



Experiments conducted in a Berlin underground station as part of the ORPHEUS project provide data for computer simulations with which the spread of smoke can be predicted.

Safely Through the Underworld

How supercomputers optimize fire safety in underground stations

Fires in underground stations can have disastrous consequences. Toxic smoke spreads through the stations, blocking the escape routes for emergency services and passengers. As part of the ORPHEUS project, experts from the Jülich Supercomputing Centre (JSC) have teamed up with partners from research and industry using supercomputers to improve safety in the event of fire.

The aim is to use simulations to predict how smoke spreads in a subterranean complex in order to identify safe escape routes, for example. The results of the project, which is being funded by the Federal Ministry of Education and Research, will also contribute to new fire protection concepts.

Reducing the cost of computation

Only supercomputers are capable of adequately managing smoke simulations for areas of this size. Jülich scientists are developing an adaptable computational-mesh model which will reduce the enormous cost of computation: crucial areas near the source of the fire or close to exits are simulated at high resolution while areas further away are represented more

roughly. By coupling simulation programs such as the Fire Dynamic Simulator (FDS) and programs simulating pedestrian dynamics (JuPedSim), the researchers can also calculate how smoke affects mobility, and how it influences the evacuation time.

Furthermore, real-time simulations of how smoke spreads are planned. In future, these may support emergency services in their operations. Experts from JSC are optimizing the codes in order to accelerate their application by means of graphics processors.

Obtaining new data

Experiments in the Berlin underground station Osloer Straße are providing the data basis for adapting the algorithms. Using trace gases and propane torches, the project partners together with the transport company Berliner Verkehrsbetriebe (BVG) are investigating how smoke spreads through the multi-storey station. Other experiments conducted as part of the project are focusing more on the human factor, particularly the requirements of people with disabilities. The insights obtained can also be applied to buildings above ground.

► [The ORPHEUS-Project \(in German\)](#)

STATEMENT



Prof. Kristel Michielsens (JSC) heads the ► [“Quantum Information Processing” research group](#)

We work on models and methods which can be used to simulate complex quantum systems on supercomputers. We are thus making a vital contribution to developing different types of quantum computers and their promising special applications.

► [see page 2](#)

Mass of Dark-Matter Particles Calculated

Axions are viewed as potential candidates for dark matter in the universe (background: Millennium Simulation, V. Springel & The Virgo Consortium)

► **Original publication:**
Nature (2016), DOI:
10.1038/nature20115

► **Comment: Nature News
and Views (2016),
DOI:10.1038/539040a**

Scientists may have come one step closer to finding the mysterious dark matter. Using large-scale computer simulations, a German-Hungarian research unit headed by the University of Wuppertal and Forschungszentrum Jülich succeeded in compiling a kind of profile of the axion. The as-yet undiscovered elementary particle is viewed as a promising candidate for the dark matter of the universe. Narrowing down its mass gives particularly important indications to search for the hypothetical particle in a targeted manner in future experiments using detectors.

According to current knowledge, only around 15% of the matter of the universe is visible. The remaining 85% is dark matter and is only noticeable due to gravity. Despite numerous efforts, physicists have not yet been able to determine what this form of matter consists of. At the same time, the existence of the axion could represent a solution to another great mystery of physics: at the core of the matter is a unique characteristic of the strong interaction, i.e. the force which holds together the elementary particles inside atomic

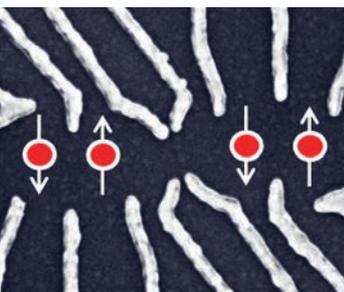
nuclei, and the question of why this force – in contrast to the other three fundamental interactions known to physics – is so surprisingly symmetrical in its properties.

An insight into the early days of the universe

According to the calculations, the mass of the axion is between 50 and 1500 microelectronvolt. The axion would thus be a very light particle, up to ten billion times lighter than the electron, which is itself a lightweight. “It must be assumed that the results presented will lead to a race for the discovery of these particles,” predicts Prof. Zoltán Fodor, head of the research unit. The researchers had to develop new calculation methods for the large-scale simulation of conditions shortly after the Big Bang, when the hypothetical particles may have formed. Forschungszentrum Jülich’s supercomputer JUQUEEN was mainly used for the calculations. The John von Neumann Institute for Computing had provided the computation time.

► Peter Grünberg Institute,
Theoretical Nanoelectronics
(PGI-2 / IAS-3)

For demonstration purposes, researchers want to integrate 50 semiconductor quantum bits (qubits) on one chip. Each electron-spin pair codes one qubit.



Millions in Funding for Quantum Computers

Quantum computers have the potential of exponentially accelerating certain applications. But their development is still in its infancy: 5 to 10 quantum bits can currently be experimentally produced, which is not enough for practical tasks. As part of the “Scalable Solid State Quantum Computing” project, researchers now want to lay the foundations for systems with several hundred quantum bits – “qubits” – as is required for quantum computers of the next generation.

