JSC News

On the Path to JUPITER

In June 2022, JSC was selected by EuroHPC Joint Undertaking (JU) as the hosting site for the first European exascale supercomputer. Over the past few weeks, two important milestones on the path to realizing the JUPITER supercomputer have been reached. On 28 November 2022, a hosting agreement between EuroHPC JU and Forschungszentrum Jülich was signed. It defines the roles, rights, and obligations of both parties over JUPITER's entire life cycle. This paved the way for the next step, which was taken on 16 January: the procurement of JUPITER was launched by EuroHPC JU in close collaboration with JSC. The vendor is to be selected by September 2023 and the installation of the supercomputer on Jülich's campus will be started in the first quarter of 2024.

JUPITER will be based on the dynamic, modular supercomputing architecture, which Forschungszentrum Jülich has developed together with European and international partners in the DEEP projects funded by the European Commission and EuroHPC JU. It will be the first system in Europe to surpass the threshold of 1 ExaFlop/s (a billion billion floating point calculations per second). This next-generation European supercomputer represents a significant technological milestone for Europe and will have a major impact on European scientific excellence. With such unprecedented capacity, JUPITER will support the development of high-precision models of complex systems and help to solve key challenges facing society, for example, climate change, pandemics, and sustainable energy production, while also enabling the intensive use of artificial intelligence and the analysis of large data volumes.

This new EuroHPC supercomputer will be co-funded with a maximum total budget of € 500 million by EuroHPC JU and German government bodies. Of this total, € 250 million is being provided by EuroHPC JU and a further € 250 million in equal parts by the German Federal Ministry of Education and Research (BMBF) and the Ministry of Culture and Science of the State of North Rhine-Westphalia (MKW NRW). JUPITER will be available to serve a wide range of European users – irrespective of where they are located in Europe – in the scientific community, industry, and the public sector. Access to the computing resources of the new machine will be jointly managed by EuroHPC JU and the respective German bodies in line with their investments. The German share will be part of the national supercomputer infrastructure provided by the Gauss Centre for Supercomputing.

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Second Phase of EuroCC Started

To facilitate access to high-performance computing (HPC) in Europe, national competence centres (NCCs) for supercomputing, artificial intelligence, and big data analytics were established by the EU in the first phase of the EuroCC project from September 2020 until the end of 2022 in 33 participating countries. These centres offer free consulting and information for companies, researchers, and public administrations in their respective countries. In Germany, EuroCC@GCS took over the role of the NCC. It consists of the GCS centres HLRS, JSC, LRZ, and SICOS BW. The first phase of the project focused on establishing the German NCC as a single point of contact for HPC topics in Germany, creating an overview of HPC-related competencies, and offering training courses for industrial and academic users. The needs of potential users were identified and a service portfolio was defined.

The second funding phase of the project (EuroCC 2) started in January 2023 and will run for the next three years. It will concentrate on offering these services to industry, academia, and the public sector, and on collaborating with the European Centres of Excellence (CoEs).

In EuroCC 2, JSC is leading the tasks "Services to and Interaction with Academia and Public Administrations" and "Collaboration". There are a growing number of activities in the project and JSC is currently looking for a new employee for EuroCC 2 (see job offer: 2023-042).

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Smart Data Innovation – Services (SDI-S) Project Started

For many years, the Smart Data Innovation Lab (SDIL) has developed approaches and implemented data science use cases based on industrial datasets. It established flexible processes and enabled SMEs and other industrial partners to leverage cutting-edge computing infrastructures. The SDIL approach thus innovates data science methods through the joint partnership of academic and industrial partners and has amassed significant experience over the years. The recently started Smart Data Innovation – Services (SDI-S) project will contribute to the SDIL by developing a service catalogue that combines this experience with concrete services offered by academic partners for SMEs and industrial partners. BMBF is providing funding for this project for a period of two years and the project coordinator is the Karlsruhe Institute of Technology (KIT). Forschungszentrum Jülich is a project partner alongside the Fraunhofer Society, the German Research Center for Artificial Intelligence (DFKI), SAP, IBM, and Software AG. The Jülich Supercomputing Centre will offer specific services for domain-specific data science approaches in remote sensing and healthcare. JSC will also provide more generally applicable services such as hyperparameter optimization and model training speed-up using distributed deep learning.

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Official Kick-Off of the Center for Advanced Simulation and Analytics (CASA)

On 26 January 2023, the Center for Advanced Simulation and Analytics (CASA) organized the first CASA Forum, which served as its official kick-off. Within CASA, Forschungszentrum Jülich pools its activities in the fields of data science and simulation. The overarching goal of CASA is to link domain- and method-oriented research throughout the research centre and to accelerate the expansion of expertise in data analysis, artificial intelligence (AI) methods, and model-based simulation using high-performance computing (HPC) in all scientific areas of Forschungszentrum Jülich. The focus is on the creation and optimal use of synergies, the application and expansion of the interdisciplinary portfolio, the long-term development of a community in the field of data and simulation-based research, and support of the use of HPC systems and data infrastructures. CASA supports the establishment of the exascale infrastructure on the campus and provides access to complex user software on HPC systems. At the heart of CASA are the CASA Labs, where cross-institutional teams work on application-related problems. There are currently five CASA Labs, all of which involve the participation of JSC. In four of these labs, a JSC Simulation and Data Lab forms the nucleus of the team, supported by researchers from other institutes. This cross-institutional collaboration is a fundamental component of all CASA Labs.

