



## Five Petaflops for Science

There was a lot of movement recently in the TOP500 – a list of the fastest supercomputers in the world. Europe, which had been poorly represented, featured with four computers among the ten best. The new Jülich supercomputer JUQUEEN made it straight to place eight in its initial configuration. In October, the system was expanded from eight racks to twenty-four. The question now is how it will fare in November, when the next TOP500 will be published.

However, even more important is the fact that JUQUEEN will probably be the first supercomputer in Europe to achieve a computing power of 5 petaflops – in other words, five quadrillion arithmetic operations per second – which will open up new opportunities in Jülich for an even broader range of working groups and for particularly computationally intensive large-scale projects. The need for computing power is increasing relentlessly, as reflected in the high utilization of the foregoing system in the past. JUGENE provided pioneering information on the basic properties of elementary particles, the origin of life, the structure of data storage materials and on elementary cell processes, an important starting point for developing new active ingredients for drugs (see p. 2).

Its successor, JUQUEEN, will also be at the service of science, and it simultaneously represents another step towards exascale – towards next-generation computers that will be a thousand times faster. Compared to JUGENE, energy efficiency has improved five times over, but it remains one of the biggest challenges today. Users throughout Germany and Europe can apply for computing time via two supercomputing alliances: via the Gauss Centre for Supercomputing and the European research infrastructure PRACE. JUQUEEN is particularly suitable for highly scalable projects, for example, for climate and atmosphere simulations, brain and galaxy models, new materials and research on elementary particles. This is also the topic of the much awaited keynote speech marking the end of the year for Jülich on 12 November 2012 in Bonn, where Professor Thomas Lippert, director of the Jülich Supercomputing Centre, will provide us with even more insights into the world of scientific computing.

Professor Achim Bachem  
*Chairman of the Board of Directors  
of Forschungszentrum Jülich*

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[www.fz-juelich.de/ias/jsc/EN](http://www.fz-juelich.de/ias/jsc/EN)

## Protons on the Frontier

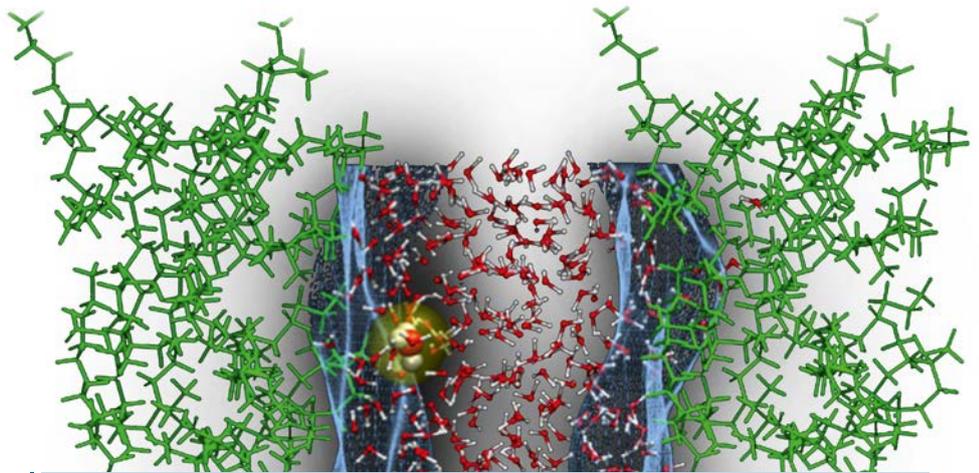
Energy conversion plays an important role in nature – in the human metabolism, for example, or in photosynthesis. In order to improve our understanding, scientists are investigating the complex processes in the smallest living unit – the cell. A key role is played here by proton transport. The protons move along the membrane walls of the cell unusually fast. This is made possible by a boundary layer, which scientists from Jülich and Linz have now discovered using simulations on the Jülich supercomputer JUGENE. In this layer, protons can move with virtually no constraints while maintaining contact with the membrane surface.

