First European Exascale Supercomputer to Be Hosted in Jülich

The European High Performance Computing Joint Undertaking (EuroHPC JU) has made its decision: Forschungszentrum Jülich will be home to Europe's first exascale computer. The supercomputer is set to be the first in Europe to surpass the threshold of one trillion calculations per second (exaflops). The system will be acquired by the European supercomputing initiative EuroHPC JU. The exascale computer should help to solve important and urgent scientific questions regarding, for example, climate change, how to combat pandemics, and sustainable energy production, while also enabling the intensive use of artificial intelligence and the analysis of large data volumes.

The overall costs for the system amount to € 500 million. Of this total, € 250 million is being provided by EuroHPC JU and a further € 250 million in equal parts by the German Federal Ministry of Education and Research (BMBF) and the Ministry of Culture and Science of the State of North Rhine-Westphalia (MKW NRW). The Jülich Supercomputing Centre (JSC) had participated in the application procedure for this high-end supercomputer as a member of the Gauss Centre for Supercomputing (GCS), an association of Germany's three national supercomputing centres – JSC in Jülich, the High-Performance Computing Center Stuttgart (HLRS), and the Leibniz Supercomputing Centre (LRZ) in Garching.

The computer, which will be called JUPITER (short for "Joint Undertaking Pioneer for Innovative and Transformative Exascale Research"), will be installed as of 2023 in a specially designed building on the campus of Forschungszentrum Jülich and will be operated by JSC. Just like Jülich's current supercomputer JUWELS, JUPITER will be based on a dynamic, modular supercomputing architecture, which Forschungszentrum Jülich developed together with European and international partners in the EU's DEEP research projects.

In its basic configuration, JUPITER will have an enormously powerful booster module with highly efficient GPU-based computation accelerators. Massively parallel applications are accelerated by this booster in a similar way to a turbocharger, for example to calculate high-resolution climate models, develop new materials, simulate complex cell processes and energy systems, advance basic research, or train next-generation, computationally intensive machine-learning algorithms.

One major challenge is the energy that is required for such large computing power. The average power is anticipated to be up to 15 megawatts. JUPITER has been designed as a "green" supercomputer and will be powered by green electricity. The envisaged warm water cooling system should help to ensure that JUPITER achieves the highest efficiency values. At the same time, the cooling technology opens up the possibility of intelligently using the waste heat that is produced. For example, just like its predecessor system JUWELS, JUPITER is set to be connected to the new low-temperature network on the Forschungszentrum Jülich campus. Further potential applications for the waste heat from JUPITER are currently being investigated.

"The EuroHPC decision enables us to take this significant step towards exascale in cooperation with research and industry, scientific users, and funding agencies", states Prof. Dr. Dr. Thomas Lippert, head of JSC, proudly. "Immense challenges exist at various levels – both technical and financial. However, it is important to realize that we are talking about a machine from which the whole of society will benefit. From traffic optimization, autonomous driving, and environmental monitoring right up to digital twins: all these challenges are extremely calculation-intensive and are reliant on new technologies, many of which we can tap into with the modular exascale system."

Further information on the planned system and statements from representatives of the funding bodies and institutions involved can be found in the press release by Forschungszentrum Jülich.

Contact: **Prof. Thomas Lippert**

Two Quantum Computers for HPCQS

HPCQS, the four-year pan-European hybrid HPC/quantum pilot project, aims to develop, deploy, and coordinate a cloud-based European federated infrastructure. Two quantum computers, each controlling 100+ quantum bits (qubits), will be tightly integrated in two Tier-0 HPC systems: GENCI's Joliot-Curie, which is operated at CEA/TGCC, and the JUWELS modular supercomputer at the Jülich Supercomputing Centre (JSC). The seamless integration of quantum hardware with classical computing resources, creating a hybrid system, is an essential step towards utilizing the power of quantum computers to enable the first practical applications.

In order to reach these goals, GENCI and Forschungszentrum Jülich – with the support of the European High Performance Computing Joint Undertaking (EuroHPC JU) and the German Federal Ministry of Education and Research (BMBF) – launched a joint public procurement of innovative solutions (PPI) procedure to acquire two quantum simulators capable of controlling at least 100 qubits. This PPI resulted in the selection of the Fresnel analogue quantum simulator provided by French start-up PASQAL, which is based on the technology of neutral atoms arranged in 2D/3D arrays of optical tweezers and interacting in their Rydberg states. Each Fresnel simulator will be coupled with a Tier-0 system and act as a quantum accelerator for specific workloads in optimization, quantum chemistry, and machine learning.

One of the Fresnel quantum simulators will be installed during the second half of 2023 at the Jülich UNified Infrastructure for Quantum computing (JUNIQ) at Forschungszentrum Jülich. In the meantime, PASQAL will provide remote early access to their in-house Fresnel system in order to advance HPCQS' activities towards the deployment of a full hybrid software stack including cloud access, resource management of hybrid workloads, tools, and libraries, benchmarking and certification, and performance analysis.

"HPCQS is the ideal continuation of the plans and activities for hybrid quantum HPC computing that we have started in Germany with JUNIQ on a European level together with our excellent partners," explains Prof. Thomas Lippert from JSC. "With HPCQS, we are the first in the world to realize deep integration between HPC and quantum computing based on modular supercomputing, and are bringing Europe to the forefront of research with this innovative technology."

Contact: **Prof. Kristel Michielsen**

TOAR Database Infrastructure Certified by CoreTrustSeal

The Tropospheric Ozone Assessment Report (TOAR) Database Infrastructure developed and operated at JSC has been certified as a Trustworthy Data Repository by the CoreTrustSeal Standards and Certification Board. The certificate is valid for three years.

