

The JURECA Cluster is Dead, Long Live JURECA!

In parallel with the ongoing deployment of the JUWELS Booster, JSC is actively preparing its next major system upgrade. In November 2020, the JURECA Cluster will have reached five years of successful operation and will require renewal. For this purpose, the Cluster module of the modular supercomputer JURECA, consisting of the Cluster module as well as the Booster module installed in 2017, will be replaced by the new JURECA “data-centric” (DC) module.

The JURECA DC module will be supplied by Atos based on the Sequana XH2000 technology that is also used in the JUWELS Booster. The module will consist of a total of 768 compute nodes, all equipped with two 64-core AMD EPYC Rome CPUs and at least 512 GB of main memory. 96 of the nodes are equipped with 1 TB main memory. A quarter of the compute partition, 192 nodes in total, are equipped with four NVIDIA A100 GPUs. The system uses a HDR100/HDR InfiniBand interconnect with a scalable DragonFly+ topology. Compared to the predecessor, all major system performance indicators are increased. The core count of the system is increased by a factor of 4, the total memory capacity by 1.6 and the peak performance by approximately 7.8; the latter in particular due to the larger number of GPU nodes.

Like its predecessor, JURECA DC will be closely integrated with the JURECA Booster, enabling the concurrent use of all resources within workflows as well as the same parallel MPI application.

While JURECA DC will provide significant speedups for current JURECA workloads, several innovative features enable it to more efficiently execute data-intensive workloads. In particular, the JURECA DC module will include a novel system-integrated NVM in addition to high-bandwidth access to the JUST storage tiers.

The JURECA DC system will be deployed in two phases. The first phase will be available from the beginning of December and is planned to provide 384 CPU and 96 GPU compute nodes. The second phase will be operational in the first quarter of 2021.

The JURECA DC module was procured as part of the PPI4HPC project co-funded by the European Commission through a joint procurement process together with three European partner centres: BSC in Spain, GENCI/CEA in France, and CINECA in Italy. All four participating sites procured innovative HPC solutions for local and European users.

Computing time on the JURECA DC module will be made available to researchers of Forschungszentrum Jülich and RWTH Aachen University. Furthermore, a share of the compute time will be available for European scientists.

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Thomas Lippert Appointed Professor at Goethe University Frankfurt

Prof. Thomas Lippert, head of the Jülich Supercomputing Centre, has been appointed professor at Goethe University Frankfurt and will occupy the newly created chair for “Modular Supercomputing and Quantum Computing” at the Institute for Computer Science. He will exercise this appointment in place of his previous position as professor at the University of Wuppertal. He will support the Center for Scientific Computing (CSC) at the Goethe University in its further development into a national high-performance computing centre. While continuing his position at JSC, Lippert is particularly excited to establishing two new research groups in Frankfurt to explore the development and practical application of modular supercomputers and quantum computers. Simultaneously with his appointment, Prof. Lippert will become a Senior Fellow at the Frankfurt Institute for Advanced Studies (FIAS). JSC wishes Thomas Lippert all the best for his new position and is looking forward to the new cooperation opportunities with the Goethe University Frankfurt.

New AI Project AlphaNumerics Zero

The Helmholtz Artificial Intelligence Cooperation Unit (Helmholtz AI) is one of five platforms initiated by the Helmholtz Information and Data Science Incubator. Its main goal is to become a driver for applied artificial intelligence (AI) through the development and distribution

of AI methods across all Helmholtz centres, effectively combining AI-based analytics with the Helmholtz Association's unique research questions and datasets.

In the first annual call for proposals, the proposal "AlphaNumerics Zero" (αN0), led by JSC together with researchers from the Steinbuch Centre for Computing at KIT, was selected for funding. The objective of this project is to rethink numerical methods on high-performance computers. Traditionally, a lot of effort goes into the design, implementation, and optimization of solvers for differential equations, numerical libraries, etc. Furthermore, performance engineering is necessary to scale simulation codes onto supercomputers. New ideas are urgently needed as developing methods for the upcoming extreme-scale supercomputers is becoming increasingly challenging. Our goal is to use reinforcement learning techniques so that the computer learns the on-average optimal numerical solution method for a given simulation problem by itself. The deliverables for the project will be a working framework and a demonstration in one application case using a time-dependent partial differential equation. This is a moonshot project that – if successful – will be the first step to changing the paradigm of how numerical simulations are designed and performed on extreme-scale computers. It would have an impact on all research fields that rely on numerical simulations.