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NIC Excellence Project Awarded to Prof. Rohlfing

The Peer Review Board of the John von Neumann Institute for Computing (NIC) regularly awards the title "NIC Excellence Project" to outstanding simulation projects. At its October meeting, the board decided to honour Prof. Michael Rohlfing (University of Münster) for his project "Spectra of 2D layered materials".

Structural and opto-electronic properties of condensed matter are determined by electronic quantum mechanics on the atomic length scale, ranging from molecules to extended crystals. This local quantum mechanics competes with the geometry structure on the nanometer scale, asking for theoretical description by ab initio (or "first-principles") techniques in which the atomic orbitals constitute the smallest active unit. This is especially true for low-dimensional materials such as monolayers of transition-metal dichalcogenides (e.g. molybdenum disulfide). The intrinsic properties of a material can be manipulated by external influences, such as deposition on a substrate, geometric strain, external electric or magnetic fields, gating from applying a voltage, and a dielectric environment, thus opening up the possibility of functional design. In this context, the theoretical understanding of the response to such external stimuli appears to be particularly important. The main topic of the project is the investigation of (opto)electronic spectra, i.e. single-particle spectra (band structures) and two-particle excitations (optical spectra) from first principles. For more details, see https://go.fzj.de/nic-ep-2022-2.

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Research Team Wins RWTH Aachen University's Innovation Award

Congratulations to Mathis Bode (JSC), Prof. Thomas Lippert (JSC), and Prof. Heinz Pitsch (RWTH Aachen/ITV) for being one of the winners of RWTH Aachen University's Innovation Award 2022 with their disruptive technology accelerator JuLES (JUelich Large-Eddy Simulation).

JuLES is an innovative platform that aims to actively contribute to achieving the 1.5-degree pathway. A starting point for the transformation of all industrial processes, which is required for the fight against climate change, is the fact that existing carbon-neutral technologies, such as renewable energy production from wind and solar energy or the hydrogen industry, need to be developed to market maturity level and become more efficient as quickly as possible. This is inconceivable without innovative technology accelerators.

On a technical level, JuLES is implemented as a software-as-a-service (SaaS) platform, which is used to develop reduced models for energy flows (e.g. flows in turbines or burners) in the shortest possible time and

with unprecedented predictive accuracy, which are considered to be a crucial technology for the carbon-neutral transformation of our industrial processes.

The scientific core of JuLES is Physics-Informed Enhanced Super-Resolution Generative Adversarial Networks (PIESRGAN) for Large-Eddy Simulation (LES). PIESRGAN for LES enables the data-driven development of reduced models for energy flows, which have already demonstrated that they are significantly superior to existing models in terms of predictive accuracy and can simultaneously reduce simulation costs by up to two orders of magnitude. It uses an artificial intelligence (AI)-based technique to "reconstruct" the smallest scales in energy flows. The combination of classical, general-establishment fluid mechanics techniques and cutting-edge AI technology allows for unprecedented predictive accuracy.

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JSC Researchers Receive Outstanding Paper Award at NeurIPS 2022

Mehdi Cherti and Jenia Jitsev from JSC received an Outstanding Paper Award at NeurIPS 2022, one of the leading international conferences for machine learning and artificial intelligence, for their publication entitled "LAION-5B: An open large-scale dataset for training next generation image-text models". Current language-vision models have risen above traditional approaches and overcome numerous limitations. This is mostly thanks to training methods based on large-scale datasets from online sources. Unfortunately, research is mainly conducted by industry labs and datasets have remained private — until now. This award-winning work provides open datasets from public internet resources that can be used to train state-of-the-art language-vision models and that are accessible to all research labs around the world. The work was performed by JSC and LAION e.V., a Hamburg-based non-profit organization strongly commit-ted to open source and open science that is co-led and was co-founded by Jitsev and Cherti. Toolsets for dataset composition and pre-trained openCLIP models are also open-sourced as a result of this work.

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PPI4HPC Project Earns 2nd Place at European Innovation Procurement Awards

The PPI4HPC project has been awarded as a 2nd place finalist at the European Innovation Procurement Awards (EUIPA) 2022 in the "Procurement leadership" category. The winners were announced during the European Innovation Council Summit in Brussels on 7-8 December 2022. Phillippe Segers, Head of European HPC Projects at GENCI, attended the award ceremony on behalf of the PPI4HPC project partners. JSC participated in the project,

which was focused on the joint procurement of HPC systems in Europe and led to the procurement and funding of the HPC system JURECA-DC at Jülich.

Calls for Computing Time Applications in January/February

The following synchronized calls for computing time applications were published on 16 January 2023. For all calls, the strict deadline for submitting proposals is 17:00 (CET) on **13 February 2023**.

The Gauss Centre for Supercomputing (GCS) issued the 29th 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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Events

ESM User Forum
Instructors: Employees from JSC, external partners
Date: 23–24 February 2023
Venue: online
https://go.fzj.de/2023-esm-user

Getting Started with AI on Supercomputers
Instructors: Alexandre Strube, Sabrina Benassou, JSC
Date: 28 February – 1 March 2023, 09:00–13:00
Venue: online
https://go.fzj.de/2023-ai-1

Introduction to Unreal Engine for Science
Instructors: Dirk Helmrich et al., JSC
Date: 3, 10, and 17 March 2023, 10:00–15:00
Venue: online
https://go.fzj.de/2023-unreal

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