## Upcoming HPC Systems in 2020

In order to provide a world-class infrastructure to its users and drive the development of high-performance computing and storage technologies for scientific cases forward, the supercomputing facility at JSC is undergoing continuous rework and upgrades. The year 2020 will be a particularly busy year.

In spring 2020, a new storage system within the Jülich Storage cluster (JUST) will be made available. The new high-performance tier leverages non-volatile memory (flash) technology to provide very high bandwidth and accelerate a range of I/O-intense simulation and machine learning workloads with the “Infinite Memory Engine” technology by DDN. It will provide separate storage pools to JUWELS, the JURECA Cluster, and JUSUF (see below) with an accumulated bandwidth of more than 2 TB/s. In a joint co-development effort, DDN and JSC are working on enabling coherent access between the storage slices attached to the three computing systems to enable workflows across the entire modular supercomputing facility at JSC. This capability is expected to be available in 2021.

Also in early 2020, the new JUSUF system, short for Jülich Support for Fenix, will go into production. JUSUF combines an HPC cluster and a cloud platform in a single system with homogeneous hardware such that resources can be flexibly shifted between the partitions. The JUSUF compute nodes are equipped with two AMD EPYC Rome CPUs, each with 64 cores operating at 2.2 GHz. One third of the compute nodes are furthermore equipped with one NVIDIA V100 GPU. The JUSUF cluster partition will provide HPC resources for interactive workloads and batch jobs. The cloud partition will enable co-location of (web) services with these resources to enable new workflows and support community platforms.

The JUST high-performance storage and JUSUF are co-funded by the European ICEI project, which is establishing the new federated e-infrastructure “Fenix”. A share of the resources will be made available to the Human Brain Project community and to European researchers via PRACE. More information about resource access to these infrastructure components will be published soon.

Later in 2020, JSC will install the new Booster module for the Tier-0/1 system JUWELS. The module will boost the peak performance of JUWELS to more than 70 petaflops. The JUWELS Booster compute nodes are equipped with multiple next-generation NVIDIA GPUs and Mellanox 200 Gb/s HDR InfiniBand adapters. The JUWELS Cluster and Booster are integrated in the same high-speed interconnect fabric enabling applications to efficiently leverage the modular architecture of JUWELS.

Finally, in late autumn, the JURECA Cluster module will have reached five years of successful operation and is scheduled for decommissioning. The procurement of the successor system will be finalized by February 2020. Due to infrastructure constraints, parallel operation of the successor and the JURECA Cluster will not be possible. Therefore, JSC intends to perform installation in phases to minimize service interruption. More details about the time schedule and the architecture of the successor system will be published in due time. The system is co-financed by the European Commission in the context of the PPI4HPC project. A share of its resources will be available to European researchers.

JSC is committed to minimizing and, where possible, eliminating service disruptions due to these deployment activities. However, in some cases additional maintenance will be required. Our thanks go to our users for their patience and continued support.

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## NIC Symposium 2020

The 10th NIC Symposium will be held at Forschungszentrum Jülich from 27 to 28 February 2020. The talks will inform a broad audience of scientists and interested members of the public about the activities and results obtained in the last two years by research projects supported through the John von Neumann Institute for Computing (NIC) using the JURECA, JUQUEEN and JUWELS supercomputers at Jülich.

Invited talks and a poster session will cover topics in the fields of astrophysics, biophysics, chemistry, elementary particle physics, condensed matter, materials science,

soft matter science, earth and environmental research, fluid mechanics, plasma physics, and computer science. To accompany the conference, a comprehensive proceedings volume will also be published. It will cover an even wider range of projects than represented by the talks. The detailed programme and the registration form are available at http://www.john-von-neumann-institut.de/nic/symposium.

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## EU Project Sano on Computational Medicine

Forschungszentrum Jülich is a partner in the 7-year EU project Sano, which officially started in August 2019. Sano received € 15 million funding from the H2020-WIDESPREAD-2016-2017 Teaming Phase 2 program and matching funds of € 15 million from Poland. The project aims at establishing, developing, and sustaining a Centre for Computational Personalised Medicine in Kraków, Poland. During the first phase, the Polish Ministry of Science and Higher Education is working through its National Centre for Research and Development (NCBR) to coordinate the consortium of six partners from Poland, the United Kingdom, and Germany.

The mission of Sano involves:

- development of new computational methods, algorithms, models, and technologies for personalized medicine,
- introducing new diagnostic and therapeutic solutions based on computerized simulations into clinical practice,
- fostering creation and growth of enterprises which develop cutting-edge diagnostic and therapeutic technologies,
- contributing to novel training and education curricula which meet the needs of modern personalized medicine.

To these ends, Sano is closely cooperating with hospitals and enterprises from the growing health and life science sector in and around Kraków.

Sano is currently in the process of recruiting a director of the centre and will establish five research groups by the beginning of 2021. Research positions at Sano are filled by way of international competitions organized by the centre's International Scientific Committee, which consists of 15 experts. Jülich's contributions, in particular in the areas of data management, computational pipelines, and high-level services, are coordinated by the SimLab Biology at JSC. Further information can be found at https://sano.science.

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## UNSEEN Project – HPC for Energy Systems Modelling Continues to Grow at JSC

October 2019 saw the launch of UNSEEN, a follow-up project to BEAM-ME, funded by BMWi for three years. The central objective is to make substantial improvements in modelling and optimizing complex energy systems using HPC infrastructure. The project's partners are DLR in Stuttgart (DLR-TT), DLR in Oldenburg (DLR-VE), the Zuse Institute Berlin (ZIB), GAMS GmbH, and TU Berlin. With its contributions to the project, JSC further corroborates its role in HPC-based energy systems modelling and analysis, which aims to account for increasing model complexity. The project focusses on the combination of machine learning methods and specific parallel optimization schemes, with the latter developed in the predecessor project BEAM-ME.

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## Early Access Programme for DEEP-EST Prototype

The Early Access Programme within the EU-funded DEEP-EST project provides academic and industrial users with opportunities to access and use the DEEP-EST prototype platform. Experienced HPC and data analytics or machine learning users are invited to port or benchmark applications and evaluate the DEEP-EST hardware and software architectures deployed on the DEEP-EST prototype platform through an application for Type1 – Selected Application Access or Type2 – Any Application Access. After the completion of each project, a brief final report is required to provide feedback. The DEEP-EST Early Access Programme call for proposals for Type1 Access and Type2 Access opened in January 2020. The single call for Type2 – Any Application Access will close on 31 January 2020, the open call for Type1 – Selected Application Access will close on 15 September 2020. Please find more information on https://www.deep-projects.eu/access.html. If you have questions or need support regarding the Early Access Programme, please contact access@deep-est.eu.

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## Awards for Bachelor's and Master's Students

On 13 December 2019, three students from Forschungszentrum Jülich received the Ehrenplakette award from Aachen University of Applied Sciences (FH Aachen). In a ceremony at Aachen's historic town hall, Prof. Baumann, rector of FH Aachen, honoured Jonas Ritz (PGI-JCNS-TA) as the best graduate from the bachelor's course Scientific Programming, and Steffen Dohmke (IEK-8) and Gitte Kremling (JSC) as the best graduates from the master's course Technomathematics.

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## Events

### Parallel and Scalable Machine Learning

Instructors: Prof. Morris Riedel, Dr. Gabriele Cavallaro, Dr. Jenia Jitsev, JSC
Date: 17-19 February 2020, 09:00-16:30
Venue: Jülich Supercomputing Centre, Rotunda
https://fz-juelich.de/ias/jsc/2020/machine-learning