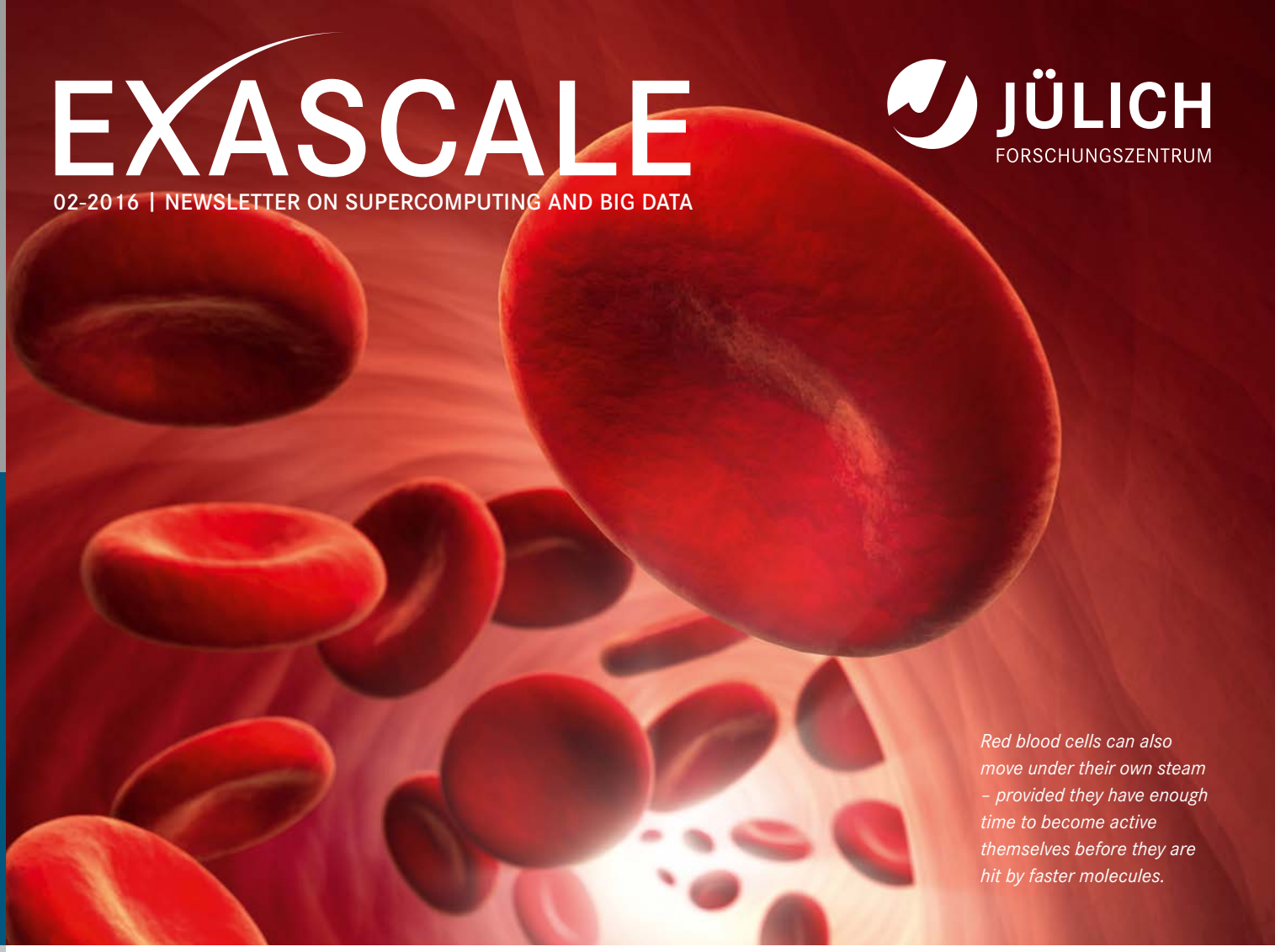
EXASCALE
02-2016 | NEWSLETTER ON SUPERCOMPUTING AND BIG DATA

JÜLICH
FORSCHUNGSZENTRUM



Red blood cells can also move under their own steam – provided they have enough time to become active themselves before they are hit by faster molecules.

Member of the Helmholtz Association

And Yet They Move

Not only external but also internal forces cause red blood cells to flicker

Scientists have discussed the issue for years: do red blood cell membranes move on their own or is this motion triggered by external forces? An international team of biophysicists has now proved that both opinions are correct. By linking physical principles and biological reality, they demonstrated how red blood cells move. They achieved this by combining innovative experiments with theoretical models and simulations on Jülich's JURECA supercomputer.

