EXASCALE

01-2016 | NEWSLETTER ON SUPERCOMPUTING AND BIG DATA

JÜLICH FORSCHUNGSZENTRUM

Using satellite images, researchers have observed how gravity waves propagate in the atmosphere. The infrared image (insert) shows the typical concentric pattern of such a wave, originating from the centre of a thunderstorm. (The thin, light-coloured lines are bolts of lightning and the large, bright areas are cities.)

A Sea of Waves in the Sky

Researchers track the complete path of gravity waves for the first time

Throwing rocks into the water and watching the ripples spread is something that most people have done during their childhood. Something similar also happens in the atmosphere: here the rocks are strong thunderstorms, tropical storms, or even volcanic eruptions. They cause the air particles of the Earth's atmosphere to oscillate. Just like in water, waves are the result: atmospheric gravity waves. In the atmosphere, they propagate sideways and upwards. They are particularly important for climate researchers because they influence winds and temperature, as well as the chemical composition of the Earth's middle and upper atmosphere. "Observing gravity waves helps to better understand and predict global circulation patterns in the atmosphere," says Dr. Lars Hoffmann, who heads the Simulation Laboratory (SimLab) Climate Science at the Jülich Supercomputing Centre.

Chance discovery in satellite data

An international team of researchers, including colleagues from Jülich, has now, for the first time, successfully measured how such waves propagate from their sources at the ground into the stratosphere (15–50 kilometres) and mesosphere (50–80 kilometres). The scientists discovered the waves on infrared images taken by Suomi-NPP, a new environmental satellite operated by the US space agency NASA. By combining their results with images taken by NASA satellite Aqua, they were able to precisely track the path of the waves through various altitudes. "Discovering this in the data was an unexpected lucky find – in fact, nocturnal cloud formations were the original focus of the Suomi-NPP measurements," explains Hoffmann, who, together with colleagues from SimLab, uses Jülich's supercomputers to analyse Aqua's data with respect to climate-relevant processes.

The researchers' aim now is to continuously observe the formation and propagation of the waves. With their new knowledge, they want to verify and improve existing climate models.

► PNAS, DOI: 10.1073/pnas.1508084112

STATEMENT

Prof. Stefan Blügel
Head of PGI-1/IAS-1

We develop quantum-theoretical methods for supercomputers in order to realize theoretical concepts in materials, such as the magnetic skyrmions. With suitable properties, these may be developed into a storage system for the information technology of the future.

> see page 3

New Insights into the Formation of Heavy Elements

Scattering of helium nuclei inside stars precisely simulated for the first time

► Nature,
DOI: 10.1038/nature16067

Stars like our Sun are gigantic, extremely hot furnaces. Inside them, atomic nuclei bond to form new elements. Thus, helium nuclei, for example, fuse to form the heavier elements carbon and oxygen. Both are important building blocks for the development of life on Earth. An international team of researchers has now developed a new method to simulate these formation processes in detail on supercomputers. The method considerably decreases the cost of computation. Using the Jülich supercomputer JUQUEEN, the researchers were for the first time able to calculate from scratch the scattering of two helium nuclei, called alpha particles.

New method shortens computation time

Simulating such processes is extremely compute-intensive, even for today's supercomputers. This is partly due to the fact that all the protons and neutrons of an atomic nucleus interact with each other. Previous simulations were therefore limited to reactions in which no more than five particles were involved. Using a trick, the German and American scientists reduced the cost of computation: they placed the protons and neutrons involved onto a virtual lattice instead of freely into space. "The state of such a lattice can be calculated very efficiently in parallel using a large number of processors," says Jülich nuclear physicist Prof. Dr. Ulf-G. Meißner, who was involved in developing the method. How well it works is shown by the researchers with the example of two helium nuclei, with a total of eight particles. "Previously, a supercomputer such as JUQUEEN would have required thousands of years for this – now it is possible in a matter of weeks," says the Jülich scientist. He and his colleagues hope for new insights into the formation of oxygen. In contrast to carbon, there are still some fundamental questions on its formation inside stars which are not yet fully understood.

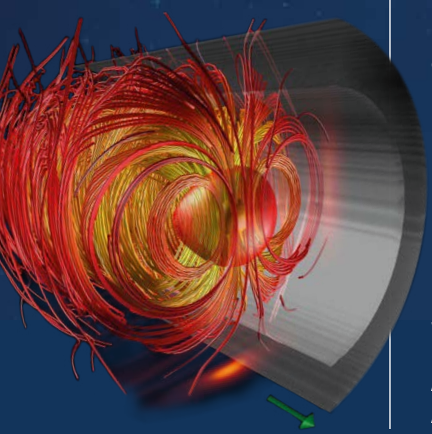
Simulated using JUQUEEN: scattering of two helium nuclei, called alpha particles

Particle Acceleration in Space

► Astrophysical Journal Letters,
DOI: 10.1088/2041-8205/803/2/L29

Outer space is full of phenomena of which we only have a rudimentary understanding so far. Among them are magnetic fields and shock waves. By means of simulations on supercomputers, Bochum plasma physicist Dr. Anne Stockem Novo wants to find out how magnetic fields are generated in outer space and how shock waves and magnetic fields influence each other. This work is a joint project conducted by physicists from Ruhr University Bochum and Instituto Superior Técnico in Lisbon, Portugal.

