EXASCALE
Newsletter of Forschungszentrum Jülich on Supercomputing

JÜLICH
FORSCHUNGSZENTRUM

Issue: 2 | June 2014

Member of the Helmholtz Association

Well Equipped for the Future

"Supercomputing involves more than the mere pursuit of records; it ranks among the world's key technologies."

Around seven years ago, I was asked by the news magazine *Der Spiegel* whether Germany had dropped out of the race for the fastest computers in the world. In my answer, I asked readers to be patient. Although it seemed as though Germany had fallen behind, at the time we were merely setting the course – on a national level with the Gauss Centre for Supercomputing, and on a European level with the PRACE supercomputing partnership. Success soon followed: in May 2009, we presented Europe's first petaflop computer, JUGENE. Its successor JUQUEEN, currently the fastest computer in Germany, performs almost six quadrillion arithmetic operations per second.

However, supercomputing involves more than the mere pursuit of records; it ranks among the world's key technologies. Simulations on supercomputers have established themselves as an independent method and have become the third pillar for obtaining scientific knowledge alongside theory and experiment. They enable us to understand complex relationships and deal with large volumes of data. Basic research, especially, requires adequate resources to break new scientific ground. At Jülich, we focus particularly on climate, materials, and brain research as well as biophysics. However, scientists from other institutions are also granted valuable computing time, for example to obtain new findings on the birth of stars and galaxies.

In June, my time as Chairman of the Board of Directors of Forschungszentrum Jülich will come to an end after eight years. I would like to wish Jülich supercomputing and its partners continued success in their activities, such as those at Gauss, PRACE, and in the collaborations with NVIDIA, Intel, and IBM. We can all look forward to groundbreaking future developments with the coming exascale generation and the Human Brain Project. My thanks also go to all you readers for your interest. Stay up-to-date with exciting developments at Jülich!

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

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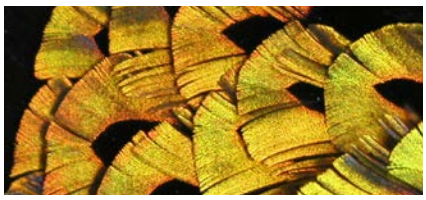
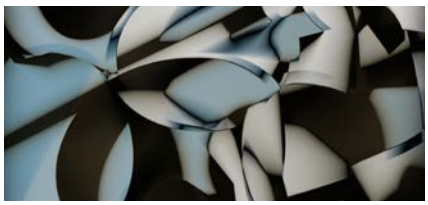




www.fz-juelich.de/ias/jsc/EN

Dance of the Colours

When birds-of-paradise perform their mating dances, they put on a real show. The males dance and sing, skilfully displaying their gloriously colourful feathers to entice the females. Biologists have long been interested in this brightly coloured spectacle staged by the songbirds, the majority of which are native to Papua New Guinea. Researchers from Jülich and Groningen have now succeeded in simulating the complex optical properties of their plumage on a supercomputer at the University of Groningen.

To do so, the physicists from the Jülich Supercomputing Centre (JSC) and their Dutch colleagues selected one representative to examine particularly closely: the male Lawes's Parotia (*Parotia lawesii*). On the sun-drenched forest floor, on which he has previously set the stage for his performance, he enacts an extraordinarily impressive ritual. While he dances, he flaunts his colourful breast feathers, which sometimes appear to shine in orange, and sometimes green or blue. What causes this iridescence is sunlight reflecting off tiny structures in the feathers. The scientists wanted to find out how exactly this works. First, they determined the optical properties of individual breast and neck feathers using a special light-scattering measurement device. They then developed a computer model which they used to simulate the reflection pattern. Their findings were almost identical. "The reflections are strongly dependent on the angle of incident light. Therefore, it is the dance that produces the dazzling iridescence, as the feathers are illuminated from constantly changing angles," explains Prof. Kristel Michielsen from JSC. Their model could also help to design nanostructured materials with interesting optical properties, for example for sensors and optical communications devices.

