High-Tech Base for the European Exascale Supercomputer JUPITER

Forschungszentrum Jülich and Eviden (Atos Group) have signed a contract for the delivery of a modular data centre (MDC) for the supercomputer JUPITER, procured by the European High Performance Computing Joint Undertaking (EuroHPC JU). JUPITER will be the first supercomputer in Europe with a performance of more than 1 ExaFlop/s and designed for simulations as well as large-scale AI applications in science and industry that require maximum computing power. The Jülich Supercomputing Centre (JSC) is taking a completely new approach in order to build a correspondingly powerful new data centre by the time JUPITER is scheduled to go into operation in autumn 2024. The data centre will be built as a modular high-performance centre (modular data centre, MDC) consisting of around 50 container modules across an area of over 2,300 square metres. The advantages of the concept include significantly shorter planning and set-up times as well as reduced construction and operating costs. Moreover, the power supply and cooling infrastructure can be flexibly adapted to new requirements in future thanks to the consistently modular design. The MDC is being financed by the Federal Ministry of Education and Research (BMBF). Furthermore, BMBF and the Ministry of Culture and Science of the State of North Rhine-Westphalia (MKW NRW) will provide funding in equal measure for the technical equipment installed in the centre.

More information: https://go.fzj.de/mdc-fuer-jupiter

Contact: jupiter@fz-juelich.de

JUPITER Research and Early Access Program (JUREAP) Has Officially Started

The EuroHPC JU supercomputer JUPITER, hosted at JSC, will come online as the first European exascale supercomputer in 2024. To rapidly enable excellent science and maximize the impact of JUPITER as well as enable a smooth start-up for hard- and software, JSC runs the JUPITER Research and Early Access Program (JUREAP). JUREAP starts with a Scalability and Performance Evaluation Phase (SPEP). During SPEP,

applications will be evaluated for their technical potential towards exascale-size simulations in collaboration between JUREAP researchers and domain scientists.

SPEP has opened on 15 January 2024 and has no formal prerequisite for applicants. However, the application needs to show a potential for scientific large-scale cases. The next phases of JUREAP will focus on performance optimization and (large-scale) deployment on JUPITER. Successful participation in SPEP is a prerequisite to continue in JUREAP and prepare for early science on the system. We strongly encourage interested JUPITER users to participate in SPEP and apply in January.

More information and the link to the application portal are available online.

Contact: jureap@fz-juelich.de

LOFAR Radio Telescope Becomes Consortium for European Research Infrastructure (ERIC)

The Low Frequency Array (LOFAR) is the world's largest radio telescope for the reception of short and ultrashort radio waves. LOFAR was previously organized as a Dutch foundation and is now being transformed into an international legal form: a consortium for a European research infrastructure. The European Commission decided to set up LOFAR as a European Research Infrastructure Consortium (ERIC) due to the Europe-wide significance of the radio telescope. LOFAR ERIC was officially established at the first meeting of the LOFAR ERIC Council on 22 January 2024.

The Jülich Supercomputing Centre has been involved in LOFAR in a variety of ways since 2009. It not only houses and operates the German part of the extensive LOFAR archive, which is the largest radio astronomy archive in Germany, but is also co-operator of the station in front of the Daubenrath entrance southeast of the campus and manages central network activities within the German LOFAR consortium.

LOFAR ERIC will significantly modernize the radio telescope's distributed infrastructure and serve the astronomy community with a cutting-edge suite of observing and data processing capabilities.

More information can be found in the press release.

Contact: Cristina Manzano, Dr. Arpad Miskolczi

Awards for Bachelor's and Master's Students

On 1 December 2023, the best students of the last two years received the badge of honor (Ehrenplakette) of the Aachen University of Applied Sciences (FH Aachen). In a ceremony at Aachen's historic town hall, Maximilian Heuwes (PGI-JCNS-TA) and René Noffke (INM-5) as the best graduates from the bachelor's course Angewandte Mathematik und Informatik (applied mathematics and computer science), and Björn Müller (JSC) and Alexander Sommer (PTJ-SPF) as the best graduates from the consecutive master's course were honoured.

Impressions of the event are in the press release of FH Aachen.

