NRW Research Minister Visited JSC on Open Day

The Open Day event ("Tag der Neugier") on 21 August at Forschungszentrum Jülich was a great success, attracting around 20,000 visitors. The JSC was also very well attended. At times, longer queues formed in front of the entrance to the main building and the JUNIQ building with the new quantum annealer JUPSI.

As a special guest, the JSC welcomed the new Minister for Culture and Science of North Rhine-Westphalia, Ms. Ina Brandes. On her tour through the research centre, accompanied by the Board of Directors as well as several politicians from the region, she was welcomed to the JSC by Prof. Kristel Michielsen, who gave a short introduction to the institute, the supercomputers, and the location of the future exascale computer JUPITER. The minister was also informed of JSC activities in the realm of quantum computing and the 3D visualization of plant root growth. She visibly enjoyed the photos of the morning reception, which were distorted with the help of artificial intelligence. Despite the short visit, Ms. Brandes was impressed by the variety of activities.

Contact: Dr. Sabine Höfler-Thierfeldt

New interTwin Project to Provide Interdisciplinary Open-Source Digital Twin Engine for Science

The Jülich Supercomputing Centre is participating in the new European project interTwin. The project has 31 partners and is coordinated by the EGI foundation. It aims at co-designing and implementing the prototype of an interdisciplinary digital twin engine, which provides a common approach on digital twins across a wide spectrum of academic disciplines. This includes artificial intelligence (AI) workflows making use of cutting-edge high-performance computing (HPC) architectures. The project has been granted a total budget of € 12.4 million for its duration of 36 months by the European Commission. It is funded within the European Union Horizon Europe Programme – Grant Agreement Number 101058386.

Modern computing workflows require capabilities of handling compute-intensive solvers along with large and fast data processing. Hence, there is an increasing demand for ready-to-use tools that are able to process and run these complex AI-based workflows in heterogeneous HPC environments. In interTwin, the ambition is to develop a digital twin blueprint architecture and an interdisciplinary digital twin engine as an open-source platform to provide generic and tailored software components for modelling and simulation and to integrate application-specific digital twins.

JSC will provide cloud computing resources that will be co-located with HPC resources and, in particular, integrated with large-capacity file systems at JSC. Furthermore, JSC is collaborating with the European Organization for Nuclear Research (CERN) on the development of an AI workflow and method lifecycle to design and develop generalizable and widely applicable AI workflows.

Contact: Dr. Andreas Lintermann

LOKI Project Launched – Local Early Warning System for Control of Infection Outbreaks

The LOKI pilot project was launched on 1 July 2022 under the leadership of the Helmholtz Centre for Infection Research (HZI) and in collaboration with the Academy of Public Health, the CISPA Helmholtz Center for Information Security, Forschungszentrum Jülich (FZJ), the German Aerospace Center (DLR), and the Helmholtz Centre for Environmental Research (UFZ). The goal is to provide health authorities with a local early warning system for epidemiologically relevant outbreaks of infection in the future – in a customizable and practical manner.

Since the pooling of data in the health sector is subject to strict requirements concerning the protection of private data, privacy and IT security are priorities in the project. The data thus obtained will be supplemented with publicly available data, and then entered into an automated modelling process.

The huge amounts of data will be fed into various equation-based and agent-based computer models that will be designed in LOKI. High-performance computers can then be used to make detailed predictions about how the outbreak might develop locally and what effect the measures taken might have.

To this end, the Jülich Supercomputing Centre is developing a secure cloud infrastructure, interfaces for connection to high-performance computing, and customized, highly automated tools for real-time analysis of infection events using artificial intelligence methods.

Contact: **Jens Henrik Göbbert**, **Stefan Kesselheim**

Advanced Computing Architectures (ACA) Pilot Project Paving the Way Towards Jülich Research in Neuromorphic Computing

Researchers from Forschungszentrum Jülich, RWTH Aachen University, the University of Manchester, and Heidelberg University came together in mid-September at Burg Obbendorf near Jülich for a final meeting of the project "Advanced Computing Architectures (ACA): towards multi-scale natural-density neuromorphic computing", which ends in November. Funded by the Helmholtz Association, ACA is a pilot project with the long-term goal of building a computer system to enable the simulation of biological learning processes in time-lapse in order to better understand learning and brain development.

During the four-year project period, the foundation was laid for future developments of architectures specifically tailored to neuroscience simulations. Ideally, such neuromorphic accelerator architectures could in the future be coupled to the Jülich modular supercomputing infrastructure. Almost 30 peer-reviewed articles have resulted from the interdisciplinary ACA project. For example, a publication on connectivity concepts in neural network modelling, which can guide the implementation of connection routines in neuromorphic hardware systems, appeared in *PLOS Computational Biology* (DOI:10.1371/journal.pcbi.1010086), while another publication on a system-on-chip (SoC) based approach for a hybrid software-hardware neuromorphic compute node architecture appeared in *Frontiers in Neuroscience* (DOI:10.3389/fninf.2022.884033). The researchers also succeeded in simulating a neuronal network consisting of 80,000 neurons connected via 300 million synapses at a previously unattainable speed. For their implementation, they used a prototype of IBM's INC-3000 FPGA-based "neural" supercomputer (*Frontiers in Neuroscience,* DOI:10.3389/fnins.2021.728460). These publications will form the basis for future research in this field at Jülich.

Contact: **Guido Trensch**

JURECA Evaluation Platforms

JURECA-DC was recently extended with three additional modules for evaluation and testing in preparation for upcoming procurements.

