EXASCALE

Newsletter of Forschungszentrum Jülich on Supercomputing

JÜLICH FORSCHUNGSZENTRUM

Issue: 3 | November 2013

Collecting data in experiments with pedestrians

BaSiGo in time lapse – to the video

Virtual Microscope Provides Breakthrough

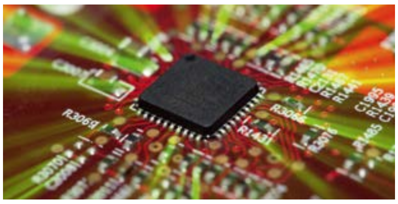
"As research questions become more and more complex, in many fields simulations on a supercomputer are the key to success."

Science delves deeper and deeper: into the building blocks of life, the evolution of the Universe or the progress of chemical and physical processes. As research questions become more and more complex, in many fields simulations on a supercomputer are the key to success. This year's Nobel Prize awards attest to this. The Nobel Prize for Chemistry went to three scientists who have made it possible to study complex molecular processes on a computer as if with a virtual microscope. Another example is the discovery of the Higgs boson, which was recognised with the award of the Nobel Prize for Physics. This too would have been inconceivable without calculations on supercomputers.

The scientific community is hoping for similar advances in research of the human brain. The successful simulation of a neural network with 10.4 trillion synapses on the K supercomputer in Japan (see page 2) serves as important groundwork for the Human Brain Project. The aim of this project, which was officially launched at the beginning of October, is to simulate the whole of the human brain on a computer. Jülich researchers have been heavily involved in both activities. But computer simulations are also needed to help solve more mundane challenges: in transport and safety, for example. The "BaSiGo" project, which stands for "Modules for Safety at Large Events", is a joint project in which researchers at the Jülich Supercomputing Centre (JSC) and their partners are developing a model to simulate pedestrian flows at large events. In the summer of 2013 they conducted a spectacular mass experiment involving 2,000 pedestrians at the Düsseldorf Trade Fair. The data collected will be used to find clues as to how congestion occurs in the first place, and at what point a bottleneck turns into a life-threatening crush. The experts at JSC already have the next priority topic in their sights: simulating fires.

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

IN THIS ISSUE



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

Currently the fourth fastest supercomputer in the world: the K computer at the RIKEN Institute in Kōbe, Japan

10.4 Trillion Synapses Simulated

Scientists from Japan and Jülich have simulated a neural network of hitherto unparalleled complexity on the Japanese K supercomputer. It comprises 1.7 trillion nerve cells, which are connected to each other by a staggering total of 10.4 contact points – also called synapses. The simulation reconstructs one second of the nerve cells' biological activity. As in the human brain, each cell is only active a few times during this time.

The nerve cells were connected to each other randomly, so it is not yet possible to deduce new neuroscientific information from this accomplishment alone: But the model sets new standards in precision for the mathematical description of biological processes. For this research, Jülich and its partners are developing the NEST (NEural Simulation Tool) software, which will be made freely available to any scientist anywhere in the world. The simultaneous multiuser access to the one-petabyte main memory of K that was required to solve a single task was only made possible by the new data structures developed by Jülich scientists together with Japanese colleagues from the RIKEN Research Institute and the Okinawa Institute for Technology. Of the four fastest computers in the world, K makes the largest storage capacity available to the individual computing nodes.

"This simulation is a direction-setting preliminary work, for the Human Brain Project for example", stresses Professor Markus Diesmann of the Jülich Institute for Neuroscience and Medicine. The Human Brain Project was started in early October with the significant involvement of Jülich researchers. Its objective is to use the JUQUEEN supercomputer and its successors to simulate complete brains. The researchers can expect a great deal more work: the human brain possesses an estimated 100 billion nerve cells.

www.fz-juelich.de/SharedDocs/Pressemitteilungen/UK/EN/2013/13-08-02LargestSimulation.html

