JSC to Build New Quantum Computing Lab with NVIDIA and ParTec

NVIDIA, ParTec, and the Jülich Supercomputing Centre are establishing a new laboratory to explore hybrid quantum-classical computing based on the NVIDIA quantum computing platform. JSC will host the lab as part of the Jülich Unified Infrastructure for Quantum Computing (JUNIQ). The goal is to run high-performance, low-latency quantum-classical computing workloads. Currently, JUNIQ uses the JUWELS booster system with 3,744 NVIDIA A100 Tensor Core accelerators for its simulations.

The NVIDIA quantum computing platform enables tight integration of quantum and classical computing through the open-source CUDA Quantum programming model and the NVIDIA cuQuantum software development kit for first-class simulations. JSC plans to test the system incrementally and will use the NVIDIA CUDA Quantum programming model to program and integrate quantum processors into the modular Jülich Exascale super-computing architecture.

The partnership between NVIDIA, JSC, and ParTec (a hardware-agnostic system provider) enables the unifica-tion of quantum computing and GPU supercomputing. This collaboration will bring quantum-classical computing to a broader audience and take a major step toward the first quantum-accelerated supercomputer. Hybrid quantum-classical systems have the potential to solve complex problems that cannot be addressed by classical computing alone. This will give scientists and researchers access to powerful tools and resources to achieve breakthroughs in chemistry and materials sciences. The new laboratory could thus also drive scientific progress in many other disciplines and industries.

Contact: Prof. Kristel Michielsen

Driving the EU-Japan Digital Partnership: The HANAMI Project

The Jülich Supercomputing Centre is part of a newly formed consortium aiming to enhance collaborations between Europe and Japan around biomedical, materials science, and environmental applications which was recently awarded funding from the EuroHPC JU. The project, called HANAMI, brings together research teams representing excellence in HPC both in Europe and Japan. Key expertise will be pooled in pre-exa and exascale systems, and the research will support organizations and industrial stakeholders involved in the developing HPC technologies for extreme-scale architectures.

The project aims to port applications in the domains identified by the EU-Japan Digital Partnership on extreme-scale supercomputers and hybrid quantum HPC systems in Europe and in Japan. All partners in the consortium support the common objective to strengthen and improve the HPC ecosystem in Japan and Europe through the co-design of applications and sharing of information and expertise around HPC. HANAMI will pursue these objectives by: 1) creating a structure to enable and promote the exchange of Japanese and European researchers and application specialists in the consortium partner organizations; 2) developing the necessary skills in the era of HPC and quantum computing in computational science and computer science both in Europe and in Japan through training and skills development, including e.g. training students through internships and creating joint doctoral and postdocs positions; 3) designing a cooperation environ-ment that is sustainable and can also accommodate and fund cooperation activities of Japanese and European organizations in the future. JSC is contributing to these goals and actions in the application domains of biomedical and materials science. The HANAMI project will officially start on 1 January 2024 and last for 3 years.

Contact: Dr. Edoardo di Napoli

2nd Call for Microprojects in SDI-S Project

The Smart Data Innovation Services (SDI-S) project published its 2nd call for data-driven microprojects on 20 July 2023. JSC is participating in this call by offering experience and computational resources to German small and medium-sized enterprises (SMEs) in the healthcare sector. JSC's new research group "AI and ML for Healthcare" offers services in few-shot learning and highly

parallel hyperparameter tuning. Interested industry partners and research institutes can apply for these services until 20 September 2023 at: https://www.sdil.de/aktuelles/open-call/sdis-2/.

The SDI-S project is coordinated by the Karlsruhe Institute of Technology and brings together Forschungszentrum Jülich, Fraunhofer Gesellschaft, the German Research Centre for Artificial Intelligence (DFKI), SAP, IBM, and Software AG. The project, established in January 2023, receives funding from the Federal Ministry of Education and Research (BMBF) for two years with the aim of developing a service catalogue of expertise and computational power for the benefit of German SMEs without additional cost to these enterprises. For more details on SDI-S, visit https://www.sdil.de/services/.

