



New Jewel in the Crown

Modular supercomputer JUWELS succeeds computing empress JUQUEEN

A new supercomputer is put into operation at the Jülich Supercomputing Centre (JSC). JUWELS is set to replace the Jülich supercomputer JUQUEEN, which at one time was the fastest supercomputer in Europe. The new system can perform up to 12 quadrillion mathematical operations per second, in other words 12 petaflops. In addition, a planned expansion in 2020 is set to multiply its computing power even further.

The Jülich Wizard for European Leadership Science is one of a new generation of modular supercomputers such as Jülich supercomputer JURECA, which was ramped up in autumn last year. "JUWELS is no off-the-shelf supercomputer. We have consciously opted for a machine that we are also able to develop ourselves. We believe modular supercomputing to be the key to an affordable technology that can be used to realize the next generation of smart European exascale systems," explains Prof. Thomas Lippert, director of JSC.

The modular concept designed at JSC envisages a supercomputer comprising several specialized building blocks. The Cluster module, which is supplied by European company Atos together with the software

specialists at the German enterprise ParTec, stands out with its versatility and ease of use. Within the next two years, it will be augmented with a second Booster module for massively parallel workloads, which are well-suited to be processed with a large number of relatively slow – but extremely energy-efficient – processor cores.

A unique feature of the Cluster module is its novel warm-water cooler, which enables the majority of waste heat to be cooled directly by outdoor air without additional cooling generators, thus helping to save energy.

The new computer is already highly sought-after by European researchers. A total of 87 projects have already been allocated computing time. The next few months are completely booked up. "The system will be used, for instance, for simulations in the fields of quantum physics, neuroscience, and materials science. There is also an extension for scientists in the field of Earth system modelling, climate research for example," explains Dr. Dorian Krause from JSC. Other applications come from engineering, life sciences, astronomy, and chemistry.



Prof. Andreas Wahner
Head of Institute at
Forschungszentrum Jülich
(IEK-8)

JUWELS makes it possible to simulate the complex chemical reactions of trace substances and pollutants of the Asian monsoon with unprecedented resolution for several phase states. In the FRONTAIR project, we are thus able to investigate the interaction of weather and extremely polluted air for next-generation climate models.

Volcanoes as a Climate Factor

For a long time, researchers believed that really only volcanoes in the tropics had a global influence on the climate. But that's not quite accurate. Eruptions that occur further north or south can also have an impact on the Earth's atmosphere as a whole. With the aid of computer simulations, scientists have now proven that the decisive factor is the time of year the eruption occurs.

ORIGINAL PUBLICATION

Wu, X., Griessbach, S., Hoffmann, L.: Equatorward dispersion of a high-latitude volcanic plume and its relation to the Asian summer monsoon: a case study of the Sarychev eruption in 2009, Atmos. Chem. Phys. (2017), DOI: 0.5194/acp-17-13439-2017

VIDEO

Volcanoes as a climate factor (duration 1:28 mins)

➤ <https://www.youtube.com/watch?v=Sob45iViBQ>

Volcanic eruptions are an important climate factor. The sulfate aerosols produced by eruptions reflect some visible solar radiation and thus help to slow down global warming. In the lower layers of the atmosphere, their lifetimes are very short. If they enter the stratosphere, however, they can survive there undamaged for months or years, which causes a cooling of the underlying troposphere.

The previous assumption was that only major volcanic events and moderate eruptions in the tropics had a global influence on the climate. One reason for this is the stratospheric circulation patterns in which air at the equator ascends, floats to high latitudes, and then descends again over the poles. Aerosol particles from volcanic eruptions at medium and high

latitudes already find themselves in a downward flow and so their influence should be limited.

"This is not the case, however," explains Dr. Xue Wu from the Chinese Academy of Sciences, who has been working as a visiting scientist at the Jülich Supercomputing Centre (JSC) for two years. Together with experts from SimLab Climate Science at JSC, she discovered that when the Sarychev volcano – located in the north – erupted in June 2009, large quantities of aerosol particles entered the tropical stratosphere. From there, the particles spread across the entire globe.