Internal activity takes time

Red blood cells transport oxygen in blood. If fast molecules impact on the blood cells, they make the cell membranes flicker. This causes the very soft and elastic cells to wriggle. "However, we discovered that the blood cells themselves also become active. If they have enough time, they fire up their own motor, which then becomes dominant rather than external forces," explains Dr. Dmitry Fedosov from Jülich's Theoretical Soft Matter and Biophysics subinstitute (ICS-2/IAS-2). The research was initiated by Jülich and the Institut Curie in Paris and was completed together with the University of Münster.

Transport proteins under suspicion

The research team stretched the blood cells using so-called optical tweezers – a concentrated laser beam. The blood cells counteracted the force of the optical tweezers if they had enough time. This means there must be forces inside the cell. Physical theories and computer simulations supported the interpretation of the experimental results. The researchers already have their suspicions about what could be the internal trigger: "Transport proteins in the membrane could generate such forces by moving ions from one side of the membrane to the other," says Jülich biophysicist Dr. Thorsten Auth, who together with Dr. Dmitry Fedosov was responsible, in particular, for the simulations. It is now up to the biologists to discover which protein it could be.

▶ Nature Physics (2016), DOI: 10.1038/nphys3621 and 10.1038/nphys3703

STATEMENT

Prof. Gerhard Gompper
Head of ICS-2/IAS-2

We develop models and methods in order to understand complex biological systems on the basis of physical principles. By means of simulations on supercomputers, we can quantify chemical and biological processes which are not amenable to direct experimental observation.

The Complex Puzzle of Combustion

► Institute for Combustion Technology, RWTH Aachen University

Gases and liquids are burned to produce energy – the principle is well known and has long been successfully applied in engines, gas turbines, and power plants. Nevertheless, the interaction of chemistry and fluid dynamics processes still has its secrets. Prof. Heinz Pitsch, head of the Institute for Combustion Technology at RWTH Aachen University, uses simulations on supercomputers in an attempt to solve this puzzle. In April, the European Research Council (ERC) provided him with an Advanced Grant for his work. This funding of € 2.5 million will help to describe combustion processes more precisely and with these insights it will be possible to optimize existing systems or develop new ones. Pitsch will also be using Jülich supercomputers for this purpose.

Combustion processes are very complex as they proceed on a huge range of different time and length scales. "Even on the basis of the most sophisticated experiments, phenomena such as ignition, extinction, and pollutant formation are very difficult to understand and explain," the Aachen researcher explains. He has frequently used supercomputers to simulate such processes with the aid of models he helped to develop, also at Jülich – for example, within the framework of the Jülich Aachen Research Alliance (JARA), an alliance of RWTH Aachen University and Forschungszentrum Jülich. The aim of such simulations is often to understand the formation of pollutants in combustion devices. "The proportion of renewable energies is constantly increasing, but we will continue to depend on the combustion of fossil fuels for many decades to come," says Pitsch. "The great challenge is to make combustion plants more efficient and environmentally friendly."

Increased Safety for the Disabled

The beginning of February 2016 saw the launch of a new research project on the Safety of People with Physical, Mental, and Age-Related Disabilities (SiME), in which the Jülich Supercomputing Centre (JSC) is also involved. Stefan Holl from JSC's Civil Security and Traffic explains the project's objectives.

Stefan Holl

Mr Holl, what is SiME all about?

If buildings have to be evacuated rapidly in case of accidents or fires, then people with disabilities often need assistance from others. Together with our project partners, we want to find out to what extent those affected can rescue themselves. On the basis of these findings, we intend to develop measures to improve their ability to save themselves. This includes efficiently preparing people for critical situations as well as an optimum design of escape routes and emergency access.

What exactly is JSC's job?

We are developing models to simulate people's movements, amongst other aspects during evacuations. We are building on experience from previous projects on the internal dynamics of crowds of people such as BaSiGo. However, we do not yet have any movement parameters for the disabled, for example the speed at which they move or the distance from other people.

How do you intend to acquire such parameters?

As in the other projects, we will perform studies – in this case with mixed groups of people with normal and restricted mobility. For example, we want to find out what effect wheelchairs or rollators have on the way people move. On the basis of such parameters, we can then create simulations, for example for evacuating residential homes or workshops.

Can the results be used for public buildings?

The initial concern is safety concepts for institutions in the social sector. Operators, specialist planners, and licensing authorities will thus be given a basis for evaluation. However, we hope that others will also consider our results in their evacuation concepts.

Mr Holl, thank you for talking to us.

► Safety of People with Physical, Mental, and Age-Related Disabilities (SiME, in German)

New Concept for Digital Data Storage

Antiferromagnets can be electrically controlled

An international team of researchers has succeeded in electrically controlling the switching and readout of the magnetic moment of an antiferromagnetic material – an important step towards storing information. These findings open up new approaches for digital data storage.

