

JSC Participates in EuroHPC Pilot Projects

Last year, the European High-Performance Computing Joint Undertaking (EuroHPC JU) issued a call for proposals with two topics: “Advanced pilots towards the European exascale supercomputers” and “Pilot on quantum simulator”. Only three proposals in this call have now been chosen to be funded by EuroHPC and co-funded by the national entities of the partners involved as pilot projects: EUPILOT, EUPEX, and HPCQS. The Jülich Supercomputing Centre is proud to be a partner of all three projects and will also take on a leading role as coordinator of the HPCQS project.

While EUPILOT and EUPEX will integrate the two processor technologies built in the EPI project (accelerator and general purpose processor, respectively), HPCQS is devoted to the integration of a quantum computer into an HPC system. The experiences in these three pilots will be very valuable for the next-generation HPC and AI infrastructures in Europe. EUPILOT and HPCQS were launched on 1 December 2021 (see articles below), while EUPEX will launch in the first quarter of 2022.

The European PILOT: Pilot using Independent Local and Open Technologies

JSC is contributing to the project entitled “The European PILOT: Pilot using Independent Local and Open Technologies” (EUPILOT, or sometimes referred to as Pilot-2). The goal of EUPILOT is to create demonstrators of RISC-V-based accelerators.

The project is the first example of a pilot HPC ecosystem designed and manufactured entirely in Europe and is aimed at power-efficient exascale supercomputers. Within EUPILOT, the RISC-V-based accelerators created as part of the EPI project will be further developed into a full ecosystem. The project’s primary goal is to integrate both open source software and open and proprietary hardware into a pilot system, and demonstrate its viability for real-world applications. The project employs a co-design approach to enable libraries and applications for the platform and to improve performance and energy efficiency.

EUPILOT is coordinated by the Barcelona Supercomputing Center (BSC). Besides JSC, 19 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). EUPILOT was launched on 1 December 2021 and will run for three-and-a-half years with a total budget of € 30 million. Further information on the project will soon be available at <https://www.eupilot.eu>.

JSC’s main contributions to EUPILOT include porting key numerical libraries for the pilot system and providing feedback about architecture requirements as part of the co-design process. Optimizing the libraries for the platform will improve the RISC-V software stack to enable smooth transitions of targeted applications. 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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HPCQS Pioneers Federated Quantum Supercomputing in Europe

The new “High-Performance Computer and Quantum Simulator hybrid” (HPCQS) project aims to develop, deploy, and coordinate a European federated infrastructure, tightly integrating two quantum simulators that each control about 100+ qubits (quantum bits) in the Tier-0 HPC systems Joliot Curie of GENCI, operated at CEA/TGCC, and the JUWELS modular supercomputer at JSC. The seamless integration of quantum hardware with classical computing resources, thus creating a hybrid system, is an essential step towards utilizing the power of quantum computers to handle the first practical applications. At JSC, HPCQS is a logical continuation of the efforts driven by JUNIQ (the Jülich UNified Infrastructure for Quantum computing) to establish tight hybrid quantum HPC simulations.

The European High-Performance Computing Joint Undertaking (EuroHPC JU) has approved the

infrastructure project within the framework of its Research & Innovation (R&I) action “Advanced pilots towards the European exascale supercomputers”. HPCQS will receive a total budget of € 12 million over the next four years, which is provided by the EuroHPC JU and the six participating member states in equal measure. HPCQS will carry out a public procurement of innovative solutions (PPI) to implement the two 100+ qubit quantum simulators and launch an ambitious research programme on 1 December 2021. Prof. Kristel Michielsen from JSC, one of the five participating European HPC centres, is coordinating the project.

HPCQS will develop the programming platform for the quantum simulator. It is based on two European software developments: the Atos Quantum Learning Machine (QLM)™ and ParTec’s ParaStation Modulo™. Together, these technologies allow the deep, low-latency integration of quantum simulators into classical modular HPC systems as a first-of-its-kind realization. In addition, HPCQS will work on the deployment of a full hybrid software stack. It will include cloud access, resource management of hybrid workloads, tools and libraries, as well as benchmarking and certification/performance analysis. Engaging users in the co-design process will lead to prototype applications in machine learning and scientific simulations.