Brain Research: Models Must Take Account of New Information

Until recently, it was commonly believed that only the transmission strength of synapses changes in the adult brain. Now, however, researchers know that new connections are being made and reorganised constantly in response to new experiences. The rules that governed this "structural plasticity" were previously unclear, but Dr. Markus Butz-Ostendorf, who began working at the Jülich Supercomputing Centre (JSC) in May 2013, and Dr. Arjen van Ooyen of the VU University Amsterdam have propounded a new theory. Their thesis: individual neurons control the formation and deletion of synapses by autoregulation of their level of electrical activity. If the level is too low, a neuron creates a new connection; if it is too high, connections are reduced – the blood sugar level regulates itself in much the same way. With the aid of an innovative simulation model developed by Dr. Butz-Ostendorf, it has been shown that the reorganisation of neural networks in the cortex of mice functions as suggested.

The activity level of neurons changes not only in learning situations, but also after the amputation of a limb or a stroke, or in the case of brain disease, for example. By processes that can sometimes take months, the brain adapts to this permanent change in incoming stimuli. The future of medicine will consist in selectively stimulating and controlling reorganisation processes in the brain. As models improve, therapies could be optimised with the aid of simulations. Today's models only consider fixed connections between neurons, and do no more than modify their strength. But structural changes and long-term growth processes must also be taken into account. The newly developed algorithms are particularly rewarding for network simulations with millions of neurons, because they enable the auto-organised growth of networks on supercomputers like JUQUEEN.

Biologist and information scientist Markus Butz-Ostendorf works at the High Performance Computing in Neuroscience Division and the Simulation Laboratory in Neuroscience at the JSC.

www.fz-juelich.de/SharedDocs/Pressemitteilungen/UK/EN/2013/13-10-11synapsenbildung-gehirn.html

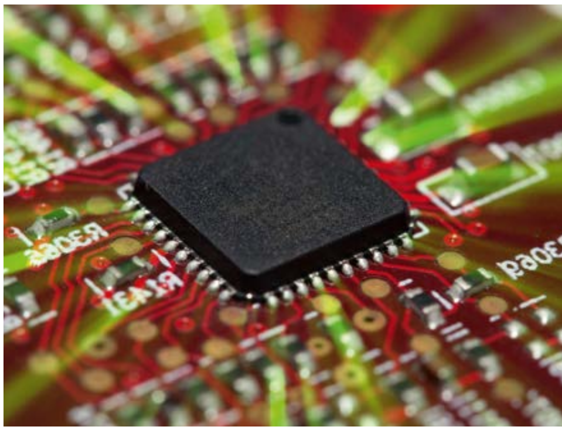
Faster and Safer with DEEP-ER

PProcessors are getting faster and faster. As they must, if Exascale computers are going to be built by 2020 as planned. “But applications will only benefit from the faster computing speed when programs are able to access and store data faster”, says Dr. Estela Suarez of the Jülich Supercomputing Centre (JSC). Dr. Suarez manages the new EU project “DEEP - Extended Reach” (DEEP-ER), which aims to solve this problem. Another objective of the project is protection from hardware failures. The enormous number of components that are included in the supercomputers of the future means that the risk of hardware failures is also greater. These can lead to the loss of interim results and data.

Starting in Jülich: At the kickoff meeting, the project partners defined next steps.

DEEP-ER, which began its work with a kickoff workshop at Jülich in early October, supplements and extends the EU project “Dynamical Exascale Entry Platform” (DEEP). In DEEP, European researchers are developing a new computer architecture for the coming Exascale class. DEEP-ER will improve the concept with new storage technologies, hardware and network components, with an efficient input/output system, for example. In order to test the benefits of the extensions, the partners are developing and building a computer prototype. Seven representative applications from medicine, geophysics, radioastronomy, quantum physics and the fields of superconductivity, oil prospecting and space weather will run on the prototype.

DEEP-ER is coordinated by Forschungszentrum Jülich, but 14 partners from seven EU countries are participating in the project. The EU will provide funding in the amount of € 6.4 million until 2016 from the Seventh Research Framework Programme.