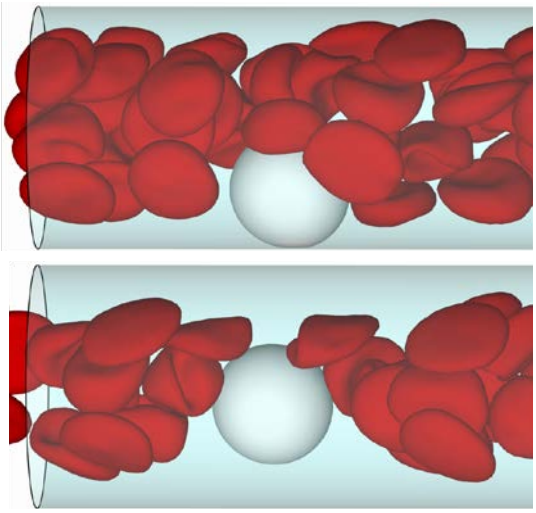
PNAS, DOI: 10.1073/pnas.1323611111

Male birds-of-paradise impress females with the iridescence of their feathers. A research team has succeeded in simulating the complex optical properties of their plumage on a computer.

Pushing the Immune System Police Over the Edge

White blood cells are the police force of our immune system. They use arteries and veins as a means of reaching every nook and cranny of the body. The problem is that the white blood cells, also known as leucocytes, do not have a self-propulsion mechanism. If they wish to leave a blood vessel, they have to be passively conveyed to the vessel wall before they can pass through it. Jülich researchers have discovered the necessary conditions for this process thanks to simulations performed on the Jülich supercomputer JUROPA.

When tissue is attacked by pathogens, it emits a neurotransmitter. This causes the spherical leucocytes to change their shape so that they can travel through narrow openings in the blood vessels to get to where they are needed. The ability of white blood cells to reach a vessel wall at all is determined by their shape and size, the concentration of red blood cells, and the velocity of the blood flow. "Using three-dimensional computer simulations, we calculated exactly what happens at given values for these factors," explains physicist Dr. Dmitry Fedosov from Theoretical Soft Matter and Biophysics. An average number of red blood cells and a low blood flow velocity will push a white blood cell to the edge of the blood vessel. However, if the number of red blood cells is too low and the flow velocity too high, a white blood cell will continue to go with the flow and cannot reach the vessel wall. "Our method could also be used to develop new technologies in medical diagnostics, for example for diagnosing malaria," adds institute head Prof. Gerhard Gompper. With this disease, it is often the case that only a small number of pathogens are present, which must be separated and concentrated to provide a reliable diagnosis.



Simulations by the Jülich researchers and still frames from the simulations. Top: An average number of red blood cells and a low blood flow velocity (from left) will push the white blood cell to the edge of the blood vessel.

Bottom: If the number of red blood cells is too low and the flow velocity too high, the white blood cell will continue to go with the flow and cannot reach the vessel wall.

Soft Matter, DOI: S10.1039/C3SM52860J

Computing for the Sake of Art

The Jülich supercomputer JUROPA is particularly suitable for CPU-intensive data analysis for areas such as medicine, biology, or climate research. Early this year, however, it was required to perform an unusual task: computing artwork.

The internationally acclaimed artist Thomas Ruff requested the help of the Jülich Supercomputing Centre (JSC) to produce artwork from his latest series, "Photograms", in the highest possible quality. Strictly speaking, photograms are black-and-white photographic images created without a camera in a darkroom. To do so, objects are arranged on light-sensitive paper and then exposed to light. Ruff's colour photograms, however, are created entirely on a computer. Yet at a size of 2.20 metres by 1.64 metres and more than nine gigabytes of data per image, the photograms pushed the artist's computers to their limits. "From our point of view, it was an excellent opportunity to determine important characteristics for the design of JUROPA's successor, for example with respect to the high demands for data storage, data rates, and local processing power," says JSC head Prof. Thomas Lippert. "It was also a good occasion to get people other than our usual clientele interested in high-performance computing."

