



Jülich Supercomputing Centre

ERC Advanced Grant for Martin Schultz

Deep learning is rapidly gaining importance for the analysis of large data volumes and has achieved spectacular successes recently. However, there are only a few researchers, who have started to use the methods of artificial intelligence in the area of environmental research. Dr. Martin Schultz, who heads the research group on Earth System Data Exploration at JSC, has now received a prestigious Advanced Grant from the European Research Council to apply deep neural networks to improve the understanding of the global distribution and trends of air pollution.

In this project entitled IntelliAQ, Schultz wants to link measurements of air pollutants with high-resolution geographic data and data from numerical weather prediction models to obtain detailed maps of regional and global air quality. Furthermore, he expects that deep learning will allow for improved air quality forecasts and automated control of data quality.

The foundations for IntelliAQ were laid in the development of the TOAR database, which contains the world's largest collection of surface ozone measurements and is hosted at JSC. Together, the JSC division Federated Systems and Data, and the Simulation Laboratories Climate Science and Terrestrial Systems, provide an ideal environment to realize the project objectives. IntelliAQ is very demanding in terms of efficient storage and processing of huge data volumes and poses interesting challenges for developers of neural network architectures due to the heterogeneity and complexity of the data involved. The project will receive funding of \in 2.5 million over 5 years.

(Contact: Dr. Martin Schultz, *m.schultz@fz-juelich.de*)

JSC@ISC'18

The International Supercomputing Conference 2018 (ISC'18) will take place from 24 to 28 June 2018 in Frankfurt am Main. JSC, together with its partners in the Gauss Centre for Supercomputing (GCS) – HLRS (Stuttgart), and LRZ (Garching) – will present its wide-ranging supercomputing activities at the GCS booth (B-1310).

The first module of our new modular supercomputer JUWELS will be presented: a Cluster component with more than 2500 compute nodes, each equipped with two Intel Xeon 24-core Skylake CPUs and 96 GiB of main memory. As another highlight, all visitors to our booth will be invited on a virtual reality (VR) tour with the HTC Vive VR system, with which they can dive into results of HPC simulations from the area of earth system science. Furthermore, news of HPC tools developed in-house, like LLview and Scalasca, will be highlighted. Flyers will present information about JSC's research and support activities, as well as the HPC infrastructure provided to national and international scientists.

JSC staff will co-organize the "International Workshop on OpenPOWER for HPC (IWOPH'18)", organize the BoF "ARM for HPC Co-Design Opportunities", and present the two tutorials "Tutorial on HPC No. 258 • May 2018

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jsc@fz-juelich.de www.fz-juelich.de/jsc Applications, Systems & Programming Languages" and "Tutorial on Machine Learning & Data Analytics" on the ISC STEM (science, technology, engineering, and mathematics) Student Day. Additionally, members of JSC will give several presentations at the conference and will co-organize the tutorial "Hands-on Practical Hybrid Parallel Application Performance Engineering". JSC staff will also be on hand at the booths of PRACE (B-1300), JARA (B-1320) and UNICORE (J-535). Detailed information on JSC's participation can be found at *http://www.fz-juelich.de/ias/jsc/isc18*.

(Contact: Dr. Florian Janetzko, f.janetzko@fz-juelich.de)

JSC Contributes to PRACE Project Access

Within the 16th call for PRACE HPC Projects, JSC will contribute about 70 million core hours on its upcoming 12 Petaflop Cluster JUWELS, as one of seven HPC systems from five hosting member institutions spread across Europe. The computing time on JUWELS was awarded by PRACE in a peer-review process to three projects from the research fields of computational chemistry, CFD, and astrophysics. The projects come from France, UK, and the Netherlands. JSC rejoins the PRACE project access after the decommissioning of JUQUEEN, which also served as an HPC resource for PRACE in earlier calls. The participation is organized by the Gauss Centre for Supercomputing (GCS) the German member of PRACE - comprising the three national supercomputing centres LRZ at Garching near Munich, HLRS at Stuttgart, and JSC. In addition to previous calls, extended user support will be provided by new PRACE High-Level Support Teams, which will be operated jointly for GCS by the three member centres. Also new is the perspective of modular supercomputing, which will be offered through additional HPC architectures which will be attached to the JUWELS core Cluster module in the near future. (Contact: Dr. Wolfgang Frings, w.frings@fz-juelich.de)

SMITH: Smart Medical Information Technology for Healthcare Project

The SMITH project started in January 2018 and has been granted funding for four years by the Federal Ministry of Education and Research as one of four consortia funded by the German Medical Informatics Initiative. The project's goal is to make better use of the wealth of patient data in order to validate the relevance of novel diagnostic and therapeutic methods in systematic trials