The reason for the unexpectedly high ascent of the aerosols was the Asian summer monsoon, which only occurs in summer and transported the aerosol particles right up into the tropical stratosphere. In winter, however, they remained in the lower atmospheric layers and were washed out of the atmosphere after a short period of time. If the aerosols from the Sarychev eruption are factored into calculations, this explains the increase from 15,000 to 20,000 tonnes of sulfate aerosols per year witnessed in the tropical stratosphere over the last few years.

48 Qubits Simulated

Software developers and engineers won't have to start from scratch when the first quantum computers become available in future. With the aid of numerical simulations it is already possible to reconstruct the behaviour of quantum computers in detail on conventional computers. The computational effort involved, however, is enormous. The amount of memory required doubles with each simulated quantum bit, or qubit. Until recently, it usually took several years to increase the maximum number of simulated qubits on supercomputers by an additional qubit.

Within the space of a few months, Prof. Kristel Michielsen from the Jülich Supercomputing Centre (JSC) has now twice succeeded in surpassing the existing record. Together with researchers from universities in Wuhan, Tokyo, and Groningen, she first simulated a quantum computer with 46 qubits followed by a quantum computer with 48 qubits. They performed their simulations on two of the world's most powerful supercomputers: China's Sunway TaihuLight and Japan's K supercomputer.

For Michielsen, these are not the first such records she has broken. In 2010, she became the first person to simulate a quantum computer with 42 qubits on the former Jülich supercomputer JUGENE. She then broke that world record in 2012 with the simulation of a 43-qubit system on JUQUEEN, the successor to JUGENE. At the end of 2017, Michielsen simulated a 45-qubit quantum system together with partners from universities in Groningen, Tokyo, and Wuhan, thus equalling a record only set in spring 2017.

The present breakthroughs cannot be attributed to immense computing power alone. The records were much more a result of an adjustment in the simulation code. The researchers optimized their software in such a way that each quantum state now only requires 2 bytes instead of 16 bytes, without the accuracy of the results being significantly reduced. Users are also set to benefit from the improvement. As a result of the simplification, the storage requirements have been reduced by a factor of eight. This now enables users to simulate a quantum computer with 32 qubits on a notebook with 16 gigabytes of memory.



Prof. Kristel Michielsen

Deep Learning for Cleaner Air

Dr. Martin Schultz conducts research on the concentration of pollutants in the atmosphere. The data specialist from the Jülich Supercomputing Centre (JSC) is one of the world's most-cited geoscientists, according to the 2017 Highly Cited Researchers list. He has received an ERC Advanced Grant – the most prestigious scientific award at European level – of € 2.5 million for his latest project, IntelliAQ.

Dr. Schultz, what is the IntelliAQ project all about?

In the project, we want to use deep machine learning methods to identify patterns that link various weather data and geographical information to air pollutant concentrations. We then want to use these correlations to close spatial and temporal gaps in the data sets and to predict concentrations of pollutants such as ozone, particulate matter, and nitrogen oxides.

Why is artificial intelligence so useful in this project?

Even after decades of development, conventional numerical models still exhibit serious errors when producing such forecasts. These errors result from insufficient spatial resolution and an incomplete un-

derstanding of the physical and chemical processes governing atmospheric composition. Using deep neural networks, however, we can derive as much information as possible directly from the measurement data. We are therefore replacing a model that includes known but incomplete equations with a system that in principle has complete information but which does not permit any conclusions about the processes.

What should we expect from such an air quality forecast?

Our initial aim is to deliver a forecast for all measurement sites, but also for places in between, which can then be used as a planning tool by cities to help keep the air clean. Further potential applications include retrospective investigations of changes in air quality to help assess health risks, for example. Furthermore, there are many ongoing initiatives, which aim to comprehensively monitor urban air quality using small, low-cost sensors. Our system might make it possible to calibrate such data later and thus make them usable.