Employees at JSC adapted the software used by Ruff so it could run on JUROPA, optimized the computing process, and created a suitable measurement environment. They also developed a new monitoring tool that will be available to all users in future. Their efforts resulted in images that are markedly more detailed but at least 18 terabytes in size. This was no problem for JUROPA, however: 1,000 of its nodes required up to 15 hours for one image, a task for which Ruff's computer would have taken over a year.

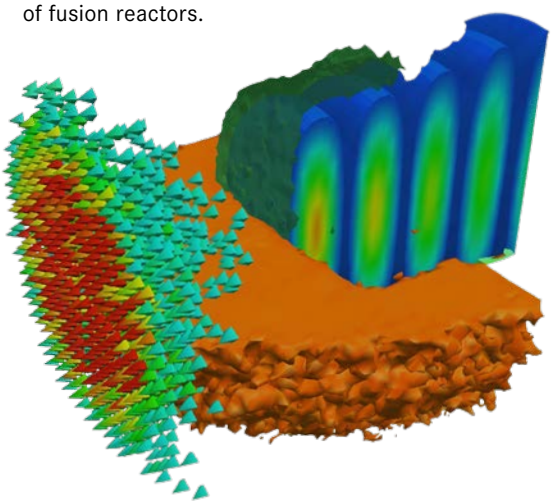
A selection of the photograms are being exhibited at the Museum of Contemporary Art (S.M.A.K.) in Ghent, Belgium, until 24 August 2014.

One of Germany's internationally best-known contemporary artists: Thomas Ruff

Laser Accelerators in the Fast Lane

Compact laser plasma accelerators have the potential to replace conventional particle accelerators in an ever growing number of fields. The latter are employed in basic scientific research or in medicine, where they are used to remove tumours. In future, laser-based systems could also be used as a source of polarized particle beams, which are required for high-precision nuclear physics experiments. This has been suggested by initial measurements conducted by Jülich and Düsseldorf scientists and confirmed by simulations on the Jülich supercomputer JUROPA.

Even laboratory-scale laser accelerators can bring particles to the required speeds. This makes them considerably less expensive to purchase and operate than large and costly conventional devices. The research group headed by Jülich scientist Prof. Markus Büscher want to enable these laser accelerators to be used in conventional physics experiments. They have developed a method that allows the polarization of particles at laser accelerators to be measured for the first time. "It was found that the 'spin' or angular momentum of the protons is not decisively altered by the strong electromagnetic fields present in the laser-generated plasma," says Büscher, who works at Jülich's Peter Grünberg Institute and at Heinrich Heine University Düsseldorf. This is an important prerequisite for using lasers to accelerate polarized particles. Whether or not this actually works will become clear by the end of the year. Fusion research may also benefit from this one day, as polarized particles could potentially increase the energy yield of fusion reactors.



If the laser pulse (ovals with blue edges) hits a thin foil (orange), the electrons (coloured particles on the left) break away from the atomic nuclei. An extremely strong electromagnetic field forms between the atomic nuclei and the electron cloud, accelerating the atomic nuclei over a very short distance.

Physics of Plasmas,
DOI: 10.1063/1.4865096

NEWS IN BRIEF

Open to Innovation

Forschungszentrum Jülich has joined the OpenPOWER Foundation. Other partners in the collaboration, which was founded in 2013, include IBM, Google, and NVIDIA. OpenPOWER advocates the use of open-source technologies based on the architecture of IBM POWER processors. Its 25 current members provide access to hardware and software in order to drive innovation for computing centres, for example for hardware acceleration and solutions for storage and networks. This will also benefit the development of new supercomputing architectures based on POWER processors and graphics processing units. This is where the Jülich Supercomputing Centre will contribute its expertise from the NVIDIA Application Lab and the Exascale Innovation Center.