Following experiments investigating proton dynamics on an interface of water and a water-repellent surface, the researchers reconstructed the phenomenon on JUGENE. Even though the scientists used a minimalistic model system, they still needed complex molecular dynamic simulations. No fewer than 40 million processor hours were required. “On a single standard PC, the calculations would have taken us almost 5,000 years; JUGENE only needed 100 days,” said Chao Zhang from the German Research

School for Simulation Sciences (GRS) at Forschungszentrum Jülich. Zhang performed the simulations within Professor Paolo Carloni’s working group for computer-assisted biophysics. GRS worked with the Jülich Institute for Advanced Simulation and the Institute of Biophysics at Johannes Kepler University Linz in Austria on the

simulations. The calculations were funded by the Partnership for Advanced Computing in Europe (PRACE).

*High-speed traveller: a proton (yellow sphere) moves along an interface of water (red and white elements) and a water-repellent surface (blue lattice).*



Original publication:

Proceedings of the National Academy of Sciences DOI: 10.1073/pnas.1121227109

## New Platform Gives Europe a Competitive Edge



Europe will only remain internationally competitive if it increases its innovativeness by making use of high-performance computing (HPC). This is one of the key messages in the Vision Paper published by the new European Technology Platform for HPC (ETP4HPC). This platform was established in June 2012 by leading companies and research institutions. “By combining our strengths, we want to consolidate Europe’s role in developing HPC technologies and drive forward technological development as a whole,” says Professor Thomas Lippert, head of the Jülich Supercomputing Centre at Forschungszentrum Jülich, which set up the platform with thirteen partners.

*Leading role: Europe can help to shape the development of the next generation of supercomputers.*

The main concern of members of ETP4HPC is that Europe is lagging behind other regions both in terms of developing and investing in technologies and software. “The Vision Paper outlines how Europe could get involved in developing computers of the next generation,” says Lippert. The first step entails drafting a strategic research agenda, which would then be implemented in dialogue with the European Commission and other institutions, such as the Partnership for Advanced Computing in Europe (PRACE). Concrete suggestions for this, including future priorities in developing hardware, are also summarized in the Vision Paper.

[www.etp4hpc.eu/documents/Joint%20ETP%20Vision%20FV.pdf](http://www.etp4hpc.eu/documents/Joint%20ETP%20Vision%20FV.pdf)

## Exploiting the Performance Potential of Graphics Cards

There are different ways of increasing the performance of supercomputers. The research community has high hopes for the use of graphics processing units (GPUs). Scientists from Forschungszentrum Jülich are working together with the American graphics card manufacturer NVIDIA in the NVIDIA Application Lab, which they set up during the summer. The partners aim to optimize scientific simulations in fields such as neurosciences, astrophysics, particle physics, materials science and biology.

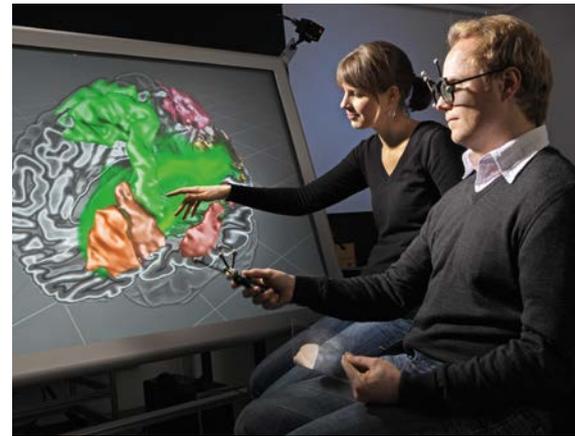
“While central processing units (CPUs) require a small number of powerful cores, GPUs perform their calculations with several weak cores. The massively parallel execution of several simple operations using GPUs requires less energy and is often much faster,” says Professor Dirk Pleiter from the Jülich Supercomputing Centre. The cluster system JUDGE is already

benefiting from this increase in speed thanks to GPUs – it is currently one of the fifty most energy-efficient supercomputers in the world.