DEEP-ER: taking aim at new storage technologies, hardware and network components

www.deep-er.eu

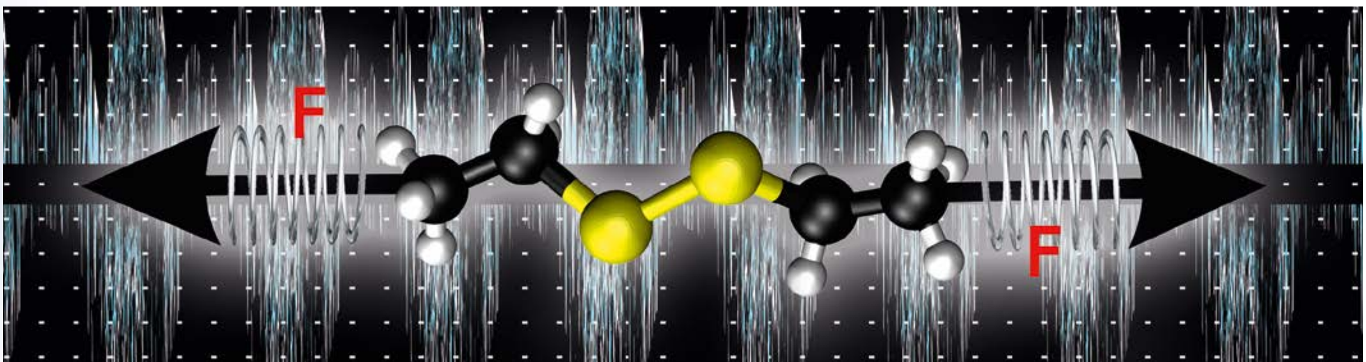
Less Is Sometimes More

The greater the force applied, the faster it goes. Until now, this has been the rule of thumb researchers in mechanochemistry have used for initiating and accelerating chemical reactions with mechanical forces. But as the theoretical chemists at the Ruhr-University Bochum discovered with the aid of the Jülich supercomputer JUQUEEN, this simple rule does not always hold true. Sophisticated simulations for a characteristic molecule have shown that it only applies up to a certain threshold value.

To investigate this, the researchers adjusted the process with the utmost precision, using the example of a small molecule having one central disulphide bridge – two sulphur atoms bonded to one another – dissolved in water. The more mechanical energy was applied to the ends of the molecule, in the form of tensile stress, the faster the chemical reaction was activated – but only up to a mechanical force of about 0.5 nanonewton. If the molecule was subjected to forces greater than this, it became so “twisted” that the molecule attacking the disulphide bridge – a hydroxide ion from the surrounding water – was no longer able to reach the reaction site easily. Consequently, the chemical reaction slowed down.

The researchers studied this mechanism on more complex models as well, including a large protein fragment. “It explains certain results from force spectroscopic measurements on titin, a protein that occurs in muscles, which were not yet understood and have been the subject of energetic debate”, says Professor Dominik Marx, the Project Leader and Director of the Centre for Theoretical Chemistry at the University of Bochum. This discovery was only possible because the researchers included the complex effects of the surrounding water in their simulations. Often, the role of such solvents is only considered superficially, in order to reduce the computing effort required.

www.fz-juelich.de/SharedDocs/Pressemitteilungen/UK/EN/2013/13-06-17-nature.html



The more, the faster: Mechanical forces accelerate chemical reactions – but only to a certain threshold value.

NEWS IN BRIEF

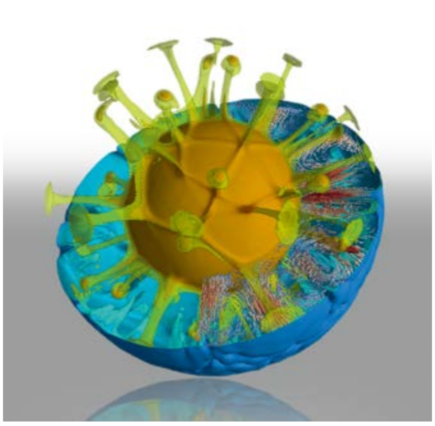
Stimulating Plasma Simulation

The Helmholtz Association has chosen the research project “Scalable kinetic plasma simulation methods” to form a “Helmholtz International Research Group”. The enterprise is a joint project led by Prof. Paul Gibbon of the Jülich Supercomputing Centre and Prof. Giovanni Lapenta from the Centre for Mathematical Plasma Astrophysics at the KU Leuven in Belgium. The researchers are investigating particle-based plasma simulation methods, which will be used for applications in fusion and solar research with the aid of supercomputers. The Helmholtz Association will provide funding of up to € 50,000 per year for three years. This contribution will be matched by the KU Leuven.