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Juwels Booster is the Fastest AI Supercomputer in Europe

A research team of AI consultants from JSC and the Karlsruhe Institute of Technology (KIT) succeeded in measuring the speed of AI applications running on the Juwels Booster as well as on the HoreKa (Hochleistungsrechner Karlsruhe) supercomputer. They were able to perform the fastest ever and most computationally intensive AI calculations in Europe. As a submission entry in the MLPerf Training HPC competition, they trained two machine learning (ML) models, utilizing the high performance of the NVIDIA A100 GPUs and the Infiniband network connection installed in both machines. On Juwels, they used up to 3072 GPUs and achieved an average computational performance of approximately 100 PFlop/s with automatic mixed precision.

The benchmark competitions are compute-intensive deep learning models. The Cosmoflow model predicts cosmological parameters from the outcome of cosmological simulations. DeepCam identifies regions of tropical storms in meteorological data. Training both models is quite data-intensive. The datasets (amounting to 8 terabytes and 5 terabytes) were stored in JSC’s file system in two large HDF5 files and the training algorithm read both files sequentially. The large main memory of the Juwels Booster ensures that it only needs to be read once. The training was performed using the ML framework PyTorch, which makes use of automatic mixed precision. The submission entry is a result of a collaboration between researchers from the Steinbuch Centre for

Computing at KIT within [Helmholtz AI](#), the cooperation unit of Helmholtz centres across Germany. Their AI consulting support will help to find new AI applications in science or to improve existing ones.

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Development Launched for EBRAINS HealthDataCloud

EBRAINS, the digital research infrastructure created by the European Human Brain Project (HBP), offers a range of resources to support brain and brain-inspired research. Large data science approaches to the brain, and to health in general, need to address an important challenge: All research needs to strictly protect privacy, and thus the freedom and rights of each individual, and to comply with the rules of the European General Data Protection Regulation (GDPR). To this end, EBRAINS will add a new service for sensitive medical brain data that is available to the scientific community – the EBRAINS HealthDataCloud. The project is coordinated by Europe’s largest university hospital, Charité – Universitätsmedizin Berlin, and is being provided with € 1 million in funding.

Over the next two years, a multinational team of academic and industrial partners in the HBP, including JSC, will develop a GDPR-compliant, federated research data ecosystem that enables neuroscience research consortia across Europe and beyond to work with sensitive neuroscience data originating from human subjects as well as defined routes for sharing the data and results. The EBRAINS HealthDataCloud will be based on the GDPR-compliant Virtual Research Environment (VRE) at the Charité, a product of the EU project Virtual Brain Cloud that is compatible with the EBRAINS infrastructure and provides a secure and scalable data platform for multi-institutional research teams. An important goal of the HealthDataCloud project is the federation of the platform and the integration of HPC centres such as JSC and other Fenix Infrastructure sites as satellite nodes for compute-intensive simulation and analysis workloads. For further information, please visit <https://www.healthdatacloud.eu/>.

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Tuning & Scaling Workshops for Juwels Booster Module

Two hands-on workshops early in 2022 will be dedicated to analysing, tuning, and scaling the HPC application codes of JSC users on the quad NVIDIA A100 GPU compute nodes of the Juwels Booster module.

The first workshop to be held will be the 41st VI-HPS Tuning Workshop organized by JSC and RWTH Aachen University from 7 to 11 February 2022. It will provide an introduction to performance measurement

and analysis of application codes executed on the JUWELS Booster module, particularly multi-node/multi-GPU application executions. Based on examples provided, participants will be given support to help them progress to working with their own application codes. Applicants are therefore encouraged to prepare suitable application test cases. Detailed information can be found at <https://www.vi-hps.org/training/tws/tw41.html>.