Shock waves are a type of moving front of electrically charged particles. They are formed when particles are deflected by interactions with electromagnetic fields. Some of these particles are then accelerated in the shock wave. How exactly this works is what astrophysicists all over the world are trying to find out. Using Jülich's supercomputer JUQUEEN, the German-Portuguese partners simulated particle streams, which themselves generate magnetic fields, and then observed the interactions. For this purpose, JUQUEEN had to calculate each individual particle and the change it undergoes by means of basic physical equations. The magnetic fields generate turbulences and scatter the particles in all possible directions, increasing the density of the particles. "These are the exact prerequisites for shock waves to form," says Anne Stockem Novo. The researchers compared their results with laboratory experiments, showing that they match well. "We are on the right track," says the Bochum physicist. Further simulations are hoped to achieve more detailed insights.



Simulation of a particle beam (red sphere in the centre) through a hollow plasma channel: the numerous circular lines represent the self-generated magnetic field which influences the path of the particle trajectories.

The Secrets of Magnetic Nanostructures

To physicists, the magnetic properties of tiny nanostructures are an exciting yet complex challenge. On the one hand, it is about understanding basic physical effects. On the other hand, new approaches may result in minute, energy-efficient, and fast data storage systems. Simulations on Jülich supercomputers are helping to reveal their properties and processes.

Millions of Funding

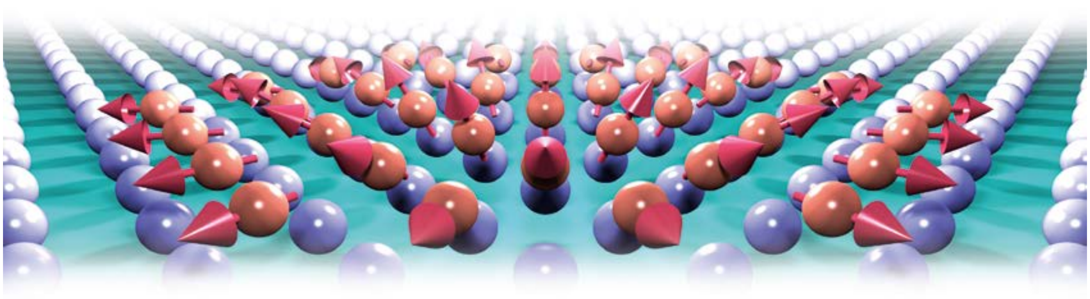
Physicist Samir Lounis attracts Consolidator Grant

In order to further expand his innovative research on tiny magnetic structures, junior professor Samir Lounis has attracted special funding: the European Research Council (ERC) has awarded him a Consolidator Grant. It is endowed with around € 2 million. This money will flow into his DYNASORE project (Dynamical magnetic excitations with spin-orbit interaction in realistic nano-structures), which is planned to take five years.

Within its scope, the physicist affiliated with Forschungszentrum Jülich and RWTH Aachen University will be concerned with magnetic structures such as the vortex-shaped skyrmions. These structures were only discovered a few years ago. With their help, data may in the future be processed and stored using very little energy in the tiniest of spaces. However, the dynamic processes that occur when skyrmions are produced and erased are still not fully understood. "We want to unravel the physical influences playing a role in this," explains Lounis. For this purpose, he and his team at the Peter Grünberg Institute will further develop a Jülich calculation method, called the KKR method (Korringa-Kohn-Rostoker Green function method). With this method, it should then be possible to describe the production and erasure of skyrmions in structures with up to several thousand atoms. The simulation method is based solely on the underlying laws of physics and does not require any additional parameters to be experimentally determined. Such *ab initio* calculation methods consume enormous computing resources and are therefore only possible using supercomputers. Samir Lounis will benefit from the close cooperation with the Exascale Innovation Centre, a joint venture by IBM and Forschungszentrum Jülich. There, the relevant program, KKRnano, will be optimized for application on the Jülich supercomputers.

Samir Lounis has attracted an ERC Grant.

► New Magnetic Effect Detects Magnetic Nano-Vortices



Complex magnetic structure (red arrows) of a nanocluster consisting of several thousand atoms.

Filter Speeds up Calculations

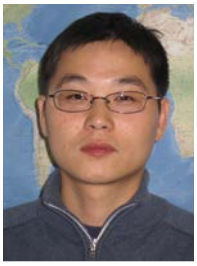
Physicist Prof. Alexander I. Lichtenstein from Universität Hamburg uses Jülich's supercomputer JUQUEEN to study the magnetic properties of crystalline solids. Such solids are usually composed of a multitude of microscopically small crystals whose atoms are arranged in a regular lattice. The John von Neumann Institute for Computing (NIC) awarded the title of 2015 NIC Excellence Project to the Hamburg researcher's project entitled "Continuous Time Quantum Monte Carlo for Materials".

