EXASCALE

Newsletter of Forschungszentrum Jülich on Supercomputing

JÜLICH FORSCHUNGSZENTRUM

Issue: 2 | July 2015

Neutrons (blue) are a tiny bit heavier than protons (yellow). For a long time, science had neither the appropriate methods nor sufficiently powerful computers to calculate the difference precisely. Using supercomputers like JUQUEEN, an international team of scientists has now succeeded in performing the calculation.

A Milestone in Computer Simulation

For two years, the Jülich supercomputers JUQUEEN and JUROPA and their colleagues in Germany and France have been working away at their calculations. Now they have finally finished the task: For the first time, an international research group succeeded in calculating the tiny difference in mass between neutrons and protons from first principles. The neutron is just 0.14 percent heavier – or, in absolute numbers, $2.3 \cdot 10^{-30}$ kilograms. This difference is minute but quite decisive. A slightly smaller or larger value of the mass difference would have led to a dramatically different universe, with more neutrons, less hydrogen, and fewer heavy elements.

Physicists are celebrating this breakthrough which, 80 years after the discovery of the neutron, has finally made it possible to calculate the difference on the basis of theoretical models. “Our simulation is further confirmation of the standard model of particle physics,” says Prof. Kálmán Szabó from the Jülich Supercomputing Centre. He and his colleague Dr. Stefan Krieg are members of the international team from Germany, France, and Hungary, who, headed by the Wuppertal researcher Zoltán Fodor, developed and performed the simulation.

Prof. Kurt Binder, chairman of the Scientific Council of the John von Neumann Institute for Computing, considers the calculation a “milestone in computer simulation”. Until now, neither the methods nor sufficiently powerful computers had been available to precisely determine this tiny difference. Only JUQUEEN, currently one of the fastest supercomputers in Europe, and new simulation methods made it possible to take all the theoretically predicted effects into consideration. The Physics Nobel Laureate Frank Wilczek also places his hopes in the new simulation tools: “Much more accurate modelling of supernova explosions and such strange objects as neutron stars could now become feasible. The dream of more refined nuclear chemistry could be within our grasp, for example improved energy storage and ultra-high-energy lasers”.

Science, DOI: 10.1126/science.1257050

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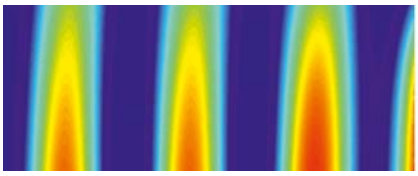

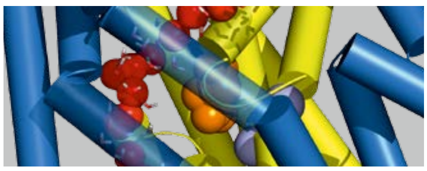

www.fz-juelich.de/ias/jsc/EN

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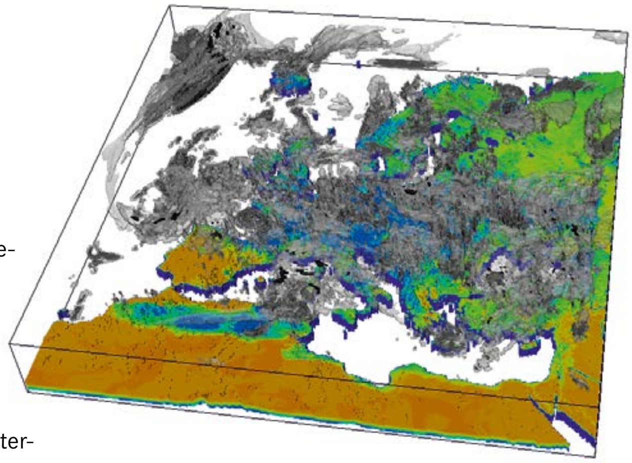
Closed Cycles

The hydrological cycle does not appear to be that complicated at first sight. Sea water evaporates and then arrives back at the Earth's surface in the form of precipitation. There, it evaporates again, infiltrates into the ground, and is transported by rivers back into the sea. This cycle is, however, influenced by complex interactions between the atmosphere, the surface of the Earth, and soils. Scientists from Jülich and Bonn have developed a modelling platform, the Terrestrial Systems Modeling Platform (TerrSysMP), which they intend to use to simulate flows of terrestrial water, energy, and nutrients for the whole of Europe.