Exclusive Computing Community

The Jülich Supercomputing Centre has established the High-Q Club for software developers. Membership is open to anyone who succeeds in creating an application that utilises all 458,752 cores on the Jülich supercomputer JUQUEEN. Since the first “JUQUEEN Porting and Tuning Workshop” in February 2013, six users have been able to scale their codes over the entire 28-rack system. The club is designed to encourage software developers to optimise their code for JUQUEEN, and thus also to promote the idea of exascale computing.

www.fz-juelich.de/ias/jsc/high-q-club



Looking inside the Earth

The John von Neumann-Institute for Computing has awarded the title “John von Neumann Excellence Project 2013” to the research project “First-principles modelling of minerals, melts and fluids at high pressures and high temperatures”, directed by Dr. Sandro Jahn. With this, the researcher from the German Research Centre for Geosciences in Potsdam, Germany receives more computing time at the Jülich Supercomputing Centre. The primary focus of the project’s studies are minerals, silicate and metal melts, and aqueous fluids that are regarded as the basic building blocks of our planet. They play a critical part in the complex geological processes that take place below the Earth’s surface. Simulating these processes in quantum mechanical terms demands enormous computing power, and the Jülich supercomputers enable realistic modelling of the interactions at the atomic level. The findings derived therefrom are not only indispensable for interpreting experimental data, they are also used to make theoretical predictions of the distribution of chemical elements or of the transport of heat and materials in the Earth’s interior. Sandro Jahn also hopes to obtain new insights into the formation of the Earth’s core. webarchiv.fz-juelich.de/nic/Projekte/jahn.html

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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:** Kevin Ward **Photos:** Forschungszentrum Jülich; ©(Sagittaria, S. 2/Background; PanOptica, S. 1 u./S. 3 o.; sudok1, S. 3 u.; C2photo, S. 4 o.) fotolia.com; Riken, S. 1 o./S. 2 o. **Contact:** Corporate Communications | Tel: +49 2461 61-4661 | Fax: +49 2461 61-4666 | Email: info@fz-juelich.de **Printed by:** Schloemer und Partner GmbH **Print run:** 300

UPCOMING EVENTS

Introduction to parallel programming with MPI and OpenMP
25-27 November 2013
at Jülich Supercomputing Centre

This training course provides an introduction to parallel programming of high-performance computers in the technical-scientific environment. Message Passing Interface (MPI) is the most important programming tool for systems with distributed memory. OpenMP is used on shared-memory systems.

Instructor: Dr. Rolf Rabenseifner, HLRS Stuttgart

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

Programming and usage of Jülich supercomputer resources
28-29 November 2013
at Jülich Supercomputing Centre

This course offers users an introduction to the supercomputers at the Forschungszentrum Jülich. Among other things, they will learn how to make the best possible use of the granted computing resources.

Instructors: Representatives of IBM, Intel and ParTec; JSC staff members

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

2nd JUQUEEN Porting and Tuning Workshop
3-5 February 2014
at Jülich Supercomputing Centre

at the Jülich Supercomputing Centre

In this workshop, users of the JUQUEEN supercomputer will learn how to port their application, how to analyse its capability and improve its efficiency.

www.fz-juelich.de/ias/jsc/events/juqueenpt14

NIC Symposium 2014
12-13 February 2014
at Forschungszentrum Jülich

The 7th NIC Symposium presents the activities of the John von Neumann Institute for Computing (NIC) and the research results obtained from NIC projects in the last two years. Several presenters will report on their work in the various scientific fields.

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

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

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