

Last Printed Issue of JSC News

Dear readers of JSC News,

Those of you who have received the printed version of JSC News so far will certainly be surprised to learn that today's issue bears the number 275. Due to the restrictions imposed by the coronavirus pandemic – at first with basic operations and then with adjusted normal operations at Forschungszentrum Jülich and the resulting reduced availability of personnel on site – it has not been possible to send the newsletter by mail in the conventional way since April. At a time when home office work had become commonplace and presence at an institute workplace rare, it was also uncertain whether printed copies would reach their recipients during these time periods. Therefore, issues 271 to 274 were sent exclusively as e-mail versions.

JSC has decided to send its newsletter only by e-mail in future and to offer it online. For this reason, this will be the last printed issue of JSC News. For almost four years now, it has been possible to subscribe to JSC News by e-mail. Anybody who wants to receive the e-mail version is invited to subscribe to the mailing list by sending an e-mail without any content to jscnews-subscribe@fz-juelich.de and confirming the registration afterwards. Furthermore, JSC News will always be available online at <https://fz-juelich.de/ias/jsc/jscnews> along with the e-mail version and PDF files.

So please stay tuned. We look forward to welcoming many of our nearly 1,000 recipients as online subscribers soon.

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New NVM Storage Resource Enters Evaluation Phase

JSC has finalized the deployment of a new innovative performance-optimized storage resource within the central Jülich storage cluster JUST. The new high-performance storage tier, JUST-IME, leverages non-volatile memory (flash) technology to provide very high

bandwidth and accelerate a range of I/O-intensive simulation and machine learning workloads with the "Infinite Memory Engine" technology by DDN. The system, which is delivered by Hewlett Packard Enterprise together with DDN, is connected to JUSUF as well as the JURECA and JUWELS supercomputers at JSC with an accumulated bandwidth of more than 2 TB/s.

The JUST-IME storage is initially being evaluated for selected use-cases before being offered to a wider audience in 2021. In parallel with this evaluation phase, development is continuing. In particular, the architecture's unique ability to tightly integrate storage with multiple supercomputers, which themselves are only loosely coupled, while still maintaining global consistency and coherency is made possible by an on-going joint co-development effort by the partners. This novel feature will enable high-performance workflows across the entire modular supercomputing facility at JSC.

The JUST-IME resource is co-funded by the ICEI project and a corresponding share of the system is to be made available for the Human Brain Project (HBP) and the broader European research community via the PRACE-ICEI calls for proposals.

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New European Centre of Excellence for Quantum Chemistry

In preparation for upcoming exascale systems, the European Commission is funding Centres of Excellence (CoE) for different application domains. Among the numerical methods that are particularly promising in terms of scalability to extremely parallel supercomputers are the Quantum Monte Carlo (QMC) methods. Using advanced and systematically improvable stochastic methods, faithful simulation of fully consistent quantum mechanical electron problems can be realized. The new CoE TREX (Targeting Real Chemical Accuracy at the EXascale) brings together domain experts who have developed QMC codes, which have been developed in Europe and are internationally recognized, as well as HPC experts.

The goal is to enable these applications for the upcoming pre-exascale and exascale systems in Europe.

One focus will be on porting these codes to compute accelerators, i.e. different types of GPUs. The project aims at developing and implementing a common library for QMC, called QMckl. This library will provide highly optimized implementations of numerical tasks for different supercomputer architectures, which can be used for different QMC applications. This new software and its integration in a service framework will help to reduce the barrier between advanced numerical simulations and scientific and industrial applications.

TREX brings together partners from 7 different countries and is coordinated by the University of Twente in the Netherlands. The project will start on 1 October 2020 and will run for 3 years. For further information, please visit <https://trex-coe.eu/>.

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CoE in Combustion to Accelerate Decarbonization of Energy

The “Center of Excellence in Combustion (CoEC)”, an EU-funded project starting on 1 October 2020 with a total budget of around € 5.6 million, brings together eleven European partners with dedicated expertise in the numerical simulation of combustion. The objective is to develop high-performance software accessible to the industrial sector for the design of innovative technologies in combustion. The simulation of turbulent combustion of real devices, such as engines and gas turbines, is extremely demanding computationally and is consistently in the group of few applications that use the largest part of the available computer time on Tier-0 machines.

The CoEC is built upon the European HPC combustion community and aims at boosting the transition of the EU combustion codes towards exascale computing. It will enable new breakthroughs towards decarbonization, by developing a portfolio of high-end exa-enabled services based on combustion simulations. The ultimate goal of the CoEC is to empower the combustion simulation community to face the current and future challenges for cleaner and more efficient power and propulsion systems.

With the upcoming exascale machines, an opportunity for the revision of simulation methodologies and the extension of the most accurate methods to a wider range of conditions becomes possible.

The project is therefore divided into four main activities: computing efficiency, modelling, data processing, and future technologies. JSC is responsible for the work package “Data processing and analysis”, dedicated to the challenges and opportunities arising from the significantly increasing amount of data available in the simulations.

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Virtual PRACE Summer of HPC Students at JSC

The PRACE Summer of HPC (SoHPC) programme, now in its eighth year, allowed 52 university students from all scientific disciplines to spend two months working together with PRACE partner organizations. In contrast to previous years, the programme was held fully remotely, which made it possible to give twice the number of students a chance to work in HPC. In addition to allowing students to work on research projects in a multidisciplinary and international environment, the aim of the SoHPC programme is to promote and disseminate scientific culture among the upcoming generation of researchers, making sure that students participating in the project will be the computational scientists of tomorrow. Furthermore, through the participants’ sharing of their experiences in blog posts and video presentations, the programme aims at ensuring that the students themselves become ambassadors for supercomputing at their respective institutions.

This year, four students, Josip Bobinac (Austria), Igor Abramov (Switzerland), Anssi Tapani Manninen (Finland), and Aitor López Sánchez (Spain) joined JSC remotely for the summer to gain first-hand experience in day-to-day research. After an online training week for all 52 students hosted by TU Wien, the four students teamed up and started working on their assigned projects at JSC. Josip and Igor were supervised by Ivo Kabadshow and worked on the Fast Multipole Method for GPUs, while Anssi and Aitor were supervised by Stefan Krieg and dealt with high performance quantum fields. They produced two video presentations that can be found at <https://bit.ly/3bWtrxA> and <https://bit.ly/3kcg8vR>.

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News from MATSE Education

At the end of August 2020, 32 mathematical and technical software developer (MATSE) trainees who started their vocational training in 2017 passed their final examinations. Despite the restrictions caused by the coronavirus pandemic like basic operations, home office, and digital learning, six of the trainees achieved the top grade “very good” and thirteen were awarded the second best grade “good”. The best result was achieved by Lars Osiewacz (ICS-TA), who achieved 97 %. Since 1964, about 1,200 trainees have successfully completed their training at JSC.

On 1 September 2020, 27 new students began their Bachelor’s degree course in “Applied Mathematics and Computer Science” at Aachen University of Applied Sciences (FH Aachen) in combination with the MATSE-training at Forschungszentrum Jülich. Of these students, 26 will complete their training at the various institutes of the FZJ, while one student was placed with an external industrial partner. The combined planned duration of the vocational training and the studies is three years. The curriculum and further information can be found at <https://fz-juelich.de/matse>.

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