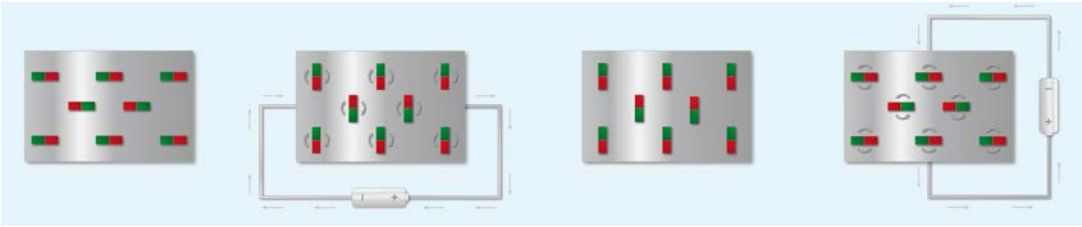
To date, it has only been possible to use antiferromagnetic materials for information technology in combination with other materials. This is due to their atomic magnetic moments, known as spins. In antiferromagnets, half of the spins point in one direction and the other half in the opposite direction. That is to say, on average they cancel each other out. This is why, in contrast to ferromagnets such as iron, they are not influenced by external magnetic fields. However, it is precisely this property of ferromagnets that is currently exploited by all common methods of magnetic data storage.

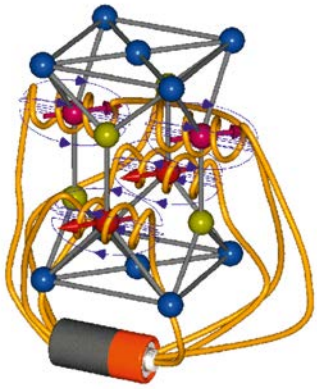
"Since antiferromagnets are more magnetically stable and can basically be switched faster than ferromagnets, we looked for a new approach," says Prof. Yuriy Mokrousov from Jülich's Peter Grünberg Institute. Using specimens made from copper manganese arsenide, researchers from the United Kingdom, the Czech Republic, Germany, and Poland were able to control the direction of the spins by means of electric pulses.

Electric current tilts spin

"The current brings about a quantum mechanical torque on individual spins and allows each of them to tilt by 90 degrees," explains the Jülich expert Dr. Frank Freimuth. Simulations on Jülich's supercomputers and special software developed at Jülich helped the researchers to understand details of how this switching occurs.

The scientists now want to develop ideas on integrating their new approach into existing data storage concepts. There is a large selection of suitable materials that are antiferromagnetic at room temperature. The phenomenon of antiferromagnetism can be found, for example, in metals, semiconductors, and insulators.





A complicated tangle of loops (yellow lines in the figure above) would be necessary to switch antiferromagnets using magnetic coils. However, as yet there are no such atomically small coils. Instead, researchers have found a way to rotate the direction of the spins (red spheres) by 90 degrees with the aid of electric pulses.

Left: spins of the copper manganese arsenide sample. A current pulse applied perpendicularly to the first pulse allows the spins to tip back into their initial position.

► Science (2016), DOI: 10.1126/science.aab1031

Human Brain Project Launches European Infrastructure

At the end of March 2016, the Human Brain Project (HBP) presented the first version of its shared European infrastructure for exploring the human brain. Researchers from 24 countries collaborated on creating this infrastructure during the past two and a half years. The new facility, which is open to all interested users, will permit detailed analyses and simulations of the brain. To this end it interconnects scientists via four large European supercomputer and data centres. One of these centres is the Jülich Supercomputing Centre (JSC). The infrastructure can be accessed via a web portal.

Together with ETH Zürich, JSC coordinates one of the six platforms of this infrastructure. The "High Performance Analytics and Computing Platform" will help store the enormous volumes of data on the human brain, integrate this data into models, and evaluate it in simulations. Furthermore, JSC and fourteen cooperation partners will provide support for European neuroscientists in using the supercomputer resources, storage systems, and user software.

New information technologies

The HBP investigates the organization of the brain and intends to contribute to a better understanding of neurological disorders. For this purpose, the scientists involved are developing new information technologies such as neurosynaptic processors, which are based on the principles governing how the human brain works. This will not only benefit neuroscience but also supercomputing and robotics.