Contact: Oliver Bücker

Using MATLAB on JSC Supercomputers

In cooperation with MathWorks, the JSC has made the MATLAB/SIMULINK software and additional products (including licenses) available on its HPC systems for non-commercial academic research since several months.

In the first "MATLAB for HPC" workshop in November 2023 about parallel computing with large computing resources, the JSC welcomed experts from MathWorks who provided detailed information about submitting MATLAB jobs to the HPC clusters, code optimisation and best practices. Similar workshops will again be organised in the future; more details will be announced timely on our JSC events page.

Access to MATLAB can be requested online by any user of the JSC's HPC systems in the section "Software" of the JuDoor Portal, where accounts, projects and resources at JSC are managed.

More information about the availability of MATLAB at JSC can be found here.

Contact: Jens Henrik Göbbert, Rajalekshmi Deepu

JuRSE Website Released

The RSE team at JSC has released a new website on the topic of research software engineering (RSE), containing information about the new JuRSE community at FZJ, the topic of RSE itself, useful tools and resources for the everyday application of RSE. Together with their Forschungszentrum-internal partners at R, UE and ZB, the team now provides a one-stop information source for everyone interested in developing software in science, from students and researchers to decision makers and funding bodies. This includes three mission statements on what the team believes are crucial steps towards establishing RSE on campus, within Helmholtz Information and in Germany.

JuRSE is an FZJ-wide initiative working to raise awareness, increase visibility and improve good practice for RSE. The initiative brings together different skills, knowledge and passion to support Research Software Engineering and Research Software Engineers from all disciplines and all career levels. The online and in-person JuRSE community is for all FZJ employees who are involved in the practice of Research Software Engineering. JuRSE aims to provide the community with the ability to share knowledge, make connections, build resources and continue their personal professional development.

The newly created website and the large variety of information it provides are a first step toward this goal. Join the community by signing up to the mailing list on the website.

Contact: Claire Wyatt

Advanced molecular simulations on JUWELS Booster pave the way for future HIV-1 treatments

The global HIV-1 pandemic, with over 40 million infections, illustrates the virus's remarkable adaptation to humans. It originated from simian immunodeficiency viruses (SIV) in chimpanzees and gorillas, with HIV-1 M being the pandemic strain. There are other non-pandemic strains, HIV-1 N, O, and P, found in a few West African individuals.

Recent research by Prof. Dr. Holger Gohlke (IBG-4, Forschungszentrum Jülich and Heinrich Heine University Düsseldorf) and Prof. Dr. Carsten Münk (University Hospital Düsseldorf) uncovered a new understanding of how HIV-1 M adapts to human cells. Human cells defend against retroviruses, like SIV, using the TRIM5α protein. However, HIV-1 M avoids this defense by binding to another protein, cyclophilin A, a trans-cis-isomerase, which suppresses TRIM5α binding.

For this, computationally intense umbrella sampling molecular dynamics simulations of HIV-capsid protein/cyclophilin A complexes were performed on the JUWELS Booster module, exploiting the excellent performance of the AMBER molecular simulation code on GPUs. Followed by configurational free energy computations, these computations indicated that capsid residue 88 can affect trans-to-cis isomerization patterns on the capsids of the tested viruses. These differential CYPA usages by pandemic and non-pandemic HIV-1 suggest that the enzymatic activity of CYPA on the viral core might be important for its protective function against human TRIM5α.

The study identifies a potential vulnerability in HIV-1, offering hope for new drugs. By suppressing the binding of cyclophilin A to the virus, researchers may develop

drugs to combat HIV-1. Published in "The Proceedings of the National Academy of Sciences (PNAS)," this study paves the way for future advancements in HIV-1 treatment.

Publication:
https://www.pnas.org/doi/10.1073/pnas.2306374120

Contact: Prof. Holger Gohlke

Destination Earth Use Case For Air Quality

Together with the Institute of Energy and Climate Research (IEK-8), JSC is developing an interactive web application to run custom-tailored numerical and machine learning simulations to forecast air quality over Europe. In a contract with the European Centre for Medium-Range Weather Forecasting (ECMWF), a demonstrator is under development that runs on a virtual machine on the JSC cloud and uses JURECA-DC resources to run simulations with the EURAD-IM regional chemistry transport model or the MLAir machine learning tool. The German Umweltbundesamt and North Rhine-Westphalia's LANUV act as core users and have provided valuable feedback on the design and functionality of this application. We make use of JSC's UNICORE software to establish secure and efficient connections between cloud and supercomputer. First trial runs of some system components on the EuroHPC system LUMI at CSC, Finland have also been performed. Ultimately, this application shall become part of the Destination Earth digital twin on extreme weather.