Contact: Dr.-Ing. Chadi Barakat

JSC Hosted 2023 Helmholtz GPU Hackathon

In May, JSC hosted the 2023 Helmholtz GPU Hackathon, together with HZDR, HIDA, and OpenHackathons. The Helmholtz GPU Hackathons have been organized annually together with HZDR since 2016. This year, JSC hosted the event for the fourth time.

In the meeting rooms of PtJ, we welcomed about 80 participants for intensive three on-site days of analysing and improving GPU-enabled applications on the JSC supercomputers. Out of the nearly 20 teams who applied from a variety of domains and organizations – Helmholtz and beyond –10 were invited to the event. Each team was assigned two expert mentors, whom they met in the preceding virtual days of the Hackathon.

During the days on site, the teams profiled their applications, identified bottlenecks, and optimized data movement and hardware utilization as well as implemented new features and algorithms. In short meetings, they presented their statuses, progress, and persisting blockers. At the end of the event, summaries were given, in which most teams shared their (partial) successes in taming GPUs and their plans beyond the event.
Read more about the GPU Hackathon in the FZJ Blogs, and watch video statements from the participating teams at: https://go.fzj.de/blog-gpu-hackathon.

Contact: Dr. Andreas Herten

Retrospective on JUNIQ's Summer School on Quantum Information Processing

From 28 August to 1 September 2023, JUNIQ hosted the Summer School on Quantum Information Processing combining expert lectures with hands-on sessions. Twenty-four participants from academia and industry across Europe came to the Jülich Supercomputing Centre to study applications of quantum computing. Additionally, about 30 participants followed the lectures online.

The students got introductory lectures on gate-based quantum computing and quantum annealing, followed by theoretical concepts of state-of-the-art algorithms that they

had to use to solve their research problems during the hands-on part. Invited speakers including Viv Kendon from Glasgow and David DiVincenzo from Jülich, complemented the school with meta-perspectives on the evolution of quantum computing (QC) and gave an outlook on future challenges and research activities.

During the hands-on sessions, the students had to solve simplified research questions directly applying the lessons learned in the lectures. For this, they used JUNIQ's cloud-programming environment, from which they could access several QC resources using a unified programming interface. During the sessions, the students were supervised by several experts from JSC's research group Quantum Information Processing. In addition to the hands-on sessions, talks, and lectures, the students presented their own research to their peer group and experts in dedicated poster sessions. This encouraged the participants to create new research ideas, initiate future collaborations, and establish new networks.

We thank all attendees for their active participation and are looking forward to hosting another group of students at next year's summer school.

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News Concerning the MaTSE Trainees

At the end of August 2023, 23 mathematical and technical software developer (MaTSE) trainees, who started their vocational training in 2019, passed their final examinations. Despite the severe restrictions in place as a result of the coronavirus pandemic, such as basic operations mode at Forschungszentrum Jülich, working from home, and digital learning, the latest group of trainees achieved good results. Three of the trainees achieved the top grade "very good" and six the second-best grade "good". The best result was achieved by Marian Dederichs (INM-1), who achieved 94%. These newly graduated trainees increase the number of MaTSE trainees successfully trained at JSC (since 1964) to 1287.
All of the graduates decided to stay at Forschungszentrum Jülich. After graduating with a bachelor's degree in "Applied Mathematics and Computer Science", some of them will continue with the corresponding master's programme at Aachen University of Applied Sciences, Campus Jülich (FH Aachen).

On 1 September 2023, 29 new students began their bachelor's degree course in "Applied Mathematics and Computer Science" at FH Aachen (Jülich) in combination with MaTSE training at Forschungszentrum Jülich. Of these students, 26 will complete their training at various institutes at FZJ, while three students were placed with an external industrial partner. Together with these new trainees, we are proud to have recruited 1500 MaTSE/MaTA apprentices over the last 60 years.

Applications for the MaTSE training course starting in September 2024 are already being accepted. The curriculum and further information can be found at https://fz-juelich.de/matse.

Contact: Oliver Bücker