Open Day at JSC

Forschungszentrum Jülich cordially invites the public to its Open Day event ("Tag der Neugier") on Sunday, **21 August 2022**. JSC will be open to visitors from 10:00 to 17:00 on the day, giving them the opportunity to take a look at the supercomputers, join guided tours of the new quantum computer JUPSI, and learn about how 3D visualisation is used in science. Special activities on the day include the "Style yourself with AI" game and the supercomputer simulator SuperResi. Young programmers also have the chance to learn their first programming steps with the "Fox in a labyrinth" exercise.

Our education team will be on hand to inform visitors about opportunities to train as a mathematical-technical software developer (MaTSE) and also about bachelor's and master's courses in Applied Mathematics and Computer Science. Furthermore, one of the questions in the ever-popular research rally for children will be about JSC's quantum computer. For detailed information on JSC's Open Day activities, see https://go.fzj.de/2022-tdn-jsc.
We look forward to seeing you there!

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Calls for Computing Time Applications in July/August

The following synchronized calls for computing time applications were published on 11 July 2022. For all calls, the strict deadline for submitting proposals is 17:00 (CEST) on **15 August 2022**.

The Gauss Centre for Supercomputing (GCS) issued the 28th 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.

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 – including time on the D-Wave Advantage™ quantum system operated by JSC within the Jülich UNified Infrastructure for Quantum computing (JUNIQ) facility – and for VSR projects.

For more detailed information and an overview of all calls, please visit the dedicated web page: "Apply for computing time".

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NIC Symposium 2022

The 11th NIC Symposium will be held at Forschungszentrum Jülich from 29 to 30 September 2022. The talks will inform a broad audience of scientists and interested members of the public about the activities of the John von Neumann Institute for Computing (NIC) and the results obtained in the last two years by research projects supported by the NIC on the supercomputer JUWELS and the JURECA Booster at Jülich.

Talks by invited speakers and a poster session will cover topics in the fields of astrophysics, biophysics, chemistry, elementary particle physics, condensed matter, materials science, soft matter science, Earth and environmental research, fluid mechanics, plasma physics, and computer science.

A comprehensive conference proceedings volume will also be published to accompany the event. It will cover an even wider range of projects than will be presented during the talks. The detailed programme and the registration form are available on the NIC Symposium homepage.

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CECAM School "Atomistic Monte Carlo Simulations of Bio-molecular Systems"

From 12 to 16 September 2022, JSC will host the CECAM school "Atomistic Monte Carlo Simulations of Bio-molecular Systems" organized by the Simulation and Data

Laboratory (SDL) Biology. Participants will be given an in-depth introduction to the theory and practice of Markov chain Monte Carlo (MCMC) methods as applied to atomistic simulations of proteins and other biomolecules. These ensemble methods offer a computationally efficient alternative to molecular dynamics simulations, in particular for studying processes with long time scales such as protein folding and peptide aggregation.

In contrast to the numerous training courses available for molecular dynamics, students rarely gain useful exposure to Monte Carlo (MC) techniques. CECAM (Centre Européen de Calcul Atomique et Moléculaire) is funding this five-day tutorial for the fourth time to address this very issue. The open-source protein folding and aggregation package ProFASi developed at the SDL Biology will be used as a demonstration tool for the highly transferable MC techniques.

Participants will have access to JSC's supercomputers for realistic tests of advanced parallel simulation techniques such as replica exchange MC or Wang-Landau. A particular focus of the course is the analysis and interpretation of MCMC simulations. The school will take place online and places are still available for any interested researchers. Detailed information about the tutorial content can be found on the CECAM school web page.

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10-Year Anniversary Workshop of NVIDIA Application Lab at Jülich

At ISC 2012, JSC and NVIDIA signed a collaboration agreement to enable and optimize scientific applications for upcoming GPU-based systems; the NVIDIA Application Lab was then founded at Jülich. Almost 10 years and about 5000 NVIDIA GPUs later, a workshop was held on 21 and 22 June 2022 to celebrate this anniversary and look back on the last 10 years of the lab.

A number of application developers with whom the Application Lab has collaborated over the years presented past developments, recent challenges, and future plans. In addition, two hardware-related talks were held, focusing on JSC's GPU installations (most importantly the JUWELS Booster) and NVIDIA's new Hopper H100 GPU processor.

The application presentations included, for example, a report about the GPU activities with JUQCS, the Jülich Universal Quantum Computer Simulator. This application is accelerated with CUDA Fortran and is able to utilize more than 2000 GPUs of the JUWELS Booster with excellent scaling and complex communication patterns. Another example is MPTRAC, an application developed in the SDL Climate Science. The application is accelerated with OpenACC and developers are currently investigating methods to deal with the large input data sets. In a talk about the fluid dynamics simulation D2Q37, a developer from the University of Ferrara/INFN Ferrara presented recent advanced transporting GPU optimizations to FPGA-based systems. D2Q37 had already been presented during the first Application Lab Workshop 10 years ago. At that time, the GPU acceleration had just started.

Lab colleagues from NVIDIA presented the new H100 GPU in detail, which introduces features such as multiprocessor clusters. Such a cluster has as many multiprocessors as an entire K20X GPU had 10 years ago – now with much more performance per multiprocessor. More information on the workshop can be found in the blog post.

Since the founding of the lab, more than 50 GPU-related activities and training courses were hosted (e.g. programming courses, hackathons, porting workshops, conference tutorials) and collaborations with various application developers were pursued. The intensive preparatory work of this lab and the experience gained in these 10 years provide an excellent basis for making applications fit for the upcoming GPU-based exascale system JUPITER.

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JuWinHPC: Jülich Women in HPC

Why are there not more women working in HPC? What started with this simple question resulted in the powerful international initiative "Women in High Performance Computing" (WHPC: https://womeninhpc.org). The members of this network are working for more equality, diversity, and inclusion in the HPC community. The initiative is active at conferences such as SC and ISC, offers workshops and mentoring programmes, and aims to raise more awareness in the HPC community with the slogan "diversity creates a stronger HPC community".

In early 2018, WHPC started with a number of groups and organizations committed to WHPC's vision and the mission to develop a programme for local chapters and affiliates. On five continents, many institutions and organizations (such as PRACE) are already working together with WHPC. While there are already several chapters in the USA, only a few have been established in Europe so far.

A team of local WHPC members recently started the process of establishing a local WHPC chapter at Forschungszentrum Jülich, the "Jülich Women in HPC" (JuWinHPC). The group's main goal is to strengthen the local community of women involved in HPC. On 28 July, JuWinHPC held its kick-off meeting as the first of a series of regular informal meetings. While the members of the chapter can use the meetings to meet new colleagues or to strengthen existing contacts, the founders are already working on further tasks behind the scenes. They aim to gain a better understanding of the gender imbalance and ensure that women in the field are more visible.

Although the network was founded by women, anyone interested in the topic of equal opportunities is welcome to join. More information can be found at https://fz-juelich.de/en/ias/jsc/juwinhpc.

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