EXASCALE
02-2018 | NEWSLETTER ON SUPERCOMPUTING AND BIG DATA

JÜLICH
Forschungszentrum

Quantum Flagship

Research initiative aims to put Europe at the forefront of quantum technologies

Data networks that are safe from eavesdropping, extremely precise measuring instruments, and the computer of the future – quantum technology raises a lot of hopes. The European Commission recently announced an extensive 10-year flagship programme that involves funding of € 1 billion for quantum technologies. In addition, the German Federal Government is contributing roughly € 650 million during the current legislative period.

Many other countries are also investing in quantum technologies. The USA is supporting research in this field with roughly $ 200 million in funding every year. In Hefei, China, a quantum laboratory is being constructed for the equivalent of almost € 9 billion. And companies such as IBM, Google, and Microsoft are competing to develop the first computer based on quantum physics, which would be vastly superior to conventional supercomputers in the completion of certain tasks.

The European initiative emerged from the "Quantum Manifesto", which was signed by more than 3,600 representatives from science and industry in the spring of 2016. "We are running the risk that expertise gained here in the EU will be developed into market-ripe applications elsewhere," warns one of the leading scientists behind the initiative, Prof. Tommaso Calarco from Forschungszentrum Jülich (PGI-8).

Jülich plays a key role in researching quantum technologies: new theories and ideas are being developed here. And thanks to Jülich's expansive infrastructure, the approaches can be experimentally verified straight away. As part of the flagship subproject OpenSuperQ, which is headed by Saarland University, researchers are planning a quantum computer with 50–100 superconducting qubits that will be developed and operated at Jülich. The aim is to establish a central European laboratory for quantum computers, which will be publicly accessible and available to the whole research community.

Prof. Kristel Michielsen hopes that this planned system will be another step towards establishing a new key area at the Jülich Supercomputing Centre (JSC): "I'm envisioning a user facility that offers access to quantum computing technologies on various stages of maturity, complemented by access to our simulators." The physicist uses high-performance computers to simulate how an ideal quantum computer would behave according to the laws of physics. This helps to estimate the error rate of real quantum computers. Because ultimately, all current approaches are still experimental: the quantum processors are too small or qubits are not yet sufficiently stable for serious calculations. The good thing for research, however, is that there is still a lot to do.

Interview with Prof. Tommaso Calarco

Prof. Tommaso Calarco, Institute head at Forschungszentrum Jülich (PGI-8)

The flagship initiative incorporates missions of the highest social relevance. In addition to designing a quantum computer, I'm talking about securing European networks by means of quantum cryptography and the development of highly sensitive sensors for navigation and medical diagnostics.

Data Awareness

The performance of state-of-the-art supercomputers in practice depends in many cases primarily on how fast data can be moved from the storage system to the processor. Many programming models and codes, however, stem from a time when the main focus was on how many floating-point operations per second a supercomputer was capable of. This is why the aim of a recently launched project entitled Maestro, coordinated by JSC, is to create a fresh appreciation for data.

"Current systems usually don't know what type of data objects are contained in memory or are communicated by an application within the system. Dependencies on other objects can also frequently not be determined. Together with European partners, we want to test a new concept for the definition of data objects, which will permit such information to be transferred via several software and hardware levels," explains project manager Prof. Dirk Pleiter.

The project aims at developing a middleware that mediates between the operating system and applications, and intelligently distributes data between different hardware and software levels. The development is guided by applications such as the ones used by the European Centre for Medium-Range Weather Forecasts (ECMWF), which is reaching its technical limits in terms of refining its globally used forecasts.

A transparent, consistent data model is also needed for novel storage concepts, which are being developed to improve access times and transfer rates for data-intensive applications. Some approaches aim at combining separate storage resources on compute and storage nodes to form a complex overall system. Other architectures focus on a mixture of different storage types which, in addition to conventional memory and hard-drive storage, also involves novel non-volatile memory and high-bandwidth memory.

These new architectures also form the focus of another project in which JSC is involved and which is coordinated by the storage manufacturer Seagate. Within the scope of the SAGE project, the project partners developed a prototype that combined several types of storage. As part of SAGE2, additional solutions are pursued for Arm processors, which are used in most smartphones today. In the European Processor Initiative (EPI), in which JSC is involved, experts pursue the development of a European supercomputer processor based on this technology.