The project is coordinated by scientists from Forschungszentrum Jülich and RWTH Aachen University. Researchers from the Karlsruhe Institute of Technology are also involved. The Helmholtz Association has chosen Scalable Solid State Quantum Computing as one of the first innovative pioneering topics and is providing €6 million in funding as part of the Initiative and Networking Fund.

For the project, the scientists are pursuing solutions for multi-qubit systems based on superconductors and semiconductors, for example. These

are the two types of materials that are most frequently used to produce qubits in solids. The focus is also on the development of new components which can be used to accurately control several hundred qubits.

Quantum speed for special purposes

Qubits, similarly to conventional bits, are the basic unit of quantum information processing. In contrast to bits, however, qubits are capable of assuming not only clearly distinguishable values such as 0 and 1 but a number of states that can be superimposed simultaneously. Certain tasks can thus be solved very rapidly: the simulation of new materials, whose atoms and electrons also obey the laws of quantum physics, could benefit. Furthermore, quantum computers are viewed as inherently safe from eavesdropping and could therefore form the basis for a new class of physically secure quantum communication networks.

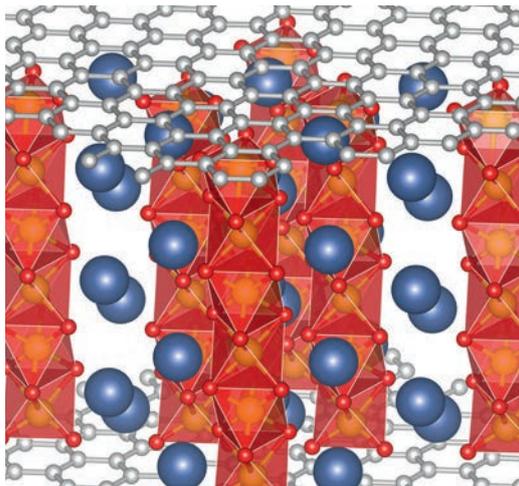
► [more](#)

New Material for Spin Transistors

For a long time, scientists have been looking for ways of using the spin of electrons to store and process information. In comparison to conventional transistors, which only make use of the electric charge of electrons, spin transistors would – theoretically – require one order of magnitude less energy and could thus revolutionize computer technology. However, the industrial breakthrough has so far been hampered by the lack of a suitable material. Early-career researcher Zeila Zanolli has now used computer simulations to identify a new combination of materials which satisfies the requirements.

The combination of graphene and barium manganese oxide makes it possible to accurately align the electron spin by means of an external field. Furthermore, the spins can move well across long distances in this material. Both properties are essential for the construction of spin transistors. Traditional semiconductors fulfil only the first requirement: the electron spins are easily controlled from the outside, but this polarization does not remain intact for very long. Carbon-based semiconductors such as graphene usually display the opposite behaviour: in these materials, spins can cover distances 100 to 200 times longer in an unhindered fashion. But due to the weak spin-orbit coupling, the spins are hard to control from the outside – which is crucial for producing a signal.

“The advantages of the two material classes complement each other if graphene is combined with a magnetic semiconductor,” explains Zanolli. The physicist, who now works at RWTH Aachen University, was able to demonstrate these remarkable properties during her time as a Marie Curie Fellow at Forschungszentrum Jülich. The Jülich supercomputers JUQUEEN and JURECA were among those used for the compute-intensive analysis.



► [Scientific Reports \(2016\)](#), DOI: 10.1038/srep31346

► [Nanospintronics Group](#)

Hybrid material for spin transistors, consisting of graphene (grey, top and bottom) and barium manganese oxide (centre)

Virtual Steel Laboratory

Tales and legends tell of the unique properties of historic steels. Even today, this adaptable material is among the most important raw materials in industry: for example in vehicle construction, where advanced lightweight high-performance steels have to withstand extreme loads. The improved properties are achieved using a carefully determined structure on the micro-scale. At the same time, the heterogeneous structure no longer permits correct predictions of the material behaviour and failure via simple material law.

As part of the EXASTEEL project, experts are working on new simulation tools aimed at permitting investigations into such lightweight high-strength steels – termed “dual-phase steels” – in a virtual environment. The realistic simulation of entire components, taking into consideration the microstructure, is extremely compute-intensive and only possible using suitable algorithms on a supercomputer of the next exascale generation.

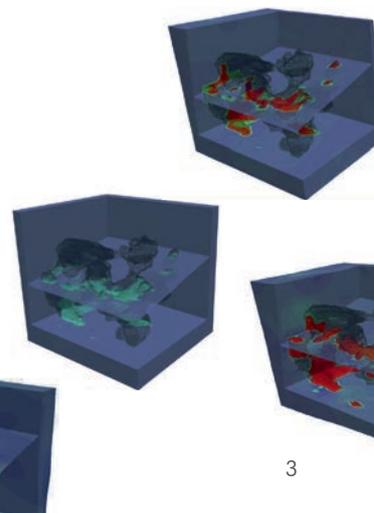
“One of our objectives is to adapt and further develop the FE2TI code for massively parallel systems,”

explains Prof. Axel Klawonn, project spokesperson at the University of Cologne. “The algorithm divides components into smaller parts according to the finite-element method in order to calculate macroscopic deformations. The simulations on the microstructure level are limited to representative bulk elements since the cost of computation will otherwise exceed the calculation capacities available in the near future.