One of the modules consists of two nodes with four AMD Instinct MI250 GPUs each. This is the same GPU generation which broke the Exascale barrier with Frontier, featuring up to 90 teraflops performance in FP64 (double-precision floating-point) while only requiring a TDP (thermal design power) of 560 Watts. The nodes have two AMD EPYC 7443 Milan CPUs and 512 GB main memory. Each GPU has 128 GB device memory and is built as a multi-chip module (MCM) with two GPU chips contained in each MI250 device package. The ROCm software stack is available on these nodes. This hardware and software combination provides the ability to evaluate the current AMD GPU platform, the successor of which might be of interest for future, bigger systems at JSC.

Two NVIDIA Arm HPC Developer Kit nodes build another module. Each node has one Ampere Altra Q80-30 CPU, an 80-core ARM CPU with a low TDP of 210 W. 512 GB of main memory are available. Two NVIDIA A100 PCIe 40 GB GPUs are installed in each node. This PCIe version of the A100 has a lower TDP of 250 W compared to the 400 W of the versions in JURECA-DC and JUWELS Booster. A full ARM software stack is currently being developed, and first software modules are available via EasyBuild. We invite everyone interested in the ARM CPU architecture to test these nodes, given the possible future HPC CPUs NVIDIA Grace and SiPearl Rhea.

Another prominent extension is a Graphcore IPU-POD4 consisting of one access server and four GC200 IPUs containing 5888 IPU cores. The system is a hardware especially developed for AI workloads. It can provide 0.999 petaflops AI (FP16.16, half-precision) or 0.2497 petaflops FP32 (single-precision) performance. Applications can make use of the IPUs through the Graphcore Poplar SDK or one of several ML frameworks that have been extended with Graphcore plugins, such as TensorFlow or PyTorch.

All systems have been added to the official JURECA documentation with additional information on how to access and use them. If you are interested, please send an informal application.

Contact: **Dr. Andreas Herten**, **Benedikt von St. Vieth**

"Dispatch" Renamed as "Office for User Services"

We would like to inform readers that JSC has introduced an "Office for User Services". Our user service team, continuing all services of the team formerly known as "Dispatch", is responsible for HPC system user administration and it supports users wishing to access the supercomputers. The service team is additionally responsible for applications to services at Forschungszentrum Jülich, such as database accounts, WLAN, and external access to JuNet. Furthermore, the service team acts as a registration office for digital certificates.

Please also note our new email address user-services.jsc@fz-juelich.de.

Contact: Christa Dohmen

Third Virtual PRACE Summer of HPC at JSC

The Summer of HPC (SoHPC) programme celebrated its ten-year anniversary. In 2022, the programme allowed 29 university students from all scientific disciplines to spend two months working on-site or remotely with PRACE partner organizations. In addition to allowing students to work on research projects in a multidisciplinary and international environment, the aim of the SoHPC programme is to promote and disseminate scientific culture among the upcoming generation of researchers, encouraging the students participating in the programme to become the computational scientists of tomorrow. Furthermore, through the participants' sharing of their experiences in blog posts and video presentations, the programme aims to ensure that the students themselves become ambassadors for supercomputing at their respective institutions.

This year, three students – Ignacio Encinas Rubio (Spain), Christopher Kirwan (Ireland), and Apostolos Giannousas (Greece) – joined JSC remotely for the summer to gain first-hand experience in day-to-day research. After an online training week for all students hosted by University of Ljubljana, the three students teamed up and started working on their assigned projects at JSC.

Ignacio was supervised by Ivo Kabadshow and worked on efficiently parallelizing the fast multipole method with MPI, while Christopher and Apostolos were supervised by Marcel Rodekamp and dealt with Kokkos for high-performance quantum fields. They produced a report and two video presentations that can be found at https://youtu.be/ehETBjaULX0 and at https://youtu.be/Wpa1UNinWt4.

Contact: Dr. Ivo Kabadshow

News Concerning the MaTSE Trainees

At the end of August 2022, 31 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, working from home, and digital learning, the latest group of trainees achieved good results. Four of the trainees achieved the top grade "very good" and twelve were awarded the second-best grade "good". The best result was achieved by Benjamin Papajewski (ZEA-2), who achieved 94%. These newly graduated trainees increase the number of MaTSE trainees successfully trained at JSC (since 1964) to 1264.

Twenty-seven 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 2022, 25 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, 23 will complete their training at various institutes at FZJ, while two students were placed with an external industrial partner. The planned duration of the vocational training and the combined studies is three years.

Applications for the MaTSE training course starting in September 2023 are already being accepted. The curriculum and further information can be found at https://fz-juelich.de/matse.

Contact: Oliver Bücker

Events

Einführung in Python
Instructors: Martin Lischewski, Matthias Richerzhagen, Sebastian Linner, JSC
Date: 17–19 October 2022, 08:30–16:30
Venue: online
https://go.fzj.de/2022-python-2

Directive-based GPU programming with OpenACC
Instructors: Dr. Andreas Herten, Dr. Thorsten Hater, Dr. Kaveh Haghighi-Mood, JSC; Jiri Kraus, Markus Hrywniak, NVIDIA
Date: 26–28 October 2022, 09:00–13:00
Venue: online
https://go.fzj.de/2022-openacc

Software Development in Science
Instructors: Guido Trensch, Wouter Klijn, JSC
Date: 15–17 November 2022, 09:00–14:00
Venue: online
https://go.fzj.de/2022-sw-devel

Introduction to Supercomputing at JSC - Theory & Practice
Instructors: JSC employees, representatives of Atos, Intel and ParTec
Date: 21–24 November 2022, 09:00–17:00
Venue: online
https://go.fzj.de/2022-sc-2

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