EXASCALE
03-2016 | NEWSLETTER ON SUPERCOMPUTING AND BIG DATA

JÜLICH
FORSCHUNGSZENTRUM

Two new pilot systems for an interactive supercomputer are being tested at the Jülich Supercomputing Centre: JULIA, manufactured by Cray (left), and JURON from IBM and NVIDIA (right). Centre: the storage system accessed by both pilot systems.

The Future is Interactive

Pilot systems for future supercomputer for Human Brain Project launched

The Jülich Supercomputing Centre has begun operation of two new pilot systems for an interactive supercomputer. The systems – JULIA, created by Cray, and JURON from IBM and NVIDIA – are specifically designed for applications in the neurosciences. The installation and test phase are part of a special procurement for the European Human Brain Project (HBP).

Jülich scientists and their colleagues from the HBP will now test how powerful the two systems are and how well they fulfil the desired functions. For this purpose, they use applications developed or co-developed by Jülich researchers, such as three-dimensional models of the human brain like BigBrain, or software including NEST and Elephant.

Intervening in processes

So far, supercomputers work on tasks in a largely autonomous way. The aim in the future is for scientists to be able to intervene in the processes of applications and to control them interactively. This means that the computers must process considerably more data than even the enormous amounts that already arise for simulations of the human brain. The special challenge for the computers of the future is that the additional data must be rapidly analysed and visualized in parallel to the main application.

Latest technologies

In order to realize their concepts, the two competitors are making use of fast computing technologies, not all of which are commercially available yet. For instance, the compute nodes communicate via networks of the latest generation. The systems also make use of new, non-volatile memory technologies which will, in the future, permit the realization of much larger computer memory capacities. Both JURON (the name is derived from JUelich and NeuRON) and JULIA (derived from JUelich and GLIA, a type of cell in the nervous system) make use of state-of-the-art graphics processing units for the visualization. The tests are to be concluded by early 2017.

► Pilot systems JULIA and JURON

STATEMENT

Prof. Katrin Amunts
Head of ► INM-1

We want to develop new 3D models of the human brain which would further improve the spatial resolution by a factor of 20. To this end, we need interactive supercomputers to directly intervene in the processes and to visualize the interim results.

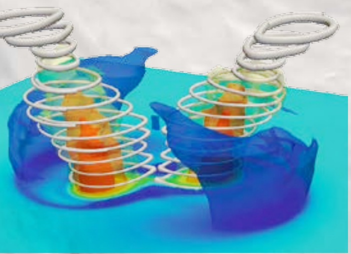
Predicting Cyclones:
Researchers Test Models

On average, around five tropical cyclones sweep over the Atlantic every year. Time and time again, they result in casualties and damaged property, as was recently the case when hurricane Matthew hit in October 2016. Computer models help predict cyclones and their routes. Heidelberg scientists are comparing models of varying complexity.

"By means of a systematic comparison, we want to find out what properties the various models have, with regard to accuracy and computation time," says Dr. Martin Baumann, who is involved in the project at the Engineering Mathematics and Computing Lab (EMCL) of Heidelberg University. "Of course, we expect the most complex model to be closest to nature. But such models require more computation time and more powerful supercomputers. The results from simpler models may be sufficient for answering many questions."

For this investigation, the researchers are using Jülich's JUQUEEN supercomputer to simulate an area of several thousand square kilometres with two cyclones by means of three models. The simplest model uses strongly idealized meteorological conditions, such as horizontally constant air density, which does not occur in reality. The most complex model would even be capable of taking into consideration the acoustic consequences of sounds that the wind produces. The third model is an intermediate stage of the two and takes only selected physical effects into consideration.

"Thanks to computation time on JUQUEEN, we can resolve even the most complex model very finely. We use its solution as a reference result," says the Heidelberg researcher. This is what the other models are measured by: is the course of the cyclones identical? Did they reshape themselves differently? Was the same wind speed simulated for the same locations? One preliminary result is that using the same computer cluster, the intermediary model produced its prediction around ten times faster than the complex model. The difference in the predicted positions of the cyclones amounted to a few kilometres, with the cyclones moving around 300 kilometres in ten hours. "In the end, users must decide which model is most suitable for their application. Our investigations result in concrete criteria which will help them do so," says Baumann.



Interaction of two idealized tropical cyclones

► Engineering Mathematics and Computing Lab (EMCL)

Mobile Technology as a Blueprint

A publication by 34 scientists from the EU project "Mont-Blanc" is among the finalists for the Best Paper Award of the world's largest supercomputing conference SC16 taking place in Salt Lake City in the US. In our interview, Dr. Dirk Brömmel from the Jülich Supercomputing Centre (JSC), one of the authors of the conference article, explains what it is about.

Dirk Brömmel

Dr. Brömmel, what did you investigate?
In our article, we describe the current prototype of the Mont-Blanc project. We compare our system architecture with other approaches – with regard to energy consumption and computing power.

