical and experimental research and also for optimizing industrial production. The demands made on supercomputers, networks, and data centres are rising exponentially with the continuously increasing complexity of the systems to be investigated. This is accompanied by increasing challenges for algorithm research, software technology, and visualization technologies. Against this background, the *Jülich Supercomputer Centre (JSC)* is devoting itself to providing supercomputers of the highest performance class and also to developing methods and tools for supporting users in the various fields of the computer sciences. JSC has a distinctly interdisciplinary character. It also has a long tradition as Germany's first national supercomputing centre and forms an important bridge to a number of research areas.

Together with our partners, we have been providing German and European science with indispensable large-scale equipment and infrastructure for more than 25 years. As a European petaflop/s supercomputing centre, from 2010 onwards JSC intends to provide supercomputing resources and services of the world's highest scalability and performance class. This goal will be supported by intensified activities in the design and construction of future high-performance systems in cooperation with European companies with the aim of providing exaflop/s power* from 2016.

Simulation laboratories are being created to support research activities in a specific and specialized manner. A core group of specialists attached to the supercomputing centre provide support for external associated members with the know-how required to achieve maximum efficiency in their simulations on the supercomputer. The first laboratories are being set up for the fields of plasma physics, earth system sciences, biology and nanosciences. On the European stage, as the project office of the "Partnership for Advanced Computing in Europe (PRACE)", we are preparing the organizational, legal and technical basis for the petaflop/s infrastructure. We are developing grid technologies – such as the UNICORE grid middleware – both for networked supercomputing at the highest performance level and also for interoperability with grids for data-intensive applications such as the D-grid funded by the German Federal Ministry of Education and Research (BMBF) and also the European EGEE and EGI initiatives.

*(10^{18} arithmetic operations per second)

Prof. Dr. Dr. Thomas Lippert is head of the *Jülich Supercomputing Centre (JSC)* and is director of the Institute for Advanced Simulation and the John von Neumann Institute for Computing. JSC operates several supercomputers of the world's most powerful performance class. It develops simulation methods, mathematical models and software tools in cooperation with users and provides support for these same users. These developments have attracted international attention.

Jülich and its partners

The *Jülich Supercomputer Centre* plays a defining role in many national and international cooperations.

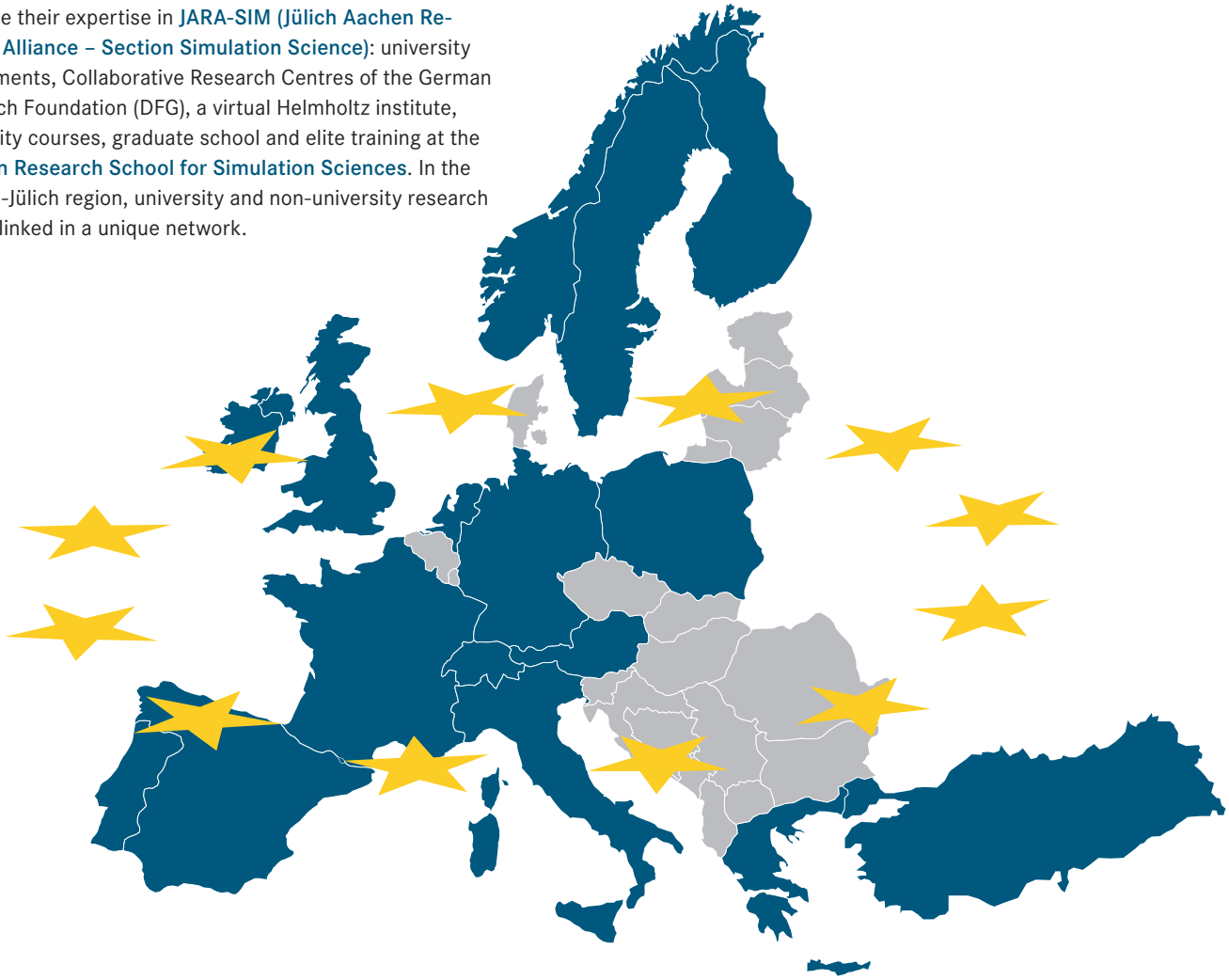
With its JSC, Forschungszentrum Jülich is promoting the development of the simulation sciences and the necessary supercomputers. These activities are based on strong supporters, partners and networks.