The project is funded by the Helmholtz Association's Initiative and Networking Fund (INF) with nearly € 200,000 and runs from August 2020 until January 2023.

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Structural Dynamics of Ion Channels and Transporters

Ion channels and transporters are present in the membranes of all living cells and mediate a variety of cell functions. Ion channels enable the rapid change in membrane permeability for ions such as sodium, potassium, and calcium. As a result, they generate and modulate electrical signals in cells. Ion transporters adjust the concentration of ions inside and outside of cells. As biomolecules that are heavily involved in basic life processes, ion channels also play an important role in understanding disease mechanisms and therapeutic approaches.

Recently, the German Research Foundation has extended the funding of the research group FOR 2518 "Functional Dynamics of Ion Channels and Transporters – DynIon", which has been investigating the functioning of these passage gates through the cell membrane for three years. The computational chemist Prof. Holger Gohlke (Institute for Pharmaceutical and Medicinal Chemistry of the Heinrich Heine University Düsseldorf; NIC research group Computational Biophysical Chemistry at JSC, Forschungszentrum Jülich) and his team will investigate hyperpolarization-activated cyclic nucleotide-gated (HCN) ion channels, dysfunction of which may give rise to diseases. At the atomistic level, the scientists want to use molecular simulations and modelling to understand how the channels are activated by way of coupling membrane

potential and ligand binding. Molecular dynamics simulations will be performed in this context on the GPU partition of JUWELS. These studies will be complemented by experimental data from the lab of Prof. Klaus Benndorf from the Friedrich Schiller University Jena.

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Calls for Computing Time Applications

The following synchronized calls for computing time applications were published on 20 July 2020. The strict deadline for submission of proposals for all calls is 17 August 2020, 5pm CEST. An overview of all calls can be found at <https://fz-juelich.de/ias/jsc/computingtime>.

The Gauss Centre for Supercomputing (GCS) has issued the 24th call for Large-Scale Projects. Researchers at German universities and publicly funded research institutions are eligible to apply. Projects are classified as "Large-Scale" if they require at least 2 % of the systems' annual production in terms of estimated availability. Available systems include the supercomputers HAWK at HLRS, SuperMUC-NG at LRZ, and JUWELS at JSC. Within this call, projects can apply for resources on the new JUWELS Booster Module for the first time.

Researchers at German universities and publicly funded research institutions can also apply for GCS/NIC Regular Projects on the JUWELS Cluster and Booster as well as on the JURECA Booster. As of now, scientists from Forschungszentrum Jülich and the RWTH Aachen University are also eligible to submit proposals for GCS/NIC Regular Projects. However, computing time on the JURECA Booster is only available via JARA/VSR (see below). For further information on GCS Large-Scale and GCS/NIC Regular projects, please visit <https://www.gauss-centre.eu/for-users/hpc-access/>.

Researchers from all HGF institutions in the research field Earth and Environment together with national cooperation partners outside the HGF may apply for resources on the ESM partition of the JUWELS Cluster and Booster. Please visit <https://fz-juelich.de/ias/jsc/esm-application> for details.

Finally, researchers from RWTH Aachen University and from Forschungszentrum Jülich can submit applications for computing time on the JARA Partition and for VSR projects. Resources on the CLAIX system located in Aachen and on the JURECA Booster Module at JSC are available through JARA. Jülich scientists can additionally apply for resources on the new JURECA DC Module. Further information is available at <https://www.jara.org/de/654>.

To account for the fact that the effective computing power per core hour differs for different modules and resources, computing time requirements expressed in units of Mcore-h for each requested resource are converted to floating point operations in units of exaFLOP (EFLOP) based on the corresponding theoretical peak performance. Further details on this conversion can be found at <https://fz-juelich.de/ias/jsc/computingtime>.

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