What makes your prototype different from other architectures?
The prototype, which was jointly developed by partners from science and industry, makes use of mobile technology in form of many highly integrated processors to reduce the energy consumption as well as the cost of future supercomputers. Such energy-efficient processors are used in smartphones, but also in washing machines and cars.

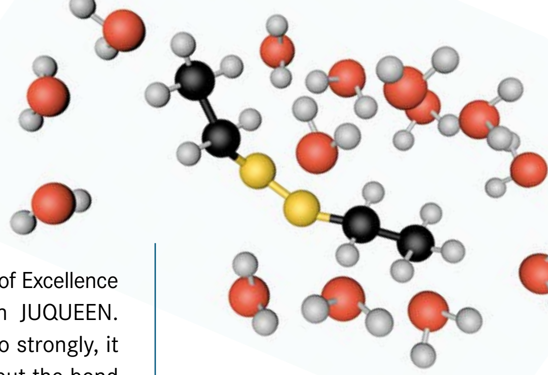
And how does the prototype perform?
In principle, our approach works well. As we hoped, our prototype's ratio of performance per energy unit was better than in the comparative system – how much better depended on the particular program code used. But we also realized that we still have to work on scalability.

What role does JSC play?
In the EU project, we support performance analysis, for example by developing the required tools. We also develop, optimize, and evaluate scientific applications. For the comparison in the article, for example, we ported applications from areas such as soft-matter physics or protein folding to the prototype and optimized them.

What does the nomination mean to you?
We are delighted to be recognized, of course. The consideration of an article for this prize alone is viewed as an accolade. And thanks to the nomination, we will have the opportunity to present our results in a special session at SC16.

Dr. Brömmel, thank you for talking to us!

► The conference article
► EU-Project Mont-Blanc



More Complex Than Expected

Disulfide bridges are essential: they serve to stabilize the structure of proteins or strengthen rubber, for example. Separating the bond between two sulfur atoms by means of mechanical forces in a basic solution, however, is more complex than previously thought. This has been revealed by researchers headed by Prof. Dominik Marx from Ruhr University Bochum using simulations on Jülich's supercomputer JUQUEEN.

It is sometimes important for bonds between two sulfur atoms to be separated – for example when disulfide bridges are supposed to switch biological processes or rubber is to be recycled. The Bochum researchers investigated what happens when both ends of a disulfide bridge in an alkaline aqueous solution are pulled in different directions. “Such mechanochemical processes occur indeed when small forces are exerted in cells, and they are used in a targeted manner when recycling rubber,” explains Dominik Marx.

The force decides

The scientists from the Bochum Cluster of Excellence Resolv simulated the entire process on JUQUEEN. The result: when the ends were pulled too strongly, it was not the disulfide bridge that ripped, but the bond between one of the sulfur atoms and a neighbouring carbon atom. However, it was not the usual chemical process of alkaline hydrolysis that drastically changed the reaction process, but the physical force. “This was previously unknown. Our results make clear that the correct interpretation of experimental data is much more complex than assumed so far,” says Marx.

The discovery was only possible because the researchers calculated all water molecules quantum mechanically just like all the other molecules and were thus able to correctly simulate the reaction in an aqueous solution. Theoreticians usually apply methods that drastically simplify the effects of the surrounding water, in order to reduce the computing power required.

▶ Exzellenzcluster Resolv

Disulfide bridges are formed by two covalently bound sulfur atoms (yellow spheres) which connect to macromolecular chains via carbon atoms (black), for instance in rubber. If sufficiently large forces are applied, it is not the disulfide bond itself that is broken, but its covalent bond to the macromolecule.

▶ Original publication:
Nature Chemistry (2016),
DOI: 10.1038/nchem.2632

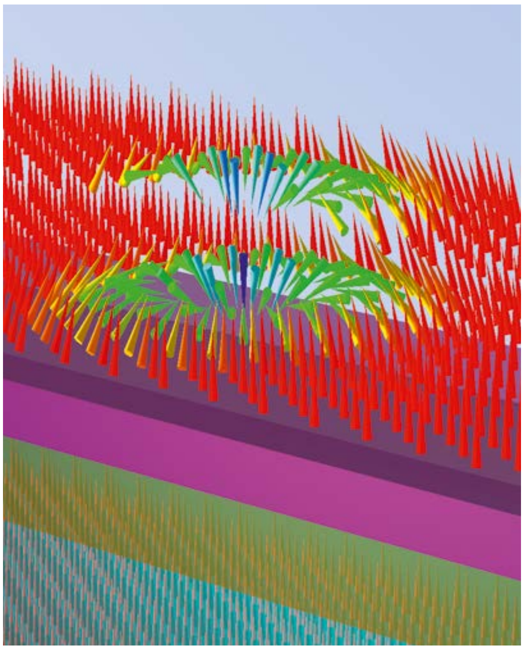
Targeted Layering

Magnetic vortices, called skyrmions, are viewed as promising candidates for storing and processing data using very little space and energy. However, until very recently, the only materials known to exhibit these vortices did so at extremely low temperatures. Using Jülich's supercomputers, scientists from Kiel and Jülich have now developed an approach that permits skyrmions to exist at room temperature.