From 7 to 11 March 2022, a Tuning and Scaling Workshop will then take place dedicated to improving performance and the scaling of applications using multiple GPUs, with opportunities to scale to the full complement of over 3600 GPUs connected by the high-speed InfiniBand network in the JUWELS Booster module. Applicants for this workshop should be able to build and run their codes correctly on multiple quad-GPU nodes of the JUWELS Booster module and demonstrate the potential for improved performance and scalability – expertise that can be obtained from the preceding VI-HPS Tuning Workshop. Detailed information can be found at <https://go.fzj.de/2022-iwb>.

Both workshops will present state-of-the-art tools and techniques for efficient multi-GPU computing, combined with interactive hands-on sessions, with instructors and mentors from JSC, NVIDIA, and VI-HPS partners. They will be held as online training events requiring separate registration for those interested in taking part in both.

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NIC Excellence Project October 2021

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. Kurt Kremer (Max Planck Institute for Polymer Research) for his project entitled "Bridging drastically coarse-grained and microscopic descriptions in hierarchical modeling of Soft Matter. Application: non-linear viscoelasticity of polymer melts".

This project investigates molecular-level mechanisms underlying polymer rheology for strong deformations, which presents tremendous challenges for basic science and industrial processing. Prof. Kremer and his group study these mechanisms by emulating rheological experiments with molecular dynamics simulations. The computational experiments must start from equilibrated samples of molten polymers that are much longer than the entanglement length – the average number of monomers between two consecutive topological constraints on chain motion. To this end, a novel strategy has been developed based on the hierarchical fine-graining of polymer melts. This backmapping method proceeds from blob-based chains down to the microscopic description and is applicable to generic polymer models (bead-spring) as well as actual materials, for example polystyrene. For more details, please visit <http://www.john-von-neumann-institut.de/nic/kremer>.

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JSC Contributes to Open Access Publication of the Month

A major contemporary challenge faced by society is the transition from an energy system based on fossil fuels and carbon to a sustainable and CO₂-neutral energy system primarily driven by renewable energy sources. JSC has dedicated intensive efforts to the subject of energy systems modeling in collaboration with various scientific partners within and outside Forschungszentrum Jülich (FZJ). In this context, the consortium of the BMWi-funded research project METIS, led by IEK-3, recently published "A modeler's guide to handle complexity in energy systems optimization" (DOI: [10.1016/j.adapen.2021.100063](https://doi.org/10.1016/j.adapen.2021.100063)). This publication was selected as the Open Access Publication of the Month by the Central Library of FZJ in October. JSC is proud and happy to be part of this important scientific endeavour and looks forward to making further contributions to this ongoing task.

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2021 End-of-Year Colloquium at JSC

Date: Thursday, 16 December 2021, 14:00–16:45

Venue: online via Zoom

Info: <https://fz-juelich.de/ias/jsc/events/eoy-2021>

- 14:00 Thomas Lippert: *Welcome*
- 14:20 Sandra Diaz: *Simulating and analyzing the structural plasticity of the brain using HPC*
- 14:45 Zahra Chitgar: *Zigzagging towards X-ray vision*
- 15:10 Stefan Kesselheim: *AI on Europe's Largest Supercomputer*
- 15:35 Alexander Schug: *Using (really) big computers to simulate life*
- 16:00 Holger Gohlke: *Enzyme function - much to understand, optimize, and discover*
- 16:25 Thomas Lippert: *The Story of a Theoretician Who Went Forth to Optimize Supercomputing*

Anyone interested is cordially invited to participate in this colloquium.

Events

AI Bootcamp for Science

Instructors: Representatives from NVIDIA

Date: 1–2 February 2022, 09:00–12:30

Venue: online

<https://go.fzj.de/2022-ai-bootcamp>

41st VI-HPS Tuning Workshop

Instructors: JSC employees, members of the VI-HPS collaboration

Date: 7-11 February 2022, 09:00-16:00

Venue: online

<https://go.fzj.de/2022-vi-hps>

For further events, talks, and training courses, please visit <https://fz-juelich.de/ias/jsc/events>