TerrSysMP helps them by providing fully coupled simulations, which means that groundwater, soil, land surface and atmospheric models actually interact with each other. Other simulations frequently use isolated models that only cover processes in the respective compartment. "Such models do not fully account for interactions. In our model, we have closed the cycles completely. Whether mass or energy, nothing gets lost," says Prof. Stefan Kollet, head of the Centre for High-Performance Scientific Computing in Terrestrial Systems (HPSC TerrSys). At the moment, TerrSysMP is applied over Europe and its watersheds with a resolution of twelve by twelve kilometres, but test runs have already been performed with three by three kilometres spatial resolution.

This does not only yield an enormous amount of data. Very diverse processes must also be covered both spatially and temporally. Some processes only take a few seconds, other days or even years. "So that the JUQUEEN supercomputer can perform the calculations as efficiently as possible, we have adapted TerrSysMP to make sure the various components all run at the same speed," says Dr. Klaus Görgen, head of Simulation Laboratory Terrestrial Systems, which is part of HPSC TerrSys. In the next step, the scientists must examine how well the simulations fit observations of the natural system. If good agreement is achieved, TerrSysMP could be used in future to analyse processes, such as the impact of groundwater on the water and energy balances. Predictions could also be used for flood and water resources management.



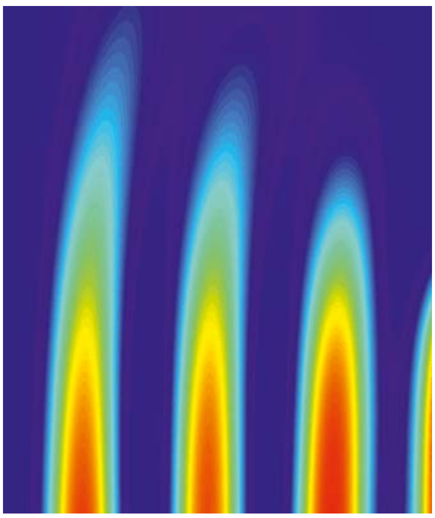
Fully coupled simulations of terrestrial water and energy cycles from aquifers across the Earth's surface into the atmosphere. The figure shows a snapshot of cloud water content (grey) and soil moisture (coloured) over Europe in June 2013.

New Approach for Terahertz Sources

Radiation in the terahertz range has a number of interesting properties: on the one hand, it penetrates textiles and plastics, while on the other hand, it is absorbed by many materials in a characteristic manner. This radiation is used, for example, in early cancer screening, for food controls, body scans, and ultrafast wireless connections. However, it is difficult to generate and until now this has only been possible to a limited extent. An international research group has now simulated a new concept for terahertz sources at Jülich's supercomputer JUQUEEN. The new method also permits tunable wavelengths.

In the electromagnetic spectrum, terahertz waves occupy an area between microwaves and infrared radiation. Since the beginning of this century, femtosecond lasers have been increasingly used to generate such waves in the range between 0.1 and 30 terahertz. In this process, a gas is bombarded by two ultrashort pulses of light. The faster laser frequencies are thus transformed into a more slowly oscillating terahertz wave.

Scientists from the Jülich Supercomputing Centre (JSC) have further developed this approach together with researchers from the University of Strathclyde in Scotland and the Institute of Physics in Beijing. "Using complex simulations, we have been able to show how the wavelengths and polarization of the terahertz radiation can be selectively influenced by a strong external magnetic field," says JSC researcher Prof. Paul Gibbon. "Imaging techniques, in particular, could benefit from the improved temporal and spatial resolution, for example, those used to investigate the dynamics of large biomolecules such as DNA," adds Dr. Wei-Min Wang, a Humboldt fellow who also works at JSC. After the successful simulation, researchers are now working on practical implementations.



Propagation of a terahertz wave: the wavelength and propagation direction can be selectively influenced by a strong magnetic field.