More information about this use case can be found on the Destination Earth website.

Contact: Sabine Schröder

EBRAINS RI secures funding for a new phase of digital neuroscience

The European Commission has signed the grant agreement providing EBRAINS 2.0, an EU co-funded collaborative research infrastructure (RI), with € 38 million until 2026. Over the next three years, the EBRAINS RI will continue to develop tools and services to widely serve research communities in neuroscience, brain medicine and brain-inspired technologies. Developed as a legacy of the Human Brain Project, EBRAINS is a digital ecosystem where researchers, clinicians, and experts converge to explore the complexity of the brain at various scales and to derive therefrom new solutions for brain medicine and technology.

The new project will foster the development and provision of the infrastructure's research technologies to the scientific community. It aims to establish a new standard for brain atlases, gather and connect multimodal neuroscientific and clinical data, and push forward the development of digital twin approaches.

The project involves 59 partner institutions from 16 European countries, including the JSC and the Institute of Neuroscience and Medicine (INM) of Forschungszentrum

Jülich. The project is coordinated by the EBRAINS AISBL, a non-profit organisation founded in Brussels during the Human Brain Project, and has started in January 2024.

More information can be found in the press releases of Forschungszentrum Jülich (German) and EBRAINS (English).

Contact: Dr. Maren Frings, Dr. Boris Orth

New Embed2Scale Project: Earth Observation and Weather Data Federation with AI Embeddings

On 15 January 2024, the EU project Embed2Scale kicked off at EUSPA, the EU Agency for the Space Programme, in Prague. This project is coordinated by MARTEL INNOVATE BV and includes ten partners, one of them being the Jülich Supercomputing Center. The true potential of the European Union's Earth Observation Copernicus Programme is unlocked when integrated with additional geo-information, such as weather models and GNSS data. However, managing hundreds of petabytes of geospatial data is challenging, as no single platform can store it all. Service providers often download data from various archives, but the vast amount of data makes some applications economically unfeasible.

Embed2Scale aims to address these challenges by facilitating efficient data exchange through AI-driven data compression. It will develop methods to convert raw geo-information into highly compressed embeddings, potentially reducing the size by up to 1000 times. The envisaged key breakthroughs include enabling decentralized applications through significant data volume reduction, enhancing the portability of geospatial analytics by reducing computational demands, minimizing data labeling through few-shot learning, and enabling near-real-time, petabyte-scale searches of earth observation and climate data. The plan is to demonstrate these advancements with practical applications in the Copernicus Programme and to foster community growth through open-source contributions and standardization. The embedding technology will be tested in four areas: maritime monitoring, aboveground biomass measurement, climate and air pollution forecasting, and early detection of crop stress and yield.

More information can be found on the project website.

Contact: Prof. Gabriele Cavallaro, Dr. Stefan Kesselheim

Hosting Entities of the EuroHPC Supercomputers Join Efforts in EPICURE to Support HPC Users

Over the last few years, the EuroHPC Joint Undertaking has been working towards taking European supercomputing to new historic heights by installing new machines capable of competing with their global counterparts: three pre-exascale, five petascale and two future exascale supercomputers. Now, the current and future hosts of said supercomputers have combined forces to provide support services to selected users. The result is the EPICURE

project (High-level specialised application support service in High-Performance Computing), featuring 16 from 14 countries partners and led by CSC – IT Center for Science.

Until now, the support provided was mainly focused on helpdesk support and resolution of operational issues. "At the moment, most of the help provided to users is short-term support which requires basic HPC skills and competences" says Emmanuel Ory, Development Manager at CSC - IT Center for Science and Coordinator of the project, "EPICURE will be ready to help users at an advanced technical level. Right now, all the different sites in Europe use different architectures, so users need to be able to move from one system to another very easily and seamlessly".

