

Europe's First Quantum Computer with More Than 5,000 Qubits Officially Launched at JSC

On 17 January 2022, a quantum annealer with more than 5,000 qubits was officially put into operation at Forschungszentrum Jülich. The Jülich Supercomputing Centre (JSC) and D-Wave Systems, a leading provider of quantum computing systems, launched the company's first cloud-based quantum service outside North America. The annealing quantum computer is part of the Jülich UNified Infrastructure for Quantum computing (JUNIQ), which was established in autumn 2019 to provide researchers in Germany and Europe with access to various quantum systems.

The launch ceremony took place as a hybrid event at JSC in the presence of Minister-President of North Rhine-Westphalia (NRW) Hendrik Wüst, European Commissioner Mariya Gabriel, and CMO, Global Marketing and Public Affairs Jennifer Houston from D-Wave Systems. The Federal Minister of Education and Research Bettina Stark-Watzinger and D-Wave CEO Alan Baratz attended via video link. In their welcoming remarks, all of the speakers emphasized that quantum computers promise enormous opportunities for our future and for research, and highlighted the importance of collaboration in the development of practical quantum applications across industry sectors and research fields. The launch of the quantum annealer within the JUNIQ user infrastructure is expected to propel Germany and Europe to an international leadership role in quantum computing. The state government of NRW and the Federal Ministry of Education and Research are each providing € 5 million in funding to support the establishment of JUNIQ.

The new quantum system is the second D-Wave quantum computer to be used within the JUNIQ user infrastructure and is the world's first Advantage™ quantum annealer to be located outside the North American continent. The Quantum Information Processing group at JSC, headed by Prof. Kristel Michielsen, will operate the system directly at Jülich, which gives JSC the opportunity to integrate it closely with its supercomputing infrastructure.

The new system is an annealing quantum computer. This type of quantum system has the potential to be particularly well suited for solving challenging optimization problems that are especially relevant to industry. These include the

efficient control of traffic flows and the training of neural networks for artificial intelligence applications. D-Wave is a leading manufacturer of such quantum systems. Clients of the company have developed early quantum applications in a diverse range of areas such as financial modelling, flight planning, election modelling, quantum chemistry simulation, automotive engineering, healthcare, logistics, and more.

The quantum annealer is housed in a new building that was especially erected for the operation of quantum computers. Quantum computing systems require a special, vibration-free location. The building's two machine halls therefore feature special vibration-damping foundations to absorb tremors. Alongside the D-Wave system, the building will host an additional quantum computer as of next year. Further information can be found at <https://fz-juelich.de/ias/jsc/juniqu>.

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EUPEX – The European Pilot for Exascale

The EUPEX consortium aims to design, build, and validate the first EU platform for HPC, with European assets covering the spectrum of required technologies end to end: from architecture, processor, system software, and development tools to applications. The EUPEX prototype will be designed to be open, scalable, and flexible, and will include a modular OpenSequana-compliant platform and a corresponding HPC software ecosystem for its modular supercomputing architecture. Scientifically, EUPEX is a vehicle to prepare HPC, AI, and Big Data processing communities for upcoming European exascale systems and technologies. A strong emphasis is put on the system software stack and the applications. Being the first of its kind, EUPEX has set itself the ambitious challenge of gathering, distilling, and integrating European technologies that its scientific and industrial partners will use to build a production-grade prototype.

EUPEX is coordinated by ATOS. Besides JSC, 16 other academic and industry partners from all over Europe are participating in the project. The project is co-funded by EuroHPC JU and the national bodies of the partners involved, including the German Federal Ministry of Education and Research (BMBF). EUPEX was launched

on 1 January 2022 and will run for four years with a total budget of € 40 million. Further information on the project will soon be available at <https://www.eupep.eu>.

JSC will bring its many years of experience in the design, installation, and operation of large HPC systems into the project. Furthermore, FZJ will contribute its well-known open-source software in the form of tools for performance measurement and analysis (Scalasca, Score-P, CUBE) and for system monitoring (LLview). Finally, JSC will port and adapt artificial intelligence (AI) applications that cover machine and deep learning. The software developed by JSC within this project will be made openly available to help support the platform within the HPC community and beyond in the long term.

