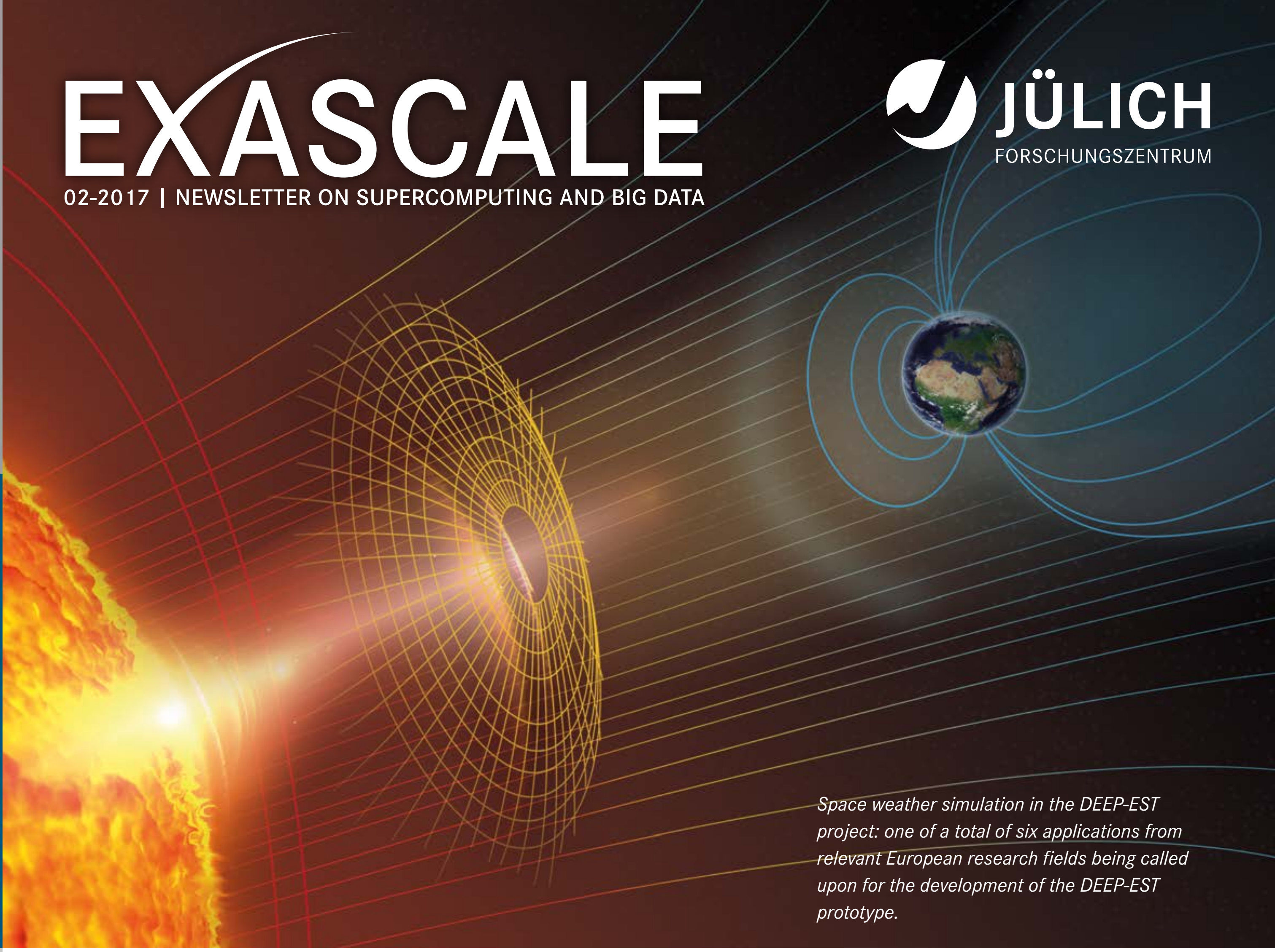
EXASCALE

02-2017 | NEWSLETTER ON SUPERCOMPUTING AND BIG DATA

JÜLICH FORSCHUNGSZENTRUM



Space weather simulation in the DEEP-EST project: one of a total of six applications from relevant European research fields being called upon for the development of the DEEP-EST prototype.