The project will provide several services, including code enablement and scaling, performance analysis and benchmarking, code refactoring and code optimisation. To this end, the project will draw on the experience and knowledge of all partners in HPC operations and support, using training activities and hackathons to share knowledge in porting, optimisation, parallelisation, and GPU programming. EPICURE will also include close collaboration with the different Competence Centres and Centres of Excellence.

Contact: Dr. Wolfgang Frings, jsc-pmo-com@fz-juelich.de

European Centres of Excellence EoCoE and POP start into their third rounds

In January 2024, EuroHPC JU relaunched the Centres of Excellence (CoE) EoCoE and POP to support research and innovation actions that will develop and adapt HPC applications for the exascale and post-exascale era. Both projects have thus entered their third funding period, which will last for three years.

The new **Energy oriented Center of Excellence (EoCoE-III)** project holds a central vision to develop comprehensive exascale applications that drive groundbreaking energy science advancements within pivotal low-carbon sectors. A primary objective lies in showcasing the remarkable potential of exascale computing within the energy domain. Firstly, employing a collaborative co-design approach encompassing library developers and HPC technology providers, the project aims to deliver fully functional exascale lighthouse production applications attaining optimal performance on the European exascale infrastructure. This endeavor resonates with objectives emphasizing operational excellence and performance optimization. Secondly, the project aims to underscore the scientific and societal significance of these applications through the execution of five exascale simulations, each illuminating the achievement of significant scientific milestones by harnessing the exascale architecture to its fullest extent.

In EoCoE-III, the Simulation and Data Lab Quantum Materials leads the Work Package 2 (WP2) with the overarching objective of enhancing the libNEGF library, culminating in the creation of a dynamic quantum simulation tool with proficiency in managing optoelectronic hetero-structures based on 2D materials, bolstered by DFT level precision. This advancement encompasses the intricate interplay of factors such as light-carrier interactions, electron-phonon scattering, and the influence of excitonic effects. Realizing this vision necessitates a multifaceted approach: transforming the libNEGF code into a scalable entity capable of seamlessly operating on both pre-exascale and forthcoming exascale systems. This transformation encompasses the development of pioneering algorithms, innovative data distribution strategies, and a repository of platform-aware kernels.

The **Centre of Excellence on Performance Optimization and Productivity** (POP CoE, https://www.pop-coe.eu) was launched in October 2015 with the fundamental goal of supporting a broad community of HPC application developers and users in both academia and industry. POP helps them to understand the performance-related problems of their applications and thus improve their efficiency and productivity. This is achieved by providing an external and objective review of code performance for all interested users, providing not only a qualitative but also a quantitative analysis using POP tools and methods. The POP CoE was funded for a second phase (POP2) for further three years in 2018.

The recently started project POP3 continues the extremely successful work of the first two phases. It is divided into three main pillars: services, users and co-design.

The POP services focus mainly on performance assessments with the aim of determining code performance and scaling, identifying the main causes of inefficiency and providing guidance and recommendations for improvement. POP3 also offers higher value services that have been expanded in scope to include proof of concept, energy efficiency and consulting studies. Although POP3 will continue to target all application scales and user types, this project will focus on upscaling applications by evaluating the execution of some so-called flagship applications of other CoEs on the current EuroHPC machines. However, POP3 will continue to provide services to all HPC users to promote efficient use of computing resources.

The aspect of co-design is pursued in two dimensions. Internally in POP3, the tools and methodology will be jointly developed so that all desired applications can be analyzed on the chosen platform at the chosen scale. Externally, POP3 will offer a database of best practices and computational algorithms to other European projects and to all developers of parallel applications. The user pillar consists of the work areas dissemination, user training, customer development and customer satisfaction.

For the project, POP3 is bringing together a consortium of eight European organizations with the necessary expertise in the required technologies and their impact on science, the market and society.