Pleiter believes that hybrid systems effectively combining CPUs and GPUs are the way forward. At the moment, however, only a few applications are capable of efficiently using several GPUs working in parallel. “In order to expand the use of GPUs, we have to know more about what computing operations they are best suited to, and what consequences this has for the architecture.” In order to determine just this, the physicist and his colleagues joined forces with their industrial partner and are taking a look at research projects that are being conducted or could be conducted on parallel GPU systems like JUDGE. For example, the JUBRAIN pilot project at the Jülich Institute of Neuroscience

and Medicine. In this project, brain researchers are creating an extremely high-resolution and multidimensional model of the human brain.

*Using GPUs to optimize 3D models of the human brain.*



[www.fz-juelich.de/SharedDocs/Pressemitteilungen/UK/DE/2012/12-06-19NVIDIA\\_Application\\_Lab.html](http://www.fz-juelich.de/SharedDocs/Pressemitteilungen/UK/DE/2012/12-06-19NVIDIA_Application_Lab.html)

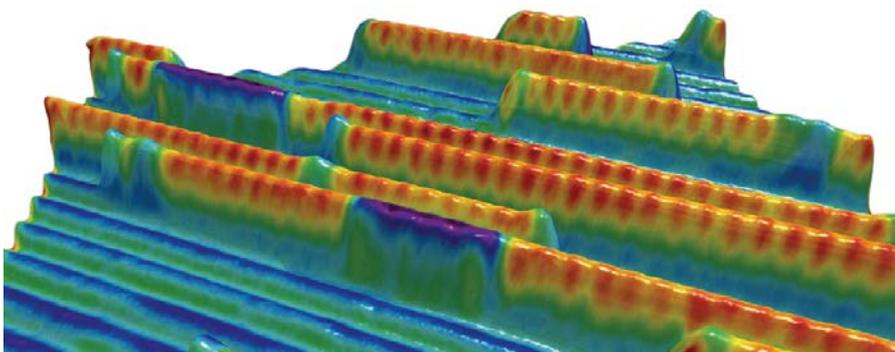
## Reading Data Using Spin Spirals

The biggest problem associated with data storage is not writing but reading – at least when broaching the physical limits. Methods of storing one bit per atom already exist. However, techniques of reading these data without destroying them are still being sought. Professor Yuriy Mokrousov from the Institute of Quantum Theory of Materials at Forschungszentrum Jülich has developed a very promising approach based on spin spirals.

Spin spirals are atomic chains in which the magnetic moments of the atoms – the spins – create a very stable spiral formation. The key characteristic is that when the topmost spin is turned, the entire chain moves with it. “It rotates like a screw, and the orientation of the bottommost spin tells us what that of the topmost spin is,” says the physicist. Usually, spins arrange themselves in parallel to their neighbours. If the topmost atom in the spin spiral touches an atom

whose magnetic angular momentum has stored information, this information could therefore be read out at the bottommost atom – in a quick and energy-efficient manner.

Mokrousov discovered this exotic formation while working together with experimental physicists from Hamburg in twin rows of 100 iron atoms on an iridium surface. The system revealed its special magnetic properties at temperatures slightly higher than absolute zero. The laws of nature, however, do not preclude the effect from also appearing at room temperature. The researcher therefore used simulations on the JUGENE supercomputer to identify conditions that would allow higher temperatures. To date, he has only reached 100 Kelvin – an icy minus 173 degrees Celsius. “For particles that do crazy things, this is hot. Usually, they only do so at temperatures a few degrees warmer than absolute zero,” says Mokrousov.



*Reading aid: by selectively modulating the magnetic order of atomic chains – here: iron (yellow/red) – stored information can be read out faster.*

Original publication: Physical Review Letters DOI:10.1103/PhysRevLett.108.197204

## NEWS IN BRIEF

## DEEP Cluster in Operation

The EU project Dynamical ExaScale Entry Platform (DEEP) has a new supercomputer cluster. An Aurora HPC 10-10 manufactured by Eurotech with energy-efficient hot-water cooling has been up and running since September at Forschungszentrum Jülich. The system uses hot water with temperatures of up to 45 °C, which releases the heat into ambient air without additional cooling. DEEP aims to develop a new computer architecture for the exascale class planned for the end of the decade. The concept envisages using the installed cluster to calculate the complex components of parallel programs. It will be augmented by another computer known as a booster. Its processors comprising 50 cores will calculate the simple, massively parallel program parts in a much more energy-efficient manner. The project, funded to the tune of € 8 million by the European Commission, involves 16 partners from science and industry. It is coordinated by Forschungszentrum Jülich.