Simplifying Big Data Analyses

Prototype planned for next-generation modular supercomputer

For smartphones and laptops, features such as cameras, network interfaces, and GPS have long been considered just as important as computing power. A similar trend can be seen in the field of high-performance computing (HPC). Big data analyses and sophisticated visualizations – which are gaining importance in addition to compute-intensive simulations – can only be performed inefficiently with current supercomputer architectures. In the DEEP-EST project, experts are therefore pursuing the development of a modular architecture which is tailored to a broad spectrum of requirements.

The aim is to build a supercomputer with various modules for different tasks. “It’s similar to building a house,” explains project leader Dr. Estela Suarez from the Jülich Supercomputing Centre (JSC). “Instead of solely employing highly trained workers - which are very expensive - you entrust the experts only with the complicated, critical work such as electrical installation. The simpler tasks can then be performed by less costly, younger workers.”

Following the EU projects DEEP and DEEP-ER, DEEP-EST now sees the project partners entering the third stage. A new data analytics module will be added to expand the Cluster–Booster architecture of the previous projects. By 2020, a prototype is to be developed in co-design that will demonstrate the advantages of the concept. For example, together with KU Leuven, the researchers aim to simulate the effect of powerful solar storms. Such rare events threaten to cause enormous damage, such as a failure of satellite communications or disrupted GPS, internet, and telephone connections.

Tests will reveal to what extent highly complex space weather simulations profit from the modular computer architecture. The analysis of satellite images of the solar activity will be transferred to the data analysis module, which has a high storage capacity and flexibly programmable FGPAs. The spread of the particle stream, in contrast, will be calculated on the cluster using high-performance general purpose processors. The simulation of the interaction with the Earth’s magnetic field will be split between the Cluster and the extremely energy-efficient Booster, which is based on interconnected, massively parallel multicore processors.

► DEEP-Project ► DEEPER-Project

STATEMENT

Prof. Dr. Dr. Thomas Lippert
Head of the Jülich ► Supercomputing Centre (JSC)

The optimization of homogeneous systems has more or less reached its limit. We are gradually developing the prerequisites for a highly efficient modular supercomputing architecture which can be flexibly adapted to the various requirements of scientific applications.

Unexpected Diversity of Shape of Red Blood Cells

Our blood vessels are often a bit like an overcrowded water slide at a swimming pool, with the red blood cells slap-bang in the middle. Almost half of our blood consists of such cells. They look similar to rubber rings with a soft sitting area in the middle instead of a hole. Thanks to their elasticity, they worm through the smallest blood vessels and rush through the heart unscathed. The faster they flow and the more it gets cramped, the more the red blood cells deform: from slightly bent to rolled-up ellipses or pyramids.

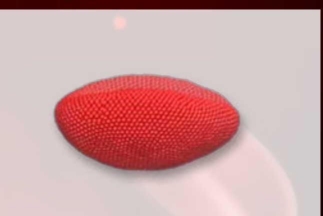
Scientists at Forschungszentrum Jülich and the University of Montpellier have for the first time detected a number of these forms. This diversity of shapes had for a long time remained undiscovered by microscopes, as much too viscous substances were selected for the liquid part of the blood. “Only when the biologists recreated the natural conditions in the experiments were they able to see the diversity of shapes calculated by us,” explains Dr. Dmitry A. Fedosov, who works at the Jülich Institute of Complex Systems (ICS-2).

In addition, the scientists found indications that the flexible deformability of the red blood cells has a decisive influence on the viscosity of the blood. This potentially plays a key role in the development of circulatory problems. “Our studies suggest that physiological phenomena – in which a drop-like movement of red blood cells had previously been assumed – need to be reinvestigated,” reports ICS director Prof. Gerhard Gompper. Diabetes, for example, causes the blood cells to stiffen. They become less elastic and no longer fit through the tightest blood vessels, the capillaries. This particularly concerns the hands and feet.