- Supercomputing in Jülich is funded by BMBF through the **Helmholtz Association** in the Helmholtz Programme "Scientific Computing". In this programme, Jülich is cooperating closely with Forschungszentrum Karlsruhe in the field of grid computing. In purchasing supercomputers, JSC is supported by BMBF and the Science Ministry of the federal state of North Rhine-Westphalia.

- Forschungszentrum Jülich and RWTH Aachen University combine their expertise in **JARA-SIM (Jülich Aachen Research Alliance – Section Simulation Science)**: university departments, Collaborative Research Centres of the German Research Foundation (DFG), a virtual Helmholtz institute, university courses, graduate school and elite training at the **German Research School for Simulation Sciences**. In the Aachen-Jülich region, university and non-university research is thus linked in a unique network.

- Within the framework of its **John von Neumann Institute for Computing (NIC)**, Jülich operates the largest and longest-established German supercomputing centre together with its Helmholtz partner institutes DESY (German Electron Synchrotron Foundation) and GSI (Society for Heavy Ion Research).

- In the **Gauss Centre for Supercomputing (GCS)** founded on the initiative of the German federal minister of education Annette Schavan in 2007, JSC cooperates with the two other national supercomputing centres in Stuttgart and Munich. GCS represents German interests on an international level.



- As head of the **PRACE consortium (PRACE – Partnership for Advanced Computing in Europe)**, Jülich is working on specific plans for extending the European supercomputing infrastructure and making it the best in the world. The EU approved about € 10 million for the preparatory phase lasting until 2010. Another € 10 million was contributed by the partners themselves, who come from 14 European countries. One objective is to install two petaflop/s systems in Germany and France by 2010. The project intends to initiate long-term developments by preparatory investigations and developments for the generation after next of supercomputers.

- As a founding member of **DEISA (Distributed European Infrastructure for Supercomputing Applications)**, together with 11 partners, JSC is developing methods to provide scientists with simple and seamless access to the European supercomputer network. Furthermore, JSC is a member of Enabling Grids in E-Science (EGEE) and also D(eutschland)-Grid and is developing the UNICORE grid software.

- Joint projects are undertaken and virtual institutes operated with supercomputing researchers from **Oak Ridge National Laboratory** and **Lawrence Berkeley National Laboratory** in the USA.

- Hardware and software are tested and developed in numerous cooperations with industry in order to create a basis for new, more powerful supercomputers.