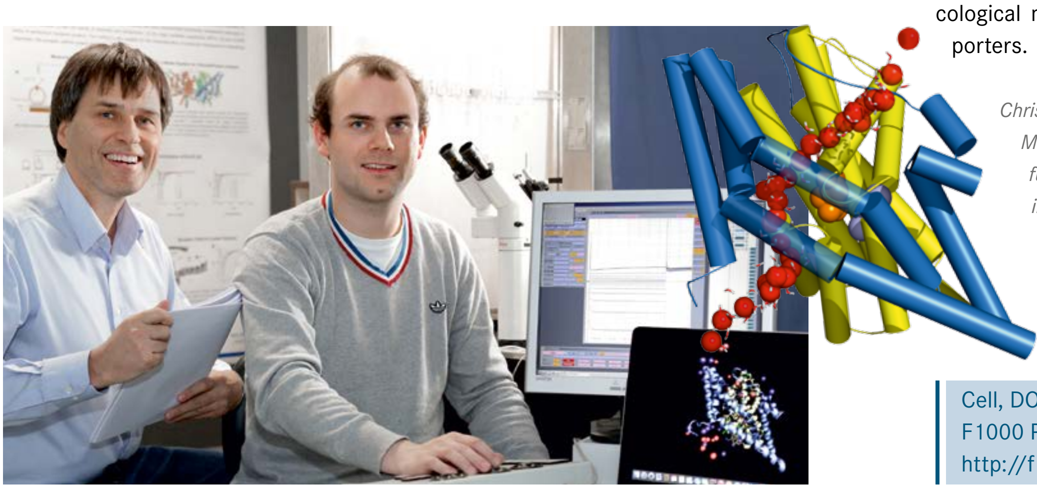
Physical Review Letters, DOI: 10.1103/PhysRevLett.114.253901

Dual Function of Glutamate Transporters Unravelled

A research group coordinated by Jülich has achieved a breakthrough in the understanding of glutamate transporters. These proteins remove the neurotransmitter glutamate from the synapses and therefore play a significant role in information transmission in the human central nervous system. With the aid of simulations on Jülich's supercomputer JUROPA, the scientists developed a model of the protein structure and were able to observe the transporters at work.

The team headed by Prof. Christoph Fahlke from Jülich's Institute of Complex Systems focused on one of the most important families of transporters: the excitatory amino acid transporters (EAATs). They do not only pump glutamate into the cell but they also mediate the selective flux of chloride ions through an ion channel – two physically completely different transport processes. "Such a dual function has been postulated for various proteins, but now for the first time we have been able to clarify how it actually works," explains Fahlke.

Attempts at unravelling the ion channel mechanism by way of experiments had always come unstuck. The breakthrough was brought about by compute-intensive molecular dynamics simulations on JUROPA. Together with colleagues from the Max Planck Institute for Biophysical Chemistry in Göttingen, the researchers developed an atomic model of an EAAT protein in a cell membrane. "This enables us to predict very accurately the structural changes in the protein leading to the ion channel opening," explains Dr. Jan-Philipp Machtens, one of the Jülich scientists. The results are in almost perfect agreement with the findings of laboratory experiments using electrophysiology and fluorescence spectroscopy performed by the researchers after the simulations. Their next step will be to exploit their new insights in order to make targeted pharmacological modifications of glutamate transporters.



Christoph Fahlke (left) and Jan-Philipp Machtens have unravelled a special function of glutamate transporters in the brain.

Cell, DOI: 10.1016/j.cell.2014.12.035
F1000 Prime Recommendation:
http://f1000.com/prime/725332607

Active Memory Cubes: Hans Meuer Award for JSC and IBM

A German-American research team has won the first Hans Meuer Award, introduced this year by the International Supercomputing Conference (ISC). The scientists from the Jülich Supercomputing Centre (JSC), the IBM Research and Development Lab in Böblingen, and the Watson Research Center in the USA will receive the award for their work on the use of active memory cube (AMC) technology for supercomputers. This work was performed in the framework of the Exascale Innovation Centre, a long-term collaboration between JSC and IBM on the development of exascale technologies. The award, which includes a cash prize of € 3000, will be presented at the ISC to be held in Frankfurt in July 2015.