In an additional step, the Jülich researchers calculated how thousands of cells behave collectively. For example, the red blood cells change their motion from a kind of free rolling into one that sees them orderly gliding and lining up. This knowledge is tremendously important, for instance in the design of stents. These are wire-mesh tubes which keep blood vessels open after a heart attack. It also plays a role in the development of blood pumps which are implanted in the body.

► PNAS (2016), DOI: 10.1073/nas.1608074113

low shearing rate or speed



moderate shearing rate or speed

high shearing rate or speed

New Findings Relating to Copper and Alzheimer’s

Junior professor Birgit Strodel has performed simulations on the high-performance computers of the Jülich Supercomputing Centre (JSC) to investigate how copper ions affect the clumping together of the body’s own amyloid beta (Aβ) protein. The entangling of Aβ peptides is directly linked to the emergence of Alzheimer’s disease.

Jun.-Prof. Birgit Strodel, head of the computational biochemistry group at Forschungszentrum Jülich (ICS-6)

Prof. Strodel, what was this study all about?

Our investigation was based on the fact that ions influence the aggregation of Aβ peptides. The role of copper ions, however, is still disputed. Experiments reveal how copper ions in some cases accelerate the formation of small aggregates, known as oligomers, and above all make them more toxic – in other words more harmful.

To what extent are these processes relevant to the emergence of Alzheimer’s disease?

In the past, fibrils were linked to the development of Alzheimer’s. These are end products of the aggregation that can be found in the brains of patients. They are relatively long – up to the nanometre range. Oligomers, in contrast, are formed during the aggregation process from individual peptides to fibrils. They are much smaller and not particularly stable. For this reason, it has not yet been possible to clarify their structure, meaning knowledge about the amyloid oligomers is still rather sketchy. What is certain, however, is that these small oligomers are toxic.

What new findings can simulations provide in this respect?

Simulations offer the advantage of allowing us to observe the peptide with atomic resolution, whereas in experiments it can often only be seen indirectly. At first glance, our results appear to be relatively random. However, statistical evaluation of the data reveals that the formation of a special folding structure of proteins – known as pleated sheets – plays an important role. In comparison to the conditions without copper, these beta pleated sheets are more likely to occur. This could mean that copper promotes the aggregation, or clumping together, of Aβ peptides. The pleated sheets are ultimately connected to both the aggregation of the oligomers and their potential for harm.

Prof. Strodel, thank you for talking to us.

► Isr. J. Chem. (2017), DOI: 10.1002/ijch.201600108

Quasicrystals from Fullerenes

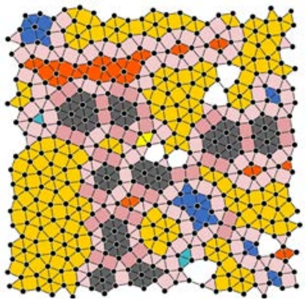
For around 35 years now researchers have been fascinated by a new kind of material class, quasicrystals, the discovery of which was honoured with the Nobel Prize in 2011. Quasicrystals were for a long time only ever found in ternary alloys, that is to say metals comprising three different types of atoms. They were subsequently also found in other systems, such as liquid crystals and perovskite films. Scientists from Forschungszentrum Jülich have now discovered another class of quasicrystals and explained using computer simulations how the special arrangement of the molecules materializes.

Quasicrystals exhibit a series of particular physical properties due to their special structure. They are today used as coatings in frying pans or as catalysts. The newly discovered class is of particular interest for optical applications, for example in the production of photonic crystals. It also creates new opportunities in the study of magnetic systems.

Conventional crystals have a periodic structure whose elementary cells are repeated at regular intervals in a chessboard-like pattern. The possibilities for such structures are limited, however. In two dimensions, for example, only twofold, threefold, fourfold, and sixfold symmetries can be joined together without gaps. Quasicrystals, in contrast, also enable other symmetries – for example fivefold symmetries or the newly discovered two-dimensional structure with twelvefold symmetry whose triangular and quadrangular basic elements consisting of fullerenes are distributed sporadically across the substrate.

