Quantum Computing at JSC

Quantum computing is a new, innovative way of computing with potential applications in quantum simulations in chemistry, materials science, optimization, and machine learning. Huge challenges and opportunities exist in developing algorithms and tools for quantum computing devices to solve very hard and hitherto intractable computational problems in science and industry. Recently, the Jülich Supercomputing Centre has strengthened its engagement in quantum computing by signing several contracts with leading companies and by launching the JUNIQ infrastructure.

Launch of JUNIQ and Contract with D-WAVE Systems

"We are counting on quantum computers": this was the motto of the event on 25 October, where JUNIQ, the new "Jülich UNified Infrastructure for Quantum computing" was put into operation. The go-ahead was given with the official signing of a user contract for a quantum annealer from the Canadian quantum computer manufacturer D-Wave Systems, making Forschungszentrum Jülich the first D-Wave Leap™ cloud-based quantum site in Europe. The event was opened with a welcoming address by Annette Storsberg, State Secretary from the North Rhine-Westphalian Ministry of Culture and Science, and a message from Thomas Rachel, Parliamentary State Secretary at the Federal Ministry of Education and Research. The state government and the Federal Ministry of Education and Research are supporting the establishment of JUNIQ with € 5 million in funding from each.

JUNIQ will be the unified portal to a number of different quantum computers – accessible via the cloud for German and European users. JUNIQ will thus offer quantum computing services similar to those that have long been available for Jülich's supercomputers: Under the guidance of experts, researchers will be able to use quantum computers – from experimental systems and prototypes to first production systems – and develop algorithms and application programs for them.

D-Wave's quantum system – a so-called quantum annealer – will be accessible via Leap™, the company's quantum cloud service. Jülich will be the site of the first European installation of D-Wave's Leap quantum cloud service. As part of the agreement, Jülich will also benefit from the upcoming release of Advantage™, D-Wave's next-generation quantum system with a new, highly connected Pegasus topology, lower-noise, and an increased qubit count.

Research Partnership with Google

Back in July, Forschungszentrum Jülich announced another research partnership in quantum computing with Google to advance this new disruptive computing technology. Google has years of experience in the development of quantum computers and quantum algorithms, which, alongside quantum materials research, are key research foci at Forschungszentrum Jülich, too.

The partnership includes joint research and expert training in the fields of quantum computing hardware and quantum algorithms. For JSC, the latter is a key component in the research collaboration. Researchers from Google and from the research group Quantum Information Processing of Prof. Kristel Michielsen will cooperate in performing simulations on supercomputers at JSC and in experimenting with Google's quantum processors for benchmarking purposes. For this research, the Jülich Universal Quantum Computer Simulator (JUQCS), developed in international collaboration and used in 2018 to set the world record for simulating gate-based quantum computers at 48 qubits, will be used. The collaboration has already commenced. For the containerization of JUQCS, Kristel Michielsen received a Google Faculty Research Award in 2018.

Contribution to Google's Demonstration of Quantum Supremacy

This collaboration is already bearing fruit: in October, Google and collaborators, including Forschungszentrum Jülich, achieved a milestone in quantum computing called quantum supremacy, as the researchers claim in the renowned journal "Nature" (DOI: 10.1038/s41586-019-1666-5). The term marks the moment when a quantum computer, for the first time, outperforms state-of-the-art conventional computers in a specific task. While the Google quantum processor takes about 200 seconds, the

world's fastest supercomputers would need approximately 10,000 years to perform the equivalent task. Researchers from Kristel Michielsen's group took part in verifying and benchmarking the quantum processor with simulations carried out on the Jülich supercomputer JUWELS.

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B2SHARE Accepted as Data Repository for Nature Publications

B2SHARE is a service developed within the EUDAT and EUDAT2020 projects. It provides a solution for storing and sharing small-scale research data from diverse contexts. The instance https://b2share.fz-juelich.de at Jülich is an offer for researchers of Forschungszentrum Jülich, who want to share or publish their results.