Complex solid state system

Lichtenstein is particularly interested in compounds consisting of cobalt and oxygen, calcium-titanium oxide (perovskites), and iron – for example iron-based high-temperature superconductors. One of the things he wants to find out is under what external conditions a material is magnetic and how it behaves under the influence of a varying electromagnetic field. However, the solid state systems he studies are very complex. This makes a theoretical description very difficult. Even with today's supercomputers, an exact calculation of their thermodynamic properties would take millions of years. Quantum Monte Carlo simulations shorten the computation time significantly by filtering the most important areas using a statistical method. The Hamburg solid-state physicist and his team helped develop new quantum Monte Carlo methods, which are now being run on JUQUEEN.

NEWS IN BRIEF

Young and Distinguished



The International Union of Pure and Applied Physics (IUPAP) has awarded Dr. Wei-Min Wang the 2015 Young Scientist Prize in Computational Physics. Thirty-five-year-old Wang, who spent the past two years at the Jülich Supercomputing Centre (JSC) thanks to an Alexander von Humboldt fellowship, received the award in early December 2015 at the IUPAP conference for computational physics held in Guwahati, India. Wang's speciality field is simulations and modelling in plasma physics. Together with JSC researcher Prof. Paul Gibbon as well as scientists from China and Scotland, he developed a new concept for a terahertz source in 2015 (see Exascale newsletter 2/2015). He was awarded the accolade for the publication of these results. With the aid of elaborate simulations at the Jülich supercomputer JUQUEEN, the researchers had shown how wavelength and polarization of the terahertz radiation can be influenced in a targeted way by a strong external magnetic field. Generating terahertz radiation is regarded as very difficult. After his fellowship had come to an end, Wang returned to the institute of physics at the Chinese Academy of Sciences in Beijing.

▶ more

NIC Symposium 2016

Around 200 scientists took part in the 8th Symposium of the John von Neumann Institute for Computing in mid-February. At the event, researchers who had used the Jülich supercomputers in the past two years presented information on the progress and results of their projects.

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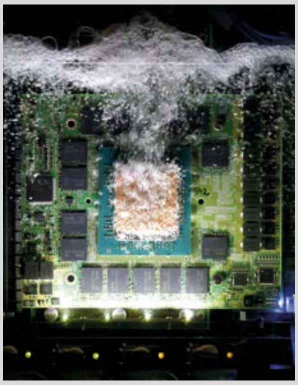
Blog on SC17

In 2017, Dr.-Ing. Bernd Mohr from the Jülich Supercomputing Centre will be the first non-American to lead the world's most important conference on high-performance computing, the US Supercomputing Conference (SC). In his blog, he offers insights into the organization and preparation of the conference.

▶ more

DEEP at CeBIT

The EU research project DEEP (Dynamical Exascale Entry Platform) will be presented at this year's CeBIT from 14 to 18 March 2016 in Hannover (hall 6, stand C30). The GreenICE Booster (pictured) of the DEEP computer will be on display. The DEEP system is based on the Cluster-Booster concept, which involves accelerating a cluster of conventional processors using a booster – a kind of turbocharger – formed by massively parallel, interconnected multicore processors. The prototype is operated at the Jülich Supercomputing Centre (see Exascale newsletter 3/2015). The GreenICE Booster, a special development within the DEEP project, possesses a very efficient cooling system. The electronic assemblies are immersed in a special liquid which evaporates even at moderate temperatures.



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UPCOMING EVENTS

▶ Introduction to Parallel In-Situ Visualization with VisIt
18 April 2016
at Jülich Supercomputing Centre
Instructors: Jens Henrik Göbbert, Dr. Herwig Zilken, JSC

▶ Introduction to ParaView for the visualization of scientific data
20 April 2016
at Jülich Supercomputing Centre
Instructor: Sonja Habbinga, JSC

▶ GPU Programming with CUDA (Training course of PRACE Advanced Training Centres PATC)
25–27 April 2016
at Jülich Supercomputing Centre
Instructors: Dr. Jan Meinke, Jochen Kreutz, JSC; Jiri Kraus, NVIDIA

▶ Node-Level Performance Engineering
28–29 April 2016
at Jülich Supercomputing Centre
Instructors: Dr. Georg Hager, Prof. Gerhard Wellein, RRZE/HPC, University Erlangen

▶ PRACEdays16
10–12 May 2016
at Prague, Czech Republic

▶ Programming and Usage of the Supercomputer Resources at Jülich
23–24 May 2016
at Jülich Supercomputing Centre
Instructors: JSC employees and representatives of IBM, Intel, and ParTec

▶ High-performance computing with Python (Training course of PRACE Advanced Training Centres PATC)
13–14 June 2016
at Jülich Supercomputing Centre
Instructors: Dr. Jan Meinke, Dr. Olav Zimmermann, JSC

▶ Here you can find an overview of events at the Jülich Supercomputing Centre