MAESTRO PROJECT:
- JSC (coordination)
- CEA
- Appentra
- ETH Zürich
- ECMWF
- Seagate
- Cray

maestro-data.eu

SAGE2 PROJECT
- Seagate (coordination)
- Atos-Bull
- CEA
- United Kingdom Atomic Energy Authority
- KTH
- JSC
- University of Edinburgh
- Kitware
- Arm

sagestorage.eu

EUROPEAN PROCESSOR INITIATIVE

https://bit.ly/2DbSQox

Geared up for Big Data

Handling large volumes of data is a crucial present-day challenge: each year, the amount of data produced by science increases. To meet the constantly growing requirements, JSC has significantly expanded its storage infrastructure this year. *more*

LARGE-SCALE MAGNETIC TAPE ARCHIVE
Name/type: IBM TS4500 Tape Library
Storage capacity: 170 petabytes, or the equivalent of roughly 36 million DVDs
Bandwidth/speed: 6 gigabytes, or roughly one DVD per second
Use: The tape drive complements the existing magnetic tape storage for backups and the long-term archiving of data.

STORAGE CLUSTER OF THE LATEST GENERATION
Name/type: JUST (Jülich Storage Cluster)
Storage capacity: roughly 50 petabytes on 7,516 hard drives
Bandwidth/speed: 500 gigabytes, or roughly 100 DVDs per second
Use: JUST is the central storage system of Jülich's supercomputers and is accessed by JUWELS and JURECA, among others.

CLOUD STORAGE FOR LARGE DATA SETS
Name/type: Multi-purpose cloud storage
Storage capacity: 40 petabytes (integrated into JUST)
Bandwidth/speed: 20 gigabytes, or roughly 4 DVDs per second
Use: The multi-purpose cloud storage system permits large data sets to remain easily accessible over long periods of time and very large sets of raw research data to be stored for processing by supercomputers.

Against Overcrowding at Stations

Congestion is becoming an issue at many train stations in Germany. Particularly during rush hour or after large public events, platforms frequently become overcrowded and are no longer able to cope with the influx of people due to steadily rising passenger numbers. As part of the CroMa project, scientists from Forschungszentrum Jülich together with their partners are working to develop new concepts and measures that will alleviate the situation and increase efficiency at train stations and underground stations.

Over a period of three years, the Federal Ministry of Education and Research (BMBF) is providing funding totalling € 2.1 million for the project, which is coordinated by the University of Wuppertal. In addition to transport companies such as Deutsche Bahn, the Swiss Federal Railways, and Kölner Verkehrs-Betriebe, the project also involves event technicians as well as the police and security authorities. Their objective is to ensure that the results can be implemented in practice.

"Conceivable measures include markings or information regarding the remaining capacities of individual train carriages. This would make it easier for passengers to spread out along the platforms, thus optimizing the boarding process. We are interested in the impact of such measures and how they affect the stress level of passengers," explains Dr. Maik Boltes, who works at Jülich's Institute for Advanced Simulation – Civil Safety Research (IAS-7).

Within the scope of CroMa, Jülich researchers are creating concepts and conducting experiments suitable for investigating the effects of various crowd management methods. The data are needed to adapt computer simulations, which can then be used for the planning and testing of train stations and large buildings.

In addition to the effects of physical and constructional systems such as crowd control barriers, the experts involved in CroMa also investigate psychological factors. In cooperation with the University of Bochum, they want to test how different ways of informing and addressing people affects the behaviour of passengers.

Project outline CroMa (in German, pdf)

Researchers Simulate Catastrophe

Jülich researchers together with two project partners use computer simulations to improve large-scale evacuations. Possible scenarios include an impending nuclear disaster, a chemical spill, or a flood. The situation is particularly critical in conurbations: if a catastrophe were to occur, roads and motorways would be jammed almost instantly. Most people would depend on trains to evacuate the danger area.

Within the KapaKrit project, the Jülich scientists aim to use the Dortmund main train station as a case study for the new simulation tools that can then be used by engineers and authorities for further planning.

The joint project, which was launched in summer 2018, involves experts from Bochum University of Applied Sciences, the engineering company bueffee, and associated partners from the field of railway operation. The Federal Ministry of Education and Research is supporting the consortium with total funding of € 1.1 million over three years.