B2SHARE handles research data in single files and in data sets across multiple files. The research data and additional metadata are stored in a record. While creating a record, the user should fill in the (community-specific) metadata. Each submitted record receives a PID (persistent identifier). A PID is a digital reference to a digital object, which allows users to find the object with a web browser. The PID can be used in publications to refer to the research data.

Since its deployment in 2017, the service has been improved to meet different needs. Since summer 2019, B2SHARE has assigned DOIs in addition to the EPIC handle PIDs for each record. In November 2019, the instance https://b2share.fz-juelich.de was accepted as an institutional repository for scientific data by Nature Publications. Although Nature does not list B2SHARE as a recommended repository, they accept the repository for the submission of scientific data from FZJ researchers. The publisher's namespace for the repository is 'FZ-Juelich B2SHARE'.

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NIC Excellence Projects November 2019

The NIC Peer Review Board regularly awards the title "NIC Excellence Project" to outstanding simulation projects. At its October meeting, the board decided to honour Prof. Frithjof Anders from TU Dortmund University and Prof. Hartmut Wittig from Johannes Gutenberg University Mainz. Both scientists were granted computing time on JUWELS and JURECA Booster.

Prof. Anders researches in the field of theoretical condensed matter and was honoured for his project, which investigates coherently controlled electron spins in an ensemble of semiconductor quantum dots which are discussed for quantum information processing. The results of this project make important contributions to spin relaxation times and to imparting nuclear spin alignment non-equilibrium distributions by periodic excitation with circularly polarized light.

The project of Prof. Wittig was recognized as an NIC Excellence Project for its contributions to elementary particle physics. The project investigates the properties of the phase transition between hadronic matter and a quark–gluon plasma, and furthermore, it investigates whether bound states of two baryons (so-called dibaryons) are predicted by quantum chromodynamics (QCD).

For more details, see http://www.john-von-neumann-institut.de/nic/anders and http://www.john-von-neumann-institut.de/nic/wittig (in German).

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New GCS Large-Scale Projects in November 2019

Twice a year, the Gauss Centre for Supercomputing (GCS) issues a call for large-scale projects on its petascale supercomputers – currently Hazel Hen/Hawk (HLRS), JUWELS (JSC), and SuperMUC-NG (LRZ). Projects are classified as large-scale if they require at least 35 million compute core hours (Mcore-h). During its October meeting at JSC, the GCS Peer Review Board decided to award the status of a large-scale project to 12 projects from various scientific fields. Three projects were granted 364 Mcore-h on Hawk, three projects were granted 84 Mcore-h on JUWELS, and six projects were granted 255 Mcore-h on SuperMUC. In total, the GCS awarded about 703 million compute core hours to large-scale projects. For more details of these projects, some of which utilize the resources of several centres, visit https://www.gauss-centre.eu/large-scale.

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End-of-Year Colloquium at JSC

Date: Tuesday, 17 December 2019, 09:30–16:00
Venue: Jülich Supercomputing Centre, lecture hall (Hörsaal)
Info: https://fz-juelich.de/ias/jsc/events/eoy-2019

09:30 Thomas Lippert: *Welcome*
09:50 Thomas Breuer: *BEAM-ME up to be UNSEEN: Tackling optimization problems for energy systems modelling on HPC systems*
10:20 Coffee break
10:50 Lukas Pieronek: *Computation of interior transmission eigenvalues*
11:20 Erik Koch: *From models to materials*
11:50 Lunch break
14:00 Jacopo De Amicis: *xPic on JURECA modular supercomputer: experiments and considerations*
14:30 Guido Trensch: *How to build a Neuromorphic Computer – The Jülich Advanced Computing Architectures Project*
15:00 Dennis Willsch: *Cute applications for quantum computers*
15:30 Thomas Lippert: *Everything you always wanted to know about PoF – but didn't care to ask*