[➤ more \(in German\)](#)



Dr. Martin Schultz

Trend Towards Artificial Intelligence

Computers can talk to us or teach themselves to become world champions in the board game Go. Similar adaptive algorithms can fine-tune photos or produce deceptively real images that do not actually exist in reality. There is no doubt that artificial intelligence (AI) has become a feature of everyday life and a trend that is gradually taking root in the world of science.

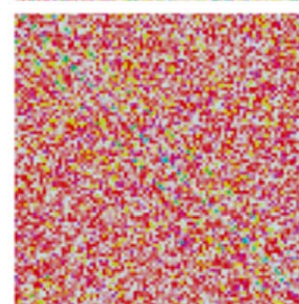
“AI is a topic that is also gaining increasing importance within the scope of high-performance computing. We know from the last allocation of computing time that around half a dozen of the projects are seeking to use AI-related processes stemming from the fields of condensed matter, fluid dynamics, meteorology, biology, and, of course, computer science,” explains Dr. Alexander Trautmann, who coordinates the allocation of computing time on Jülich supercomputers via the John von Neumann Institute for Computing (NIC).

One of these projects is the recently announced NIC Excellence Project “Simulation of quantum-mechanical many-fermion systems”. The researchers are teaching adaptive neural networks to recognize novel material properties that have no equivalent in

classical physics. Simulations on the JURECA Booster form the foundation for this. The Jülich supercomputer module was installed last autumn and has been optimized for extreme computing power.

“One thing that interests us is the high-temperature superconductor mechanism, which has been puzzling physicists for 30 years,” explains project leader Prof. Simon Trebst from the University of Cologne. Another phenomenon is spin liquids: materials whose electron spin, at ultracold temperatures, interacts in a similarly chaotic manner to molecules in a liquid.

Both properties can be seen in fermion systems. In contrast to bosons, fermions do not have integer spin – only half-integer spin. “Bosons can be very easily simulated – hundreds of thousands of particles are possible. Fermions, however, are much more complex to calculate due to their different wave function,” the physicist explains. For a long time, it was only possible to simulate just over 20 electrons. A new formulation was then discovered a few years ago, significantly reducing the computational effort for a certain class of electron problems, and allowing several hundred electrons to be simulated today.



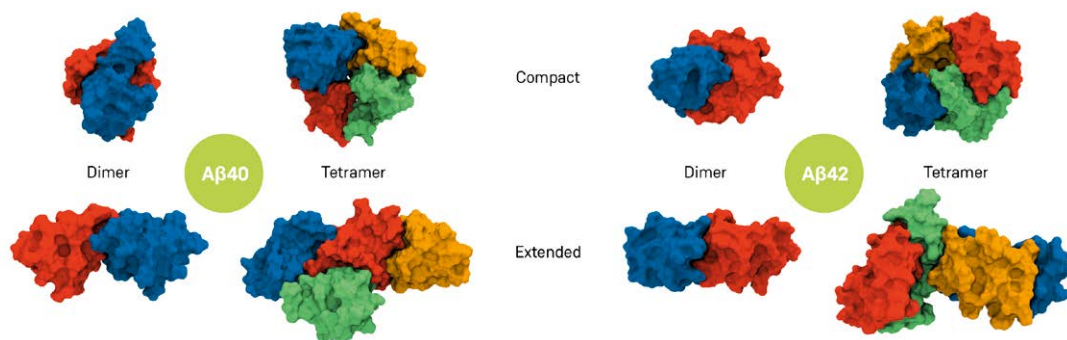
Insulator (top) and metal (bottom): Artificial intelligence can distinguish different phases. The images were “captured” during the simulation of a many-fermion system.

Alzheimer's Research

Deposits of beta-amyloid plaques in the brain are typical of Alzheimer's disease. The plaques are less likely to be caused by the deposits themselves, which are visible with a microscope, and much more a result of their precursor aggregates: oligomers, which are harmful to nerve cells in various ways. With the aid of simulations on the Jülich supercomputer JURECA, researchers from Jülich's Institute of Complex Systems – Structural Biochemistry (ICS-6) have now

investigated the role of different oligomer shapes. They found that elongated or extended oligomers are the main driving force behind the formation of the deposits typical of Alzheimer's. These oligomers often consist of a long-chain version of the beta-amyloid peptide, which is considered to be particularly harmful.