The researchers, together with transport and security services, want to investigate how large numbers of people can be evacuated in an emergency via train stations in large cities. Such numbers are fundamental for planning and are expected to provide new impetus for new technical and organizational measures.

"Using our JuPedSim software, we can already predict fairly accurately how fast people can be evacuated from a room. But the case we are investigating now is more complex," explains project leader Dr. Stefan Holl from Forschungszentrum Jülich. "People first have to get to the train station. Once there, they have to be guided through the station to the correct platform. And there then has to be a train waiting for them to get on."

Dortmund main station is one of the largest train stations in Germany with around 130,000 passengers per day. In the event of an evacuation, however, many more people would have to be brought to safety. On top of the city's 600,000 inhabitants, there would be an additional 5 million inhabitants from the surrounding commuter area of the Ruhr region. The recommendation to use trains in emergencies stems from the working group of the federal interior ministers, which was convened after the 2011 nuclear disaster in Fukushima, Japan.

Project outline KapaKrit (in German, pdf)

Launch of JUWELS

From left to right: Chairman of the Board of Directors Prof. Wolfgang Marquardt, NRW Prime Minister Armin Laschet, Federal Research Minister Anja Karliczek, and JSC director Prof. Thomas Lippert

In September, German Federal Research Minister Anja Karliczek and NRW Prime Minister Armin Laschet together with Jülich's Board of Directors officially launched Jülich's new supercomputer JUWELS. The Federal Government and the federal state of NRW are providing more than € 145 million until 2025 for the further development of supercomputing at Jülich. The first component of the novel, modular supercomputer system has a theoretical peak performance of 12 petaflop/s, which corresponds to the computing power of roughly 60,000 state-of-the-art PCs. For 2019, an expansion is in the offing, which will again substantially increase JUWELS' computing power. *more*

Ozone in China

China has seen a substantial increase in ozone pollution over the past few years, while Europe and the USA have registered a general decrease. This was revealed in a new study by Chinese, American, and Jülich scientists. "According to our knowledge, no other region in the world has such high levels of ozone as frequently as China," explains Dr. Martin Schultz from Jülich Supercomputing Centre. *more*

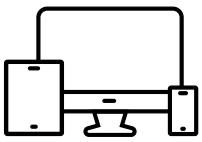
Environ. Sci. Technol. Lett. (2018), DOI: 10.1021/acs.estlett.8b00366

Smart Computer

Together with transmission grid operator TenneT TSO GmbH, experts from JSC have developed a computer system for the simulation of load flows in the electricity grid. The "smart" new system can be used to accelerate such calculations by a factor of more than 30. The simulations will help to adapt the electricity grid to the requirements of the transformation of the German energy sector (*Energiewende*). In northern Germany, it is often the case that more wind power is produced at peak times than can be transported to the south and west of the country. *more*

New Chair of PRACE Council

Prof. Thomas Lippert, head of JSC, was elected as the new Chair of the PRACE Council. As advisor to the founding chair Prof. Achim Bachem, he was involved in the development of the European supercomputing organization from an early stage. Lippert believes his current task for PRACE is to bring together the exascale systems of the coming EuroHPC Joint Undertaking with science and industry in Europe. *more*



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UPCOMING EVENTS

Training course: "Software Development in Science"

19–20 November 2018
at the Jülich Supercomputing Centre
Instructors: Guido Trensch, Wouter Klijn, JSC
more

Training course: "Introduction to the usage and programming of supercomputer resources in Jülich"

22–23 November 2018
at the Jülich Supercomputing Centre
Instructors: Representatives of Intel and ParTec, JSC staff members
more

Training course: "Advanced Parallel Programming with MPI and OpenMP"

26–28 November 2018
at the Jülich Supercomputing Centre
Instructors: Dr. Rolf Rabenseifner, HLRS; JSC employees
more

Training course: "Introduction to parallel programming with MPI and OpenMP"

18–22 March 2019
at the Jülich Supercomputing Centre
Instructors: Benedikt Steinbusch, Thomas Breuer, JSC
more

Training course: "GPU Programming with CUDA"

1–3 April 2019
at the Jülich Supercomputing Centre
Instructors: Dr. Jan Meinke, Jochen Kreutz, Dr. Andreas Herten, JSC; Jiri Kraus, NVIDIA
more

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