Contact for EoCoE-III: Dr. Edoardo di Napoli
Contact for POP3: Dr.-Ing. Bernd Mohr

FAST-EO Project Launched

The FAST-EO project was officially launched on 5 February 2024, aiming to advance AI Foundation Models (FMs) for Earth Observation (EO). Funded by the European Space Agency (ESA), the consortium is led by the German Aerospace Center (Deutsches Zentrum für Luft- und Raumfahrt; DLR) and includes Forschungszentrum Jülich, KP Labs, and IBM Research. Each partner brings unique strengths to the project, ranging from satellite data expertise to advanced AI and machine learning research as well as high-performance computing, with the goal to enhance the use of FMs within the EO community. By addressing key challenges such as adapting models to EO-specific data, enhancing the models' ability to process multimodal data, and reducing the computational and financial costs associated with model training and application, FAST-EO aims to make advanced EO technologies more accessible. Looking forward, as the project progresses, updates and outcomes will be shared with the community. The collaboration between these organizations aims not only to achieve the specific goals of FAST-EO but also to lay a foundation for future advancements in EO technologies.

More information can soon be found on the project website.

Contact: Prof. Gabriele Cavallaro, Dr. Stefan Kesselheim

Helmholtz GPU Hackathon 2024

Together with NVIDIA and the OpenACC organization, Helmholtz will host a hybrid Open Hackathon taking place on six days in total: on April 8 and 15 (online), and on April 23-26 (in-person in Görlitz).

Open Hackathons are multi-day, intensive hands-on events designed to help computational scientists and researchers port, accelerate and optimize their applications on a variety of data center architectures including CPUs and GPUs. The event pairs participants with dedicated mentors experienced in programming and targeted application areas to realize performance gains and speedups using a variety of programming models, libraries, and tools.

Participating teams should leave the event either with their applications accelerated and/or optimized on the latest supercomputing hardware or with a clear roadmap of the next steps needed to leverage these resources. At least three team members should participate throughout the event, who are fluent with their codes or projects, which can be classic simulation or also large scale AI models. Teams can use almost any programming model to do so, provided we find mentors for support. Each team will receive two mentors to help in the process.

Attendance and mentoring are free of charge (but participants have to cover their travel expenses to Görlitz). The Jülich HPC Systems (JURECA-DC, JUWELS Booster) will be used for the hackathon. Registration for Teams has closed in February.

More information can be found on the event website.

Contact: Dr. Andreas Herten

Guest Student Programme 2024: Registration is Open

In summer 2024, JSC will again offer a guest student programme. It is supported by the Centre Européen de Calcul Atomique et Moléculaire (CECAM). Within this programme, students with a major in natural sciences, engineering, computer science or mathematics get the opportunity to familiarise themselves with different aspects of scientific computing. Together with local scientists, the participants work on different recent research and development topics. Depending on prior knowledge and on the participant's interest, the assignment can be chosen out of different areas. These fields include mathematics, physics, chemistry, neuroscience, software development tools, visualization, distributed computing, operating systems and communication. A special emphasis is placed on the use of supercomputers.

The participants are expected to have knowledge and experience in the computer-oriented branches of their subjects. The students should already have completed their first degree but have not yet finished their master's course. Additionally, a letter of recommendation from a university lecturer or professor is required for application. The programme will last ten weeks and takes place at JSC from 5 August to 11 October 2024. Students are encouraged to apply for the programme online. The closing date is 30 April 2024.

Further information can be found on the web at https://go.fzj.de/gsp.

Contact: Dr. Ivo Kabadshow via jsc-gsp@fz-juelich.de

Events

Introduction to Bayesian Statistical Learning (online)
Instructor: Dr. Alina Bazarova, JSC
Date: 18-22 March 2024, 09:00-13:00
https://go.fzj.de/2024-bayesian-sl

GPU Programming Part 1: Foundations
Instructor: Dr. Jan Meinke, Dr. Andreas Herten, Dr. Kaveh Haghighi-Mood, JSC; Jiri Kraus, Markus Hrywniak, NVIDIA
Date: 8-10 April 2024, 09:00-16:30
Venue: JSC; Ausbildungsraum 1
https://go.fzj.de/2024-gpu-cuda

Parallel I/O and Portable Data Formats
Instructor: Ilya Zhukov, Jolanta Zjupa, Chew Junxian, Aravind Sankaran, Jan Ebert, JSC
Date: 22-24 April 2024, 09:00-16:30
Venue: JSC; Ausbildungsraum 1
https://go.fzj.de/2024-parallel-io

Interactive High-Performance Computing with JupyterLab (online)
Instructor: Jens Henrik Göbbert, Christian Witzler
Date: 23-24 April 2024, 09:00-13:00
https://go.fzj.de/2024-interactive-hpc