Researchers from the universities of Cologne, Freiberg, Erlangen, Duisburg-Essen, Dresden, and Lugano are involved in the project, which is supported by the German Research Foundation (DFG) through the SPPEXA priority programme. Computation time is supplied by the Gauss Centre for Supercomputing. While adapting the code, they have already been able to achieve some success: since 2015, FE2TI has been a member of the High-Q Club. In order to be granted membership, all 458,752 processor cores of Jülich’s top computer JUQUEEN have to be efficiently used to capacity.

► [Projekt Exasteel - Bridging Scales for Multiphase Steels](#)

EXASTEEL combines macro- and microsimulations for material tests on future exascale computers.



NEWS IN BRIEF

NIC Excellence Project

The Peer Review Board of the John von Neumann Institute for Computing (NIC) has awarded a project aiming to calculate the magnetic moments of muons the title of 2016 NIC Excellence Project. The DESY project is searching for discrepancies from the conventional value that the electron's heavier relative displays. The difference is down to pure quantum effects and could reveal insights into theories beyond the standard model of high-energy physics. [▶ more](#)

HBP Substantiates Objectives

The Human Brain Project (HBP) has re-defined its research goals and published them in the journal *Neuron*. The scientists are looking to decode how the brain works. To do so, the HBP is creating a European research infrastructure capable of examining the most complex processes and structures of the brain using detailed analyses and simulations. [▶ more](#)



Germany's Brightest

Julia Valder from the Jülich Supercomputing Centre has been honoured for her excellent final grade in her training as a mathematical-technical software developer – MATSE for short. At the Chamber of Industry and Commerce's official event in late 2016, she received the award for the best MATSE trainee in both North Rhine-Westphalia and the whole of Germany. Federal Minister for Family Affairs Manuela Schwesig gave the official speech at the event. [▶ more](#)

European Data Service

Together with 14 other European computer and data centres, the Jülich Supercomputing Centre has founded the EUDAT Collaborative Data Infrastructure (EUDAT CDI). The partners want to create a reliable and long-term infrastructure for research data, which will be independent of project durations. EUDAT CDI is based on the EUDAT2020 project, which is being funded as part of Horizon 2020. [▶ more](#)

Helmholtz Data Federation

The Helmholtz Association is providing funding totalling €49.5 million for the establishment of an international network infrastructure for research data until 2021. The aim of the Helmholtz Data Federation is storing data and making them publicly available in the long term. So far, a total of six establishments are involved, including the Karlsruhe Institute of Technology as project coordinator and Forschungszentrum Jülich. [▶ more \(in German\)](#)

UPCOMING EVENTS

▶ PATC training course:
GPU Programming with CUDA
24–26 April 2017 at the
Jülich Supercomputing Centre
Instructors: Dr. Jan Meinke, Jochen
Kreutz, JSC; Jiri Kraus, NVIDIA

▶ Training course:
**Introduction to the usage and
programming of supercomputer
resources in Jülich**
22–23 May 2017 at the
Jülich Supercomputing Centre
Instructors: Employees from Intel
and ParTec; JSC employees

▶ PATC training course:
**High-performance
computing with Python**
12–13 June 2017 at the
Jülich Supercomputing Centre
Instructors: Dr. Jan Meinke, Dr.
Olav Zimmermann, JSC

▶ Training course:
**High-performance scientific
computing in C++**
20–21 June 2017 at the
Jülich Supercomputing Centre
Instructor: Dr. Sandipan Mohanty,
JSC

▶ 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
In-Situ Visualization with VisIt**
29 June 2017 at the
Jülich Supercomputing Centre
Instructors: Jens Henrik Göbber, Dr.
Herwig Zilken, JSC

▶ Overview of events at the
Jülich Supercomputing Centre

Also available for smartphones and tablets!

- ▶ Exascale-Newsletter
- ▶ effzett – the crossmedia magazine
- ▶ 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, Christian Hohlfeld
Graphics and Layout: Graphical Media, Forschungszentrum Jülich **Translation:** Language Services, Forschungszentrum Jülich **Photos:**
p. 1: Forschungszentrum Jülich/Ralf Eisenach, Weissblick/fotolia.com; p. 2 top: V. Springel & The Virgo Consortium; p. 2 bottom: RWTH
Aachen University/2nd Institute of Physics; p. 3 top: RWTH Aachen University/Zanolli; p. 3 bottom: D. Brands, A. Klawonn, M. Lanser,
O. Rheinbach, L. Scheunemann, J. Schröder; p. 4: DIHK/Schicke/Ebner, Jezper/fotolia.com **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

