Europe's Fastest Supercomputer Goes Online at JSC

After more than two years of extensive preparation, co-design, and deployment work, JSC – along with its project partners Atos, ParTec, and NVIDIA (including Mellanox Technologies, formerly Mellanox) – proudly unveiled the JUWELS Booster module at the 2020 Supercomputing conference. The new supercomputer module, which is tightly coupled with the Cluster system installed in 2018 and thus follows JSC's modular supercomputing paradigm, fully lives up to its name and has boosted JUWELS to new heights.

The JUWELS Booster, which provides a peak performance of 73 PF/s in double precision, is now the fastest European supercomputer and the 7th fastest supercomputer worldwide, according to the Top500 ranking. Ranking 5th on the HPCG list and with a performance of 110 multi-precision PF/s on the new HPL-AI benchmark, the system is ideally suited for a broad range of scientific applications, including artificial intelligence and deep learning workloads. With a Gigaflop-per-Watt ratio of more than 25, the JUWELS Booster ranks 3rd on the Green500 list and is the most energy-efficient supercomputer among the top 100 supercomputers worldwide. The success of the co-design efforts, which have enabled JSC and its partners to couple the most energy-efficient processor technologies with highly effective system packaging and a direct liquid cooling design in a balanced system, also underlines JUWELS' position as an architectural prototype for an upcoming European exascale system in the coming years.

During the installation phase, JSC worked with a number of early access users, who were able to port codes to the new architecture at an early stage and provide valuable feedback about the capabilities of the system. They also supported optimization and problem resolution efforts. Since 23 November, the JUWELS Booster has been officially in operation and JSC continues to optimize the system together with its users.

The modular supercomputer JUWELS is operated by JSC as a member of the Gauss Centre for Supercomputing and is funded by the Federal Ministry of Education and Research (BMBF) and the Ministry of Culture and Science of the state of North-Rhine Westphalia. Information on the technical specification can be found at https://fz-juelich.de/ias/jsc/juwels.

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Porting & Tuning Workshops for JUWELS Booster Module

With the JUWELS Booster module now in service at JSC, users are encouraged to take advantage of two workshops early next year dedicated to porting and tuning HPC application codes for its quad NVIDIA A100 GPU compute nodes.

The first workshop will be the JUWELS Booster Porting Workshop, which begins with a full-day colloquium on 20 January 2021 reviewing the successes and experiences gained from the JUWELS Booster Early Access Programme. The next two days (21-22 January) will focus on GPU programming for neophytes (with parallel applications not yet exploiting GPU accelerators) followed by two days (25-26 January) dedicated to more experienced GPU application developers needing to adapt their codes to multi-node/multi-GPU execution on the JUWELS Booster module. When registering, please specify which aspect(s) of the workshop you are interested in. For detailed information, please visit https://fz-juelich.de/ias/jsc/2021/jwb-porting.

The second workshop will be the 38th VI-HPS Tuning Workshop organized by JSC and RWTH Aachen University from 8-12 February 2021. It is dedicated to performance analysis and the optimization of multi-node/multi-GPU application codes executed on the JUWELS Booster module. Application teams with such codes from the porting workshop will be prioritized. Detailed information can be found at https://www.vi-hps.org/training/tws/tw38.html.

Both workshops place an emphasis on hands-on work with small teams of application developers coached by expert instructors and assisted by JSC support staff. The

training events will be held online, requiring separate registrations for those interested in both workshops.

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Production Start on JURECA-DC

On 30 November, we bid farewell to the JURECA Cluster after five years of operation. As announced in July, the successor system, the JURECA-DC ("data centric") module, will take its place and complete the revised JURECA supercomputer, consisting of the new JURECA-DC module and the Intel Xeon Phi-based Booster module, for the coming years.

The deployment of the JURECA-DC module started in July following the decommissioning of the first half of the JURECA Cluster. From the beginning of December, the first phase of the JURECA-DC module will be available to users with only a short service interruption.