Researchers at Jülich's Peter Grünberg Institute (PGI-1, PGI-5, PGI-7) deposited the fullerenes, which are also known as "football molecules", on a platinum–titanium alloy. By performing compute-intensive ab initio simulations on the Jülich supercomputer JUQUEEN, they successfully attributed the arrangement of the fullerenes to the specific interaction with the underlying alloy. Detailed findings might in future make it possible to produce customized quasicrystals with certain qualities.

► Original publication:
Nature Communications (2017),
DOI: 10.1038/NCOMMS15367



Two-dimensional quasicrystal structure consisting of fullerenes with twelvefold symmetry

Heat Transport on the Nanoscale

Metals, which are good current conductors, usually also transfer heat well. In both cases, the energy is mainly transported by means of the same particles: freely moving electrons. Using supercomputers, scientists have now successfully verified that the connection between the two properties persists even if only the interactions between individual atoms are considered. The insights are decisive for developments such as micro- and nanoelectronic circuits, particularly for cooling computer chips of decreasing size.

As early as the 1980s, scientists had measured the – quantized – transport of electric charges between individual atoms. Using novel methods of scanning tunnelling microscopy, researchers from the US University of Michigan have now succeeded in observing heat transport on the atomic scale – which is much harder to detect. To do so, they used one of the thinnest wires imaginable: a chain of individual gold atoms.

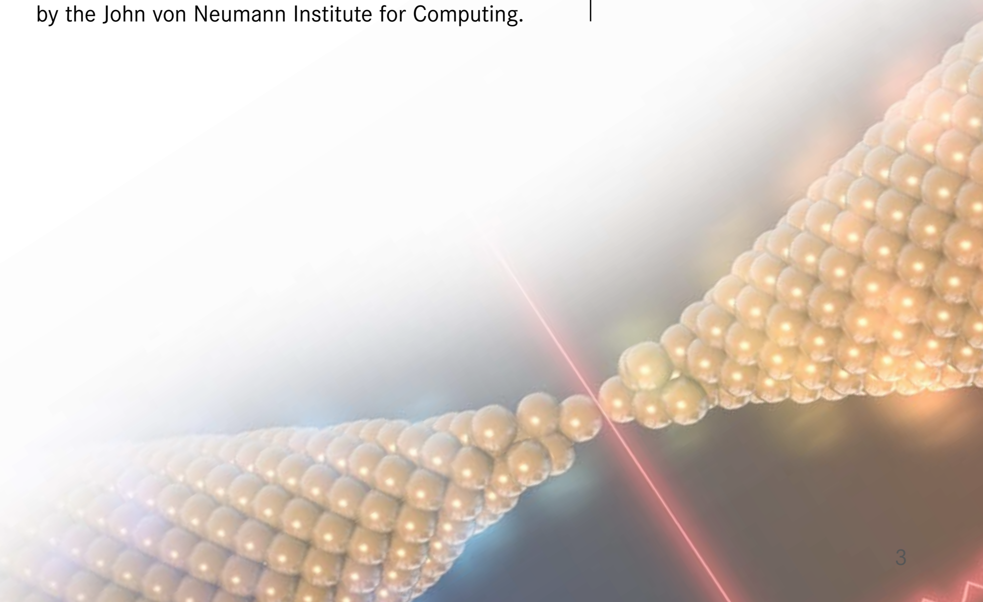
A team headed by Prof. Peter Nielaba from the University of Konstanz used the Jülich supercomputer JURECA to show that the Wiedemann–Franz law retains its validity even on the atomic scale. The law describes the relation between electric and thermal conductivity in classical physics. For atomic dimensions, however, a quantum-mechanical description is required. In addition to the atomic positions, the researchers calculated the charge and heat transport, ascertaining a proportionality between electric and thermal conductivity in atomic gold and platinum wires.

The result permits further research into other nanosystems and fundamental quantum phenomena, for example within the scope of thermoelectricity. The work will be continued as part of a project recently announced as the 2017 NIC Excellence Project by the John von Neumann Institute for Computing.