► The six platforms of the European infrastructure

► *The Human Brain Project explores the organization of the human brain. The newly launched European infrastructure will facilitate detailed analyses and simulations.*

NEWS IN BRIEF

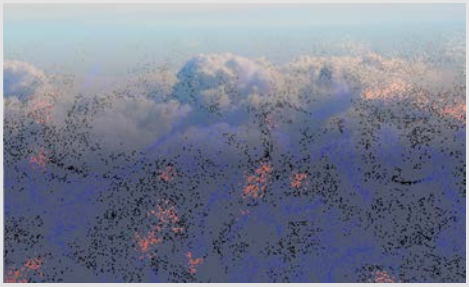
New SPXXL President

Dr. Michael Stephan from Jülich Supercomputing Centre is the new president of the SPXXL user group. SPXXL is a user group for institutions operating large installations of IBM or Lenovo equipment. The aim is to further develop, together with the vendors, large-scale scientific and technical computing on scalable parallel computers.

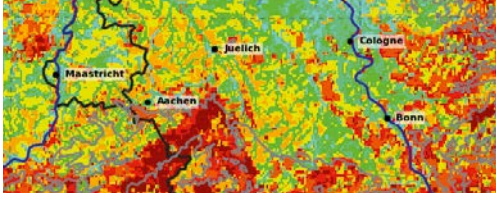
▶ more

Insights into Rain Clouds

Big data experts at the Jülich Supercomputing Centre (JSC) have optimized an algorithm frequently used for data analysis. By parallelizing DBSCAN (Density-Based Spatial Clustering for Applications with Noise), large volumes of data can be processed more rapidly on supercomputers. It also considerably reduced memory storage. The new variant HPDBSCAN is currently being used at Jülich and is also available as open-source software. Together with partners from RWTH Aachen University, the JSC researchers want to better understand droplet formation in rain clouds.



In a sea of clouds: raindrops are formed by particles becoming compressed. DBSCAN identifies flow lines (dark blue dots in the lower part of the image) and other accumulations (orange), thus revealing the formation of precipitation.



Daily Updates on YouTube

Every day, the "Centre for High-Performance Scientific Computing in Terrestrial Systems" publishes updated simulations regarding important state variables of the terrestrial water cycle. They show how, for example, the groundwater level changes in the course of a day or how much water is available for plants in the soil – for North Rhine-Westphalia and also for Europe. The simulations are performed on the Jülich supercomputers JUQUEEN and JURECA with the aid of the Terrestrial Systems Modeling Platform, TerrSysMP, (see Exascale Newsletter 2015/2).

▶ more (in German)
▶ YouTube channel

Contact for Industry

In January 2016, a dedicated contact point was set up for companies wishing to make use of the facilities at the Jülich Supercomputing Centre (JSC). The Industry Relations Team helps businesses to access the Jülich supercomputers and purchase computation time. The team also coordinates research projects relevant to industry and facilitates contacts between external clients and JSC experts.
Tel: + 49 2461 61-8808
Email: ha.fischer@fz-juelich.de

▶ more

JUQUEEN Undergoes Performance Test

From 14 to 20 June 2016, Jülich Supercomputing Centre will be holding a Big Blue Gene Week. During this time, exclusively applications using at least four Blue Gene/Q racks or 65,536 processor cores will be implemented on the JUQUEEN supercomputer. The test days are intended to help users scale their programs more easily and efficiently.

▶ more

Also available for smartphones and tablets!

▶ Exascale newsletter
▶ effzett – the crossmedia magazine
▶ Facts and figures

PUBLICATION DETAILS

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UPCOMING EVENTS

▶ **International Supercomputing Conference**
19 – 23 June 2016
at Messe Frankfurt, Germany
Jülich research: booth 1310 (Jülich Supercomputing Centre), booth 1320 (JARA|HPC), booth 1340 (European Exascale Projects), booth 1201 (PRACE), booth 553 (UNICORE)

▶ **High-performance scientific computing in C++**
27 – 28 June 2016
at Jülich Supercomputing Centre
Instructor: Dr. Sandipan Mohanty, JSC

▶ **International Workshop on Quantum Annealing and its Applications in Science and Industry (QuAASI'16)**
26 – 28 July 2016
at Jülich Supercomputing Centre

▶ **Introduction to Parallel Programming with MPI und OpenMP**
9 – 12 August 2016
at Jülich Supercomputing Centre
Instructors: Dr. Florian Janetzko, Dr. Alexander Schnurpfeil, JSC

▶ **CECAM Tutorial: Atomistic Monte Carlo Simulations of Bio-molecular Systems**
19 – 23 September 2016
at Jülich Supercomputing Centre

▶ **HPSC TerrSys Fall School 2016**
10 – 14 October 2016
at University of Bonn, Germany

▶ **Introduction to GPU Programming using OpenACC**
24 – 25 October 2016
at Jülich Supercomputing Centre
Instructors: Anke Zitz, Dr. Andreas Herten, Dr. Paul Baumeister, all JSC, Jiri Kraus, NVIDIA

▶ **Overview of events at the Jülich Supercomputing Centre**