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Open Data Impact Award for JSC Scientists

The Open Data Impact Award was created by Stifterverband as part of its innOsci programme, the Forum for Open Innovation Culture, and is awarded in cooperation with the magazine *DUZ*. It aims to create initiatives to make research data open and thus more widely usable. It especially highlights the potential of Open Data in research for innovation and society. Every year, a jury of open data experts from the fields of science, business, and civil society selects three projects from various research areas. Stifterverband provides a total of € 30,000 in funding for the award.

One of the projects selected for the Open Data Impact Award 2021 involves Clara Betancourt, Jianing Sun, Sabine Schröder and their colleagues from JSC. The JSC scientists received second prize and € 10,000 in funding for their project "TOAR App, Tropospheric Ozone Assessment Report database". The TOAR database is one of the largest collections of global near-surface ozone measurements. To further facilitate the reuse of this data, they are developing a smartphone app that farmers can use to quantify ozone-related damage to their crops.

The virtual award ceremony for the Open Data Impact Award took place in December 2021 as part of the innOsci "unKnOwn unKnOwns" festival. The award winners introduced themselves and their research to the public and demonstrated how open research data can benefit society as a whole. Further information on the Open Data Impact Award can be found at <https://www.stifterverband.org/innosci/open-data-impact-award>.

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Preparatory Study for the Helmholtz Platform for Research Software Engineering Started

Scientific software is becoming increasingly important to ensure the success of research and generate new knowledge. However, the impact of code for science has not yet been recognized at the national level. Moreover, existing evaluation measures for research do not yet support sustainable work on scientific software. The

situation is further complicated by the fact that conventional, industrial software engineering methods cannot be transferred one to one to scientific software. Therefore, Research Software Engineering (RSE) is forming as a new subject of investigation in Europe, Germany, and the Helmholtz Association.

In this context, the concept behind the Helmholtz Platform for Research Software Engineering (HiRSE) sees the establishment of central activities in RSE and the targeted, sustainable funding of strategically important software by Community Software Infrastructure (CSI) groups as mutually supportive aspects of a single entity.

In a first preparatory study, HiRSE_PS will evaluate the core elements of the HiRSE concept and how they interact in practice over the funding period of two years. One work package deals with the operation of CSI groups, in particular for young code, and a second with consulting and networking. The study is led by Forschungszentrum Jülich (Markus Diesmann) and Karlsruhe Institute of Technology (Achim Streit), which are joined by HZB and Hereon. JSC will play a key role in consulting and networking activities and will help code developers to make use of modern continuous integration, testing, and delivery techniques, especially in the context of high-performance computing.

The goal of the preparatory study is the further refinement of the concept, which can then be rolled out to the entire Research Field Information, or, if desired, to the entire Helmholtz Association with high prospects of success and high efficiency.

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Update on Pilot Lab Exascale Earth System Modelling

Since 2019, around 30 scientists from 8 Helmholtz Centres have been working together to create Earth System Models (ESMs) that are fit for the next generation of supercomputers, i.e. ready for exascale. Recently, Martin Schultz from JSC, the coordinator of the Pilot Lab Exascale Earth System Modelling (PL-ExaESM), presented the background and rationale of this project and some recent results at the Center for Earth System Observation and Computational Analysis (CESOC). CESOC was established in 2021 to strengthen collaboration between Earth System scientists and computer scientists in the Rhineland region and to support Germany's successful bid to become a new host of the European Centre for Medium-Range Weather Forecasts (ECMWF). ECMWF pioneered a technology-oriented perspective on ESM development with its scalability programme, and this work has led to a European Centre of Excellence (ESiWACE) and a series of projects (ESCAPE). With PL-ExaESM, the Helmholtz Association has joined forces and strengthened the connection with leading ESM developers in Europe. The underlying concern of PL-ExaESM is the observation that new supercomputer technologies

present a disruptive change to more specialized and diverse computing and storage components. While scientific progress with ESMs in the past partly relied on the exponential growth of supercomputing resources due to miniaturization (Moore's law), it is no longer possible to simply run existing code on more processors. Instead, fundamentally new concepts must be developed to exploit the capabilities of accelerators such as GPUs and to optimize workflows and storage concepts. Furthermore, new algorithms and the embedding of machine learning techniques in ESM models and ESM output post-processing need to be explored. As ESM code represents some of the largest and most complex supercomputing applications, the analysis of ESM requirements and bottlenecks can also help in designing the supercomputing architectures of the future. PL-ExaESM has made substantial progress in all of these areas and has helped to build a new community of interdisciplinary researchers who will create the next generation of ESMs with enhanced resolution, better representations of physical processes, and a better user experience, thus contributing even more to the solving of society's grand challenges.