► Science (2017), DOI:
10.1126/science.aam6622

► Science Perspective (2017),
DOI: 10.1126/science.
aam9362

Computer simulations show that the laws of classical physics also apply to heat transport in atomic dimensions



NEWS IN BRIEF

People to Watch

The journal HPCwire has included Dr. Bernd Mohr from the Jülich Supercomputing Centre (JSC) in its list of "People to Watch 2017". Every year, the journal presents about a dozen experts from whom new impulses are expected for the field of high-performance computing. Bernd Mohr is one of the few individuals to have featured on the list twice – in 2015 and 2017. He will this year be the first non-American to coordinate the most important HPC conference, the SC17 taking place in the US. ► more

10 Years of GCS

The Gauss Centre for Supercomputing (GCS) is celebrating its 10th anniversary. Germany's three major computing centres in Stuttgart (HLRS), Jülich (JSC), and Munich (LRZ) have pooled their activities in this alliance since 2007 to create a joint supercomputing infrastructure that sets international standards. In future, there are plans in place to expand the current computing capacity (20 Petaflop/s) as well as to provide extended user support with courses and more intensive supervision of software development. ► mehr

Booster for JURECA

Intel and Forschungszentrum Jülich together with ParTec and Dell have agreed on a cooperation to develop and deploy a modular supercomputing system. Three of the partners have previously co-operated closely in the EU projects DEEP and DEEP-ER. Building on the work of these projects, agreement has been reached on the expansion of the Jülich supercomputer JURECA to include a highly scalable booster with a peak performance of 5 Petaflop/s. ► mehr

Successor Wanted

Almost six years after its installation, the Jülich supercomputer JUQUEEN will be going into well-deserved retirement at the start of 2018. JUQUEEN will then be replaced by a modular supercomputer which when finished will consist of several closely coupled modules. The procurement process for the first module was launched in May. The module will be based on an integrated architecture with multicore processors and is scheduled to be connected to JUQUEEN's operation as seamlessly as possible. ► more

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- ► Facts and figures

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, Brigitte Stahl-Busse **Graphics and Layout:** Graphical Media, Forschungszentrum Jülich **Translation:** Language Services, Forschungszentrum Jülich **Photos:** p. 1: cglightNing/fotolia.com, Kerbusch/fotolia.com; p. 2 left: eranicle/fotolia.com; p. 2 right: Forschungszentrum Jülich/Ralf-Uwe Limbach, p. 3 top: DOI: 10.1038/NCOMMS15367 (CC BY 4.0)/Forschungszentrum Jülich; p. 3 bottom: Enrique Sahagun; p. 4 top: SC16 Conference, Jo Ramsey; p. 4 bottom: Forschungszentrum Jülich/Ralf-Uwe Limbach **Contact:** Corporate Communications Tel.: +49 2461 61-4661 | Fax: +49 2461 61-4666 | Email: info@fz-juelich.de **Printed by:** Schloemer & Partner GmbH **Print run:** 200

UPCOMING EVENTS

► **Training course: Introduction to ParaView for the visualization of scientific data (in German)**
28 June 2017
at the Jülich Supercomputing Centre
Instructor: Sonja Habbinga, JSC

► **Training course: "Introduction to parallel programming with MPI and OpenMP"**
15 – 18 August 2017
at the Jülich Supercomputing Centre
Instructor: Benedikt Steinbusch, JSC

► **International HPSC TerrSys Fall School 2017**
25 – 29 September 2017
at the University of Bonn
Organization: Stefan Kollet, Wendy Sharples, Centre for High-Performance Scientific Computing in Terrestrial Systems (HPSC TerrSys)

► **Training course: "Porting code from Matlab to Python"**
9 – 10 October 2017
at the Jülich Supercomputing Centre
Instructors: Sandra Diaz, Lekshmi Deepu, Dr. Alexander Peyser, Wouter Klijn, JSC

► **Training course: "Introduction to GPU programming using OpenACC"**
16 – 17 October 2017
at the Jülich Supercomputing Centre
Instructors: Anke Kreuzer, Dr. Andreas Herten, Dr. Paul Baumeister, JSC Jiri Kraus, NVIDIA

► **Training course: "Software Development in Science"**
20 November 2017
at the Jülich Supercomputing Centre
Instructors: JSC employees from the Simulation Laboratory Neuroscience

► **Overview of events at the Jülich Supercomputing Centre:**