CoreTrustSeal is an international, community-based, non-governmental, and non-profit organization promoting sustainable and trustworthy data infrastructures. The certificate requires the infrastructure to provide open data and data management policies that call for the long-term storage and accessibility of data as a basis for data sharing. This has to be proven by complying with a set of 17 requirements concerning the background, organizational infrastructure, digital object management, and technology.

The TOAR Database Infrastructure contains one of the world's largest collections of near-surface air quality measurements and considers FAIR data principles as integral. A special feature of its data service is the on-demand processing and product generation of several air quality metrics directly from the underlying database. For the application for the CoreTrustSeal certification, the TOAR Database Infrastructure provided the necessary evidence through extensive documentation of the database, its structure, metadata, and processes, as well as the services offered.

Contact: **PD Dr. Martin Schultz**

NIC Excellence Project April 2022

The John von Neumann Institute for Computing (NIC) Peer Review Board regularly awards the title "NIC Excellence Project" to outstanding simulation projects. At its April meeting, the board decided to honour Prof. Jörg Schumacher (TU Ilmenau) for his project "Mesoscale convection: Numerical analysis of compressibility".

Turbulent convection flows in nature typically span a wide range of lengths and times, ranging from thousands of kilometres to centimetres and from days to seconds. In the intermediate mesoscale range, turbulent convection is often organized in nearly regular flow patterns that we observe, for example, as cloud streets in the atmosphere or as a honeycomb network of granules on the surface of the Sun. Of the several reasons for this order on the mesoscale, one specific aspect – the effect of compressibility – will be investigated in more detail in this project by means of direct numerical simulations. In compressible flows, the density of the fluid varies and gives rise to additional instabilities as well as new structures such as density jumps. Their influence on mesoscale patterns and heat transport will be clarified in the project. For more details, see https://go.fzj.de/2022-nic-exc-proj (in German).

Contact: **Dr. Alexander Trautmann**

New GCS Large-Scale Projects Started in May 2022

Twice a year, the Gauss Centre for Supercomputing (GCS) issues a call for large-scale projects on its petascale supercomputers – Hawk (HLRS), JUWELS (JSC), and SuperMUC-NG (LRZ). Projects are

classified as large-scale if they require at least 2 % of the systems' annual production in terms of estimated availability.

While computing time quantities were previously specified in core hours, the modularity of JUWELS requires the introduction of a new computing time unit. JSC currently specifies computing time based on the peak floating point operations per year (FLOP/a) of the computing devices (CPU or GPU) available to approved projects. Computing time on Hawk and SuperMUC-NG continues to be specified in core hours. Therefore, projects are only categorized as large-scale if they require at least 100 Mcore-h on Hawk, or 45 x 10^{21} FLOP/a on JUWELS, or 45 Mcore-h on SuperMUC-NG.

At the end of April, the GCS Peer Review Board decided to award the status of large-scale project to 17 projects from various scientific fields. In total, two projects were granted 1057 Mcore-h on Hawk, five projects were granted 295 x 10^{21} FLOP/a on JUWELS, and ten projects were granted 585 Mcore-h on SuperMUC-NG.

For more details of these projects, visit https://www.gauss-centre.eu/results/large-scale-projects/.

Contact: Dr. Alexander Trautmann

Gabriele Cavallaro Appointed Adjunct Associate Professor at University of Iceland

Dr.-Ing. Gabriele Cavallaro joined JSC in 2016 as deputy head of the High Productivity Data Processing research group led by Prof. Dr.-Ing. Morris Riedel. In 2022, he became head of the AI and Machine Learning (ML) for Remote Sensing (RS) Simulation and Data Lab, which bases its work and research activities at the intersection of remote sensing applications and parallel machine learning methods that can scale on advanced computing technologies such as high-performance computing (HPC) and quantum computing. His lab collaborates closely with the Simulation and Data Lab RS of the Icelandic HPC community (University of Iceland) and other international institutions in joint activities that include community support, research projects, and the organization of special sessions and tutorials at international conferences. Gabriele is also the Chair of the High-Performance and Disruptive Computing in Remote Sensing (HDCRS) Working Group of the IEEE Geoscience and Remote Sensing Society (GRSS), as well as a Visiting Professor at the Φ-Lab of the European Space Agency (ESA) in the context of the Quantum Computing for Earth Observation (QC4EO) initiative.

In June 2022, Gabriele was appointed Adjunct Associate Professor at the Faculty of Industrial Engineering, Mechanical Engineering and Computer Science, School of Engineering and Natural Sciences, University of Iceland. He will retain his position at JSC according to the Jülich model. The joint position will strengthen the existing collaborations with the University of Iceland, including lecturing and supervising students at different academic levels in topics that address large-scale remote sensing applications with high-performance and advanced ML methods.

JSC wishes Gabriele all the best for his new position.

Edoardo Di Napoli Distinguished as 2021 Outstanding Associate Editor

Dr. Edoardo Di Napoli from JSC was distinguished as a 2021 outstanding associate editor by *Frontiers in Applied Mathematics and Statistics* in recognition of his contributions to the journal. The journal especially wished to honour his dedication in ensuring a fair and constructive peer review and stated that his contributions further strengthen its Open Access model and philosophy. Edoardo started editing for this fairly new journal about two years ago. Congratulations!

Events

Introduction to parallel programming with MPI and OpenMP
Instructors: Benedikt Steinbusch, Thomas Breuer, JSC
Date: 9–13 August 2022, 09:00–16:30
Venue: online
https://go.fzj.de/2022-mpi-intro-2

For further events, talks, and training courses see https://fz-juelich.de/en/ias/jsc/events