The team used computational fluid dynamic simulations based on the lattice Boltzmann method and simulations of lattice quantum chromodynamics (LQCD) to examine the impact of active memory cubes on performance and energy efficiency. With the active memory cubes developed by IBM, the data are largely processed directly in the memory module. This means that they do not need to be passed backwards and forwards to the central processing unit (CPU), thus improving performance and saving energy. The novel hardware has not yet been constructed, but the results based on cycle-accurate simulations demonstrate the great potential of this pioneering technology.

Hans Meuer Award

The award is named after the founder of the ISC conference series, Hans Meuer, who died in 2014, and will in future be presented annually at the ISC. Meuer, who was also involved in introducing the TOP500 list of the fastest supercomputers in the world, worked at Jülich from 1962 to 1973 before he was appointed professor at the University of Mannheim.

NEWS IN BRIEF

New Chairman for GCS

Prof. Thomas Lippert, head of the Jülich Supercomputing Centre (JSC), is the new Chairman of the Board of Directors of the Gauss Centre for Supercomputing (GCS). At a regular GCS assembly meeting in mid-April 2015, Lippert was elected successor to Prof. Michael M. Resch, whose two-year term of office had come to an end. GCS combines the three German supercomputing centres – JSC, the Leibniz Supercomputing Centre in Garching, and the High Performance Computing Center Stuttgart – into one national institution.

Successful Acquisition of Funding

The Jülich Supercomputing Centre is involved in four projects that will be receiving funding from the EU's Horizon 2020 programme in the field of centres of excellence for computing applications. The Energy-oriented Centre of Excellence (EoCoE) will promote the transition to a low-carbon energy supply. Materials Design at the Exascale (MaX) intends to speed up the development of new materials. The E-Infrastructure for Software, Training and Consultancy in Simulation and Modelling (E-CAM) is concerned not only with new materials but also with biological processes. Finally, Performance Optimization and Productivity (POP) will help users from science and industry to apply supercomputers even more effectively. All four projects are due to start this autumn.

Fire Protection in Underground Stations

A fire in an underground station can easily turn into a hazard. A new project at the Jülich Supercomputing Centre aims to increase passenger safety and improve smoke exhaustion concepts. The ORPHEUS project was launched in February 2015 and will be funded for three years by the Federal Ministry of Education and Research. The partners will work on fire protection concepts for planned and existing stations with the aid of real fire experiments, small-scale models, and numerical smoke and fire simulations. They also intend to investigate the way in which the emergency services, station operators, and other facilities involved (shops, markets) work together.

www.orpheus-projekt.de

ORPHEUS

JURECA Ready to Replace JUROPA

A new supercomputer will come online at Jülich in September. JURECA (Jülich Research on Exascale Cluster Architectures) will replace the JUROPA system, which has been in operation since 2009. When fully operational, JURECA will consist of about 1850 nodes. This system, supplied by the Russian company T-Platforms, will achieve a peak performance of about 1.8 petaflop/s. This is almost eight times as fast as its predecessor JUROPA.

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UPCOMING EVENTS
at Jülich Supercomputing Centre

11–14 August 2015

Introduction to parallel programming with MPI and OpenMP for JSC guest students

Instructors: Dr. Florian Janetzko, Dr. Alexander Schnurpfeil, JSC

14–18 September 2015

Workshop "Computational Solar and Astrophysical Modeling"

14–16 October 2015

Workshop "Lattice Practices 2015"

19–20 October 2015

Introduction to GPU programming using OpenACC

Instructors: Anke Zitz, Thorsten Hater, Dr. Paul Baumeister, all JSC, Jiri Kraus, NVIDIA

9–11 November 2015

Data analysis and data mining with Python

Instructors: Dr. Jan Meinke, Dr. Olav Zimmermann, JSC

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

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

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 **Photos:** p. 1 top: Bergische Universität Wuppertal/Thavis, Forschungszentrum Jülich; p. 2 top: Forschungszentrum Jülich/Universität Bonn, Meteorologisches Institut; p. 1 right, p. 2 bottom, p. 3 top, p. 4: Forschungszentrum Jülich; p. 3 bottom: © vege/fotolia.com; **Contact:** Corporate Communications | Tel: +49 2461 61 - 4661 | Fax: +49 246 61 -4666 | Email: info@fz-juelich.de **Printed by:** Schloemer & Partner GmbH **Print run:** 300