In 2007, the leading computing centres within Europe joined together to form the PRACE partnership. According to a joint plan, they intend to establish a supercomputing infrastructure in Europe that will be the best in the world.

"Supercomputing – A job for national research centres"

Interview with Thom Mason, ORNL

What part does supercomputing play in science?

Today, science is trying to solve complicated issues involving several degrees of freedom. This can only be done by utilizing high-performance computers. Materials science models, for instance, contain thousands of atoms which interact in a complex manner, and climate models reduce the grid size from several hundred to just a few kilometres. In these two fields we need better and more precise predictions of system properties. This requires computers with the necessary memory capacity and processing speeds capable of simulating scenarios on a long time scale within a short time.

What part will large research institutions such as Jülich and ORNL play in this field?

Computers have become more powerful. However, at the same time it has become more complicated to install and operate them. In order to achieve a leading position we need the potential available at a national research centre. The infrastructure requirements are becoming more and more demanding with respect to electric power, cooling and capital expenditure. It must therefore be ensured that the total capacity of the resources can be effectively exploited. This is difficult for small groups. As national research centres, we are well equipped to deal with this challenge and to make these resources available to a wide research community.

Which research areas that employ supercomputers do you consider to have common interests and projects?

Supercomputing is indispensable for the material sciences if experimental data are to be compared with theoretical models. This is done in both Jülich and in Oak Ridge. Joint projects can be conceived for fields that employ both experiments and supercomputers. The topic of climate in general is also becoming increasingly important. Nuclear fusion could represent a third field.

Dr. Thom Mason is Director of Oak Ridge National Laboratory (ORNL). ORNL is the largest science and energy research institution of the US Department of Energy. With a staff of 4,200, 20 large-scale facilities and a budget of approx. US$ 1.2 billion, it pursues research in the fields of material sciences, energy research and supercomputing.

Forschungszentrum Jülich

Forschungszentrum Jülich pursues cutting-edge interdisciplinary research on solving the grand challenges facing society in the fields of health, energy and the environment, and information technology. In combination with the two key competencies – physics and supercomputing – work at Jülich focuses on long-term, fundamental and multidisciplinary contributions to science and technology as well as on specific technological applications. With a staff of about 4,400, Jülich – a member of the Helmholtz Association – is one of the largest research centres in Europe.

Together with its partners, the *Jülich Supercomputing Centre* at Forschungszentrum Jülich has been operating the first German supercomputing centre since 1987, and with the *Jülich Institute for Advanced Simulation*, founded in early 2008, it is continuing the long tradition of scientific computing at Jülich. Computing time at the highest performance level is made available to researchers in Germany and Europe by means of an independent peer-review process. About 120 experts and contacts for all aspects of supercomputing and simulation sciences work in JSC. As a member of the German Gauss Centre for Supercomputing, the *Jülich Supercomputing Centre* and its partner the French research organization CEA intend to set up the first two European supercomputers with a power of more than a petaflop/s in Germany and France, respectively, by 2010.

Facts and Figures: Jülich Supercomputing Centre

Staff:	120 in total
including:	approx. 70 scientists
	approx. 20 university lecturers
Computing power:	ca. 280 teraflop/s
Storage capacity:	approx. 1 petabyte on hard drives
	approx. 10 petabytes on tapes
Air-conditioned floor space:	approx. 1700 m^2
	6-megawatt cooling capacity
External projects per year:	approx. 200
	about 20 large-scale projects
Distribution of computing time:	40 % universities
	40 % Helmholtz Association
	10 % EU projects
	5 % Max Planck Society
	5 % industrial research
Allocation of computing time:	peer-review process
Simulation labs:	plasma physics
	nanophysics and material sciences
	earth system sciences
	biophysics and bioinformatics
Participations:	more than 20 EU-, DFG- and BMBF-funded projects
Member of:	GCS, PRACE, JARA-SIM, NIC, OGF, OASIS, DEISA

Facts and Figures: Forschungszentrum Jülich

Partners:	Federal Republic of Germany (90 %)
	Federal State of North Rhine-Westphalia (10 %)
Share capital:	€ 511,291
Budget:	€ 360 million per year (including special tasks)
Staff:	4,399 in total
including:	scientists 1,278
	inc. PhD students and fellows 377
	technical staff 1,460
	trainees 348
Visiting scientists:	more than 800 from over 50 countries each year

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