[www.deep-project.eu](http://www.deep-project.eu)

## Accounting for the Time Factor

More and more processor cores, increasingly complex computer architectures and applications – enhanced computing capacity can only be utilized efficiently if special tools are used. Developers of parallel simulation codes are now receiving support from the Performance Dynamics of Massively Parallel Codes (LMAC) project. As part of the project, the analysis tools Vampir, Scalasca and Periscope are being extended with an additional feature: the automatic examination of time-dependent performance behaviour, also referred to as performance dynamics. Existing tools often provide detailed data on the performance behaviour of parallel codes, but neglect differences over time. However, detailed information on these dynamics is required to minimize performance bottlenecks.

The project is coordinated by the German Research School for Simulation Sciences and also involves Forschungszentrum Jülich, GNS mbH, RWTH Aachen University, and the universities of technology in Dresden and Munich. The University of Oregon in the USA is an associated project partner.

<http://www.vi-hps.org/projects/lmac>

## Saving Electricity without Losing Time

Scientists working on the eeClust project have developed a new method of reducing the electricity consumed by computer clusters. They used analysis software to investigate the time taken to execute tasks and the energy required by parallel programs to do so. Their findings showed that cluster components temporarily not in use can be switched off. The decisive advantage here is that this does not affect computing time. Other methods to date were unable to overcome this risk. The Jülich Supercomputer Centre is already using tools and methods developed by eeClust in ongoing projects. One example is the Exascale Innovation Center (EIC), which it jointly operates with IBM.

[www.eeclust.de](http://www.eeclust.de)

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[www.fz-juelich.de/app\\_en](http://www.fz-juelich.de/app_en)



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Android

### PUBLICATION DETAILS

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## UPCOMING EVENTS

Introduction to the programming and usage of the supercomputing resources at Jülich

22 – 23 November 2012

Jülich Supercomputing Centre

New users of the supercomputing resources at Forschungszentrum Jülich will be given an overview of the systems and their applications. The course will also explain how efficient use can be made of the allocated resources.

**Instructors:** JSC employees and representatives of IBM, Intel and ParTec

[www.fz-juelich.de/ias/jsc/events/sc-nov](http://www.fz-juelich.de/ias/jsc/events/sc-nov)

Introduction to parallel programming with MPI and OpenMP

26 – 28 November 2012

Jülich Supercomputing Centre

The course will provide an introduction to parallel programming on supercomputers in the area of technical and scientific computing. The two most commonly used programming models will be presented: OpenMP and Message Passing Interface (MPI).

**Instructor:** Dr. Rolf Rabenseifner, HLRS Stuttgart

[www.fz-juelich.de/ias/jsc/events/mpl](http://www.fz-juelich.de/ias/jsc/events/mpl)

Introduction to parallel computing

12 December 2012

Jülich Supercomputing Centre

In this course, participants will learn about the basic concepts, methods and technologies associated with supercomputing systems, as well as the essential parallel programming. Future technologies and research issues will also be dealt with.

**Instructor:** Dr. Bernd Mohr, JSC

[www.fz-juelich.de/ias/jsc/events/parcomp](http://www.fz-juelich.de/ias/jsc/events/parcomp)

Workshop HYBRID2013

4 – 7 March 2013

Jülich Supercomputing Centre

The Workshop on Hybrid Particle-Continuum Methods in Computational Materials Physics targets scientists working in computer-assisted materials science who conduct research on complex liquids and solids.

[www.fz-juelich.de/ias/jsc/HYBRID2013](http://www.fz-juelich.de/ias/jsc/HYBRID2013)

You can find an overview of events at the Jülich Supercomputing Centre at:

[www.fz-juelich.de/ias/jsc/events](http://www.fz-juelich.de/ias/jsc/events)