www.fz-juelich.de/SharedDocs/Pressemitteilungen/UK/EN/2014/14-04-23OPF.html

Science on Board

The MS Wissenschaft exhibition ship will be touring around Germany and Austria until 28 September with an exhibition on board about the digital world. The exhibition presents what researchers have discovered about the benefits and opportunities – as well as the risks and challenges – of the digital revolution brought about by computers and the Internet. Experts from the Jülich Supercomputing Centre demonstrate how computer simulations can help to prevent dangerous situations at large public events. For example, visitors to the exhibition can simulate on a computer how several hundred people can be evacuated from a room.

www.fz-juelich.de/SharedDocs/Pressemitteilungen/UK/EN/2014/14-04-30ms-wissenschaft.html

Inhospitable Centre

The Jülich supercomputer JUDGE has helped astrophysicists from Heidelberg University to gain new insights into the formation of stars. Evidently, the process is different at the centre of the Milky Way than at its edge, for example in the area around our sun, which is located at a distance of some 25,000 light years from the galaxy's centre. This difference is due to the extreme conditions at the centre. Black holes and extremely hot or exploding stars cause powerful "radiation winds". Simulations performed on the JUDGE extension "Milky Way" revealed that the radiation field at the centre must be 1,000 times stronger than that at the edge of the Milky Way. This strong field heats the interstellar gas found between the stars of a galaxy, which is important for star formation. The scientists from the German Research Foundation's Collaborative Research Centre 881, "The Milky Way System", believe that this influences the formation process.

DOI: 10.1088/2041-8205/768/2/L34

www.zah.uni-heidelberg.de/sfb881/

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PUBLICATION DETAILS

EXASCALE NEWSLETTER of Forschungszentrum Jülich **Published by:** Forschungszentrum Jülich GmbH | 52425 Jülich | Germany **Conception and editorial work:** Dr. Anne Rother (responsible according to German press law), Tobias Schlößer, Christian Hohlfeld **Graphics and layout:** Graphical Media, Forschungszentrum Jülich **Translation:** Language Services, Forschungszentrum Jülich **Images:** p. 1: Forschungszentrum Jülich, ©fotolia.com/Photobank/virtua73; p. 1 centre and p. 2 top: Justin Marshall; p. 2 bottom and p. 3 top: Forschungszentrum Jülich; p. 3 bottom: Jülich Supercomputing Centre; p. 4 top: ©fotolia.com/virtua73; p. 4 bottom: Ilja Hendel/ Wissenschaft im Dialog **Contact:** Corporate Communications | Tel: +49 2461 61-4661 Fax: +49 2461 61-4666 | Email: info@fz-juelich.de **Printed by:** Schloemer & Partner GmbH **Print run:** 300

UPCOMING EVENTS

High-Performance Computing with Python
26 – 27 June 2014
Jülich Supercomputing Centre
Parallel programming with Python; performance optimization with various tools
www.fz-juelich.de/ias/jsc/events/hpc-python

Introduction to Parallel Programming with MPI and OpenMP
5 – 8 August 2014
Jülich Supercomputing Centre
Parallel programming for supercomputers in a scientific and technical environment; training course as part of the JSC Visiting Student Programme
www.fz-juelich.de/ias/jsc/events/mpi-gsp

Atomistic Monte Carlo Simulations of Biomolecular Systems
15 – 19 September 2014
Jülich Supercomputing Centre
CECAM tutorial on the open-source software ProFASi, which enables Markov Chain Monte Carlo simulations of biomolecules at the atomic level
www.fz-juelich.de/ias/jsc/events/cecam-mc-2014

Data Analysis and Data Mining with Python
10 – 12 November 2014
Jülich Supercomputing Centre
Introduction to analysis and evaluation programs for Python: matplotlib for visualization, pandas for time series analysis, and scikit-learn for data mining
www.fz-juelich.de/ias/jsc/events/data-mining

Programming and Usage of Supercomputing Resources
27 – 28 November 2014
Jülich Supercomputing Centre
Introduction for new users, e. g. on how to make optimal use of allocated computing resources
www.fz-juelich.de/ias/jsc/events/sc-nov

You can find an overview of events at the Jülich Supercomputing Centre at:
www.fz-juelich.de/ias/jsc/events