Skyrmions were first observed in 2009 in exotic crystals at temperatures close to absolute zero, i. e. around -245 °C. The stable vortices are only a few nanometres in size and can efficiently be moved by electric currents. Since then, these unique magnetic structures have also been found at metallic interfaces which are used in today's magnetic sensors and hard drive read heads.

In order for skyrmions to be used as a storage medium, three conditions must be fulfilled: the interfaces should be producible on a large scale, they must have sufficient magnetic material, and the magnetic vortices must occur at room temperature. The approach pursued by the scientists from Kiel University and Forschungszentrum Jülich involves layering various metals on top of each other, with each layer only a few atoms thick. “We were able to show that in this way, skyrmions occur near room temperature and that the magnetic properties of the interfaces can be set in a targeted manner,” says Jülich physicist Dr. Gustav Bihlmayer.

The results obtained by means of quantum-mechanical calculations on various supercomputers now have to be verified in practice. Researchers from Kiel and Jülich together with colleagues from several countries are working on the EU project MAGicSky to develop magnetic data storage systems. From the scientists' point of view, however, there is still a long way to go until the first storage applications will become available.



▶ Original publication:
Nature Communications (2016),
DOI: 10.1038/ncomms11779

▶ Project „Magnetic Skyrmions for Future Nanospintronic Devices“ (MAGicSky)

Skyrmions in a metallic layer structure: at the centre of these tiny magnetic vortices, the “atomic bar magnets” of the iron atoms (blue arrows) align in the opposite direction to those in areas without vortices (red arrows).

NEWS IN BRIEF

Stable Injection

The John von Neumann Institute for Computing (NIC) awarded the title of 2016 NIC Excellence Project to Dr. Alberto Martinez de la Ossa's research project on plasma-based accelerators. One of the greatest challenges faced by such accelerators is the stable injection of electron packages in plasma waves. The scientist from the German electron synchrotron DESY investigates them using "particle-in-cell" (PIC) simulations. ▶ more

Improved Analyses

The transformation of the energy sector ("Energiewende") confronts Germany with new challenges. This applies not only to energy generation, distribution and storage: methods and computer models for the analysis of energy systems are also becoming more and more complex. As part of the BEAM-ME project, the Jülich Supercomputing Centre and five other partners are tackling this task by developing new algorithms and strategies to improve energy systems analysis using high-performance computing. ▶ more

Federal President Visits

In September, Federal President Joachim Gauck (right) visited Forschungszentrum Jülich. During his two-hour stay, he learnt about advances in brain research as well as supercomputing. Prof. Katrin Amunts from the Institute of Neuroscience and Medicine presented the Jülich brain model BigBrain, which is currently the most accurate model of the human brain. ▶ more (in German)

ParaPhase Project Launched

As part of the Federal Ministry of Education and Research's ParaPhase project, the Jülich Supercomputing Centre together with five partners is developing new methods and software for the efficient large-scale calculation of phase field problems. Phase field models play an important role in numerous physical and technical processes, for example in cracks and damage in solids or when growing crystals. ▶ more

Dance of the Droplets

High-pressure fuel injection systems ensure that the optimal amount of fuel reaches the diesel engine at the exact right moment. During the injection, complex flow processes occur, forming bizarre-looking droplets. Researchers from RWTH Aachen University simulate these flows on Jülich supercomputers to improve engine performance and reduce pollutant emissions. ▶ more

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- ▶ Facts and figures

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UPCOMING EVENTS

▶ Introduction to the Usage and Programming of Supercomputer Resources at Jülich
24–25 November 2016
at Jülich Supercomputing Centre
Instructors: Employees from Intel and ParTec; JSC employees

▶ Advanced parallel programming with MPI and OpenMP
28–30 November 2016
at Jülich Supercomputing Centre
Instructors: Dr. Rolf Rabenseifner, HLRS Stuttgart; Dr. Markus Geimer, JSC

▶ Introduction to Parallel Programming with MPI and OpenMP
31 January to 3 February 2017
at Jülich Supercomputing Centre
Instructor: Benedikt Steinbusch, JSC

▶ Parallel I/O and portable data formats
(course by PRACE Advanced Training Centres PATC)
13–15 March 2017
at Jülich Supercomputing Centre
Instructors: Sebastian Lührs, Dr. Michael Stephan, Benedikt Steinbusch, Dr. Kay Thust, JSC

▶ Vectorisation and portable programming using OpenCL
16–17 March 2017
at Jülich Supercomputing Centre
Instructors: Andreas Beckmann, Willi Homberg, Ilya Zhukov, JSC; Prof. Dr. Wolfram Schenck, University of Applied Sciences Bielefeld

▶ Overview of events at the Jülich Supercomputing Centre