This first phase of JURECA-DC consists of 384 CPU nodes, each with 128 AMD Rome EPYC cores per node, and 48 nodes additionally equipped with four NVIDIA A100 GPUs. The system thus contains about two thirds of the final system's CPU nodes and 25 % of the GPU nodes. The staggered deployment, which is required due to facility limitations prohibiting a parallel installation of the JURECA-DC module during operation of the Cluster module, also implies that some features – e.g. the system-integrated non-volatile memory partition – will only be available with the full installation, which is scheduled to be fully deployed in the first quarter of 2021. For detailed information on JURECA, please visit https://fz-juelich.de/ias/jsc/jureca.

Since summer, the reduction in size of the JURECA Cluster has led to a noticeable increase in wait times for users. While this shortage of compute resources could be seen to underline the continuing appeal of the JURECA Cluster, JSC saw the need to provide users with additional access to the JUSUF system in order to alleviate the impact of the transition phase. It is expected that the availability of the first phase of JURECA-DC, which – with approx. 49,000 cores and 192 A100 GPUs – already significantly exceeds the capabilities of the old JURECA Cluster, will restore the job wait times and system backlog to the expected level.

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NIC Excellence Project November 2020

The NIC Peer Review Board regularly awards the title "NIC Excellence Project" to outstanding simulation projects. At its October meeting, the board decided to honour Dr. Markus Heyl (Max Planck Institute for the Physics of Complex Systems) for his project entitled "Quantum many-body dynamics from neural networks with GPU acceleration". Enormous advances in experimental techniques have been made during the past two decades, such as the development of various quantum simulators and ultrafast pump-probe techniques, allowing unprecedented control and time-resolved measurements on quantum systems with many interacting degrees of freedom. These developments have shifted the focus to a number of fundamental yet challenging open theoretical questions, which stem from microscopic quantum many-body models. This project follows a novel route by employing artificial neural networks to encode the complex quantum many-body wave function. The project thus aims to advance the theoretical description of non-equilibrium quantum matter, addressing the challenging regimes of two spatial dimensions and of long-time dynamics. For more details, see http://www.john-von-neumann-institut.de/nic/heyl (in German).

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New GCS Large-Scale Projects in November

Twice a year, the Gauss Centre for Supercomputing (GCS) issues a call for large-scale projects on its petascale supercomputers – Hawk (HLRS), JUWELS (JSC), and SuperMUC-NG (LRZ). Projects are classified as "large-scale" if they require at least 2 % of the systems' annual production in terms of estimated availability.

Currently, the JUWELS Booster module is being installed and made available to applicants for the first time in this call. Whilst computing time quantities were previously specified in core hours, the modularity of JUWELS requires the introduction of the new computing time unit EFLOP, which reflects the amount of floating-point operations per year available to approved projects. The computing time on Hawk and SuperMUC-NG continues to be given in core hours. From now on, these projects will only fall into the "large-scale" category if they require at least 100 Mcore-h on Hawk, 45,000 EFLOP on JUWELS, or 45 Mcore-h on SuperMUC-NG.

The GCS Peer Review Board took the decision to award large-scale project status to 16 projects from various scientific fields. Three projects were granted 1130 Mcore-h on Hawk, eight projects were granted 408,000 EFLOP on JUWELS, and five projects were granted 277 Mcore-h on SuperMUC-NG. For more details of these projects, visit https://www.gauss-centre.eu/results/large-scale-projects/.

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Martin Schultz Ranks among Highly Cited Researchers again

Dr. Martin Schultz from JSC ranks among the 6,167 Highly Cited Researchers of 2020, a list compiled every year by Clarivate Analytics. For this list, more than 10 million articles from around 11,000 journals are evaluated in 21 research fields. Researchers receive the accolade if they are among the top 1 % of most-cited authors in their field. In the case of Martin Schultz, the field was geosciences. Schultz has contributed to several major international assessments of tropospheric ozone and atmospheric aerosols. After featuring on the list in 2017, this was the second time he received this accolade.
JSC congratulates him on this recognition.