Journal of the American Chemical Society (2018), DOI: 10.1021/jacs.7b10343



Compact oligomers (top) are relatively stable, while extended forms (bottom) are rather short-lived. Variants of long-chain peptide building blocks (A β 42, bottom right) are regarded as particularly toxic

Germany's Best MATSE

Simply the best: Svenja Schmidt, a former JSC trainee, had the best examination marks among trainee mathematical-technical software developers (MATSEs) in Germany. She was presented with an award at an event in Berlin organized by the Chamber of Industry and Commerce (IHK) honouring the best trainees. Schmidt is still employed at Forschungszentrum Jülich and works in the Institute for Advanced Simulation – Civil Safety Research (IAS-7), while also completing a master's at the Aachen University of Applied Sciences. [↗ more](#)

Europe's Next Flagship

The selection of the EU's next flagship project with up to €1 billion in funding is heading into the next phase. Scientists from Forschungszentrum Jülich are involved in four applications, which have made it into

the second of three rounds in total. These projects are: ExtremeEarth-PP, a prediction of extreme natural phenomena; BATTERY 2030+, an energy research project; SUNRISE, a synthetic fuels and raw materials project; and DigiTwins, a personalized medicine project.

ORPHEUS Project Completed

For three years, the ORPHEUS project coordinated by JSC focused on fires in underground stations. The project came to a close at the start of this year at a public meeting in Berlin, during which the parties involved presented their results. Shortly before this, three articles also received Best Paper Awards at conferences and demonstrated the scientific relevance of the project, which was funded by the German Federal Ministry of Education and Research. [↗ more](#)

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

Graphics und Layout: SeitenPlan GmbH

Translation: Language Services, Forschungszentrum Jülich

Photos: p. 1 top: Forschungszentrum Jülich/Ralf-Uwe Limbach/SeitenPlan; p. 1 bottom: Forschungszentrum Jülich/Sascha Kreklau; p. 2-3 top: Gennady Tepplitskiy/Shutterstock; p. 2 bottom: Forschungszentrum Jülich/Ralf-Uwe Limbach; p. 3 top: Forschungszentrum Jülich/Ralf-Uwe Limbach; p. 3 bottom: Universität zu Köln/Simon Trebst; p. 4: Forschungszentrum Jülich/Birgit Strodel

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Printed by: Schloemer & Partner GmbH

Print run: 300



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UPCOMING EVENTS

Training course: Introduction to parallel programming with MPI and OpenMP

13–17 August 2018
at the Jülich Supercomputing Centre
Instructors: Benedikt Steinbusch, Thomas Breuer, JSC

[↗ more](#)

Extreme Data Workshop

18–19 September 2018
at the Jülich Supercomputing Centre
Organizers: Dr. Martin Schultz, Prof. Dirk Pleiter, Daniel Mallmann, JSC

[↗ more](#)

CECAM tutorial: Atomistic Monte Carlo Simulations of Biomolecular Systems

24–28 September 2018
at the Jülich Supercomputing Centre
Instructors: Dr. Sandipan Mohanty, Dr. Olav Zimmermann, Dr. Jan Meinke, JSC

[↗ more](#)

Training course: Porting code from Matlab to Python

8–9 October 2018
at the Jülich Supercomputing Centre
Instructors: Sandra Diaz, Lekshmi Deepu, Dr. Alexander Peyser, Wouter Klijn, JSC

[↗ more](#)

Training course: Introduction to GPU programming using OpenACC

29–30 October 2018
at the Jülich Supercomputing Centre
Instructors: Dr. Andreas Herten, JSC, Jiri Kraus, NVIDIA

[↗ more](#)

↗ Overview of events at the Jülich Supercomputing Centre: fz-juelich.de/ias/jsc/events