The PL-ExaESM project, which is funded by the Helmholtz Initiative and Networking Fund, runs until September 2022. Its main activities will then be continued under the umbrella of a Joint Lab. For further information, please visit <https://www.exaesm.de/>.

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Jülich CECAM Node Activities 2022

The Jülich CECAM node supports and runs workshops, tutorials, and internships within the international CECAM network, which consists of the CECAM headquarters in Switzerland and 17 nodes located in 10 countries in Europe and Israel. The network's calendar of activities had to be adjusted due to the pandemic, which made it difficult or impossible to organize on-site events. Although a large number of activities had to be postponed or cancelled during the first year of the pandemic, many workshops or tutorials could be held last year, either remotely or as hybrid events. This form of organization has brought some flexibility and offers hope that the planned activities for 2022 can go ahead as scheduled.

The next event will be the workshop "Recent Advances in Machine Learning Accelerated Molecular Dynamics", which will take place in Pisa on 16–18 March as a co-organized multi-node event. It continues a series of workshops on biomolecular simulations and aims to foster an exchange of ideas in the emerging field of machine learning techniques.

The workshop "Virtual Materials Design", planned for 18–21 July, will take place at KIT and reflects the activities and members of the Helmholtz Joint Laboratory Virtual Materials Design. A similar workshop was organized in July 2021 as a full online event, using the conference program gather.town. The large number of more than 200 participants encouraged the organizers to repeat the event in 2022.

On 12–16 September, the bi-annual tutorial "Atomistic Monte Carlo Simulations of Biomolecular Systems" will be organized at JSC. It will give a broad introduction to Monte Carlo methods ranging from basic to advanced, including Markov Chain Monte Carlo methods and generalized ensemble techniques. Participants will also gain hands-on practice of these methods on JSC's HPC systems.

Another multi-node event entitled "Ions, Membranes and Channels: Multiscale Simulations from Quantum to Coarse-Grain", organized by the French, Italian and UK nodes as well as Jülich, will take place on 27–29 October in Rome. This workshop, held in honour of Mike Klein, had to be postponed in 2020 due to the pandemic.

Finally, the regular annual event "International Guest Student Programme on Scientific Computing" is being organized for the timeframe 1 August – 7 October, for which a separate report will follow in due course.

While we are still optimistic that we will be able to organize the various events as on-site meetings, our experience from the last two years has shown that even remote or hybrid events can be efficiently organized, and therefore CECAM will continue to keep international networking active. Further information can be found at <https://fz-juelich.de/ias/jsc/cecam>.

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Calls for Computing Time Applications

The following synchronized calls for computing time applications were published on 17 January 2022. For all calls, the strict deadline for submitting proposals is 17:00 (CET) on 14 February 2022.

The Gauss Centre for Supercomputing (GCS) issued the 27th call for large-scale projects on Hawk at HLRS, SuperMUC-NG at LRZ, and JUWELS at JSC. Furthermore, researchers at German universities and publicly funded research institutions can now apply for regular GCS/NIC projects on the JUWELS Cluster and Booster modules as well as on the JURECA Booster module.

Researchers from all HGF institutions in the Research Field Earth and Environment together with their national cooperation partners outside HGF are invited to apply for resources on the ESM partition of JUWELS.

Finally, researchers from RWTH Aachen University and Forschungszentrum Jülich can submit applications for computing time on the JARA Partition – for the first time including time on the D-Wave Advantage™ quantum system operated by JSC within the Jülich UNified Infrastructure for Quantum computing (JUNIQU) – and for VSR projects.

For an overview over all calls and detailed information please visit

<https://www.fz-juelich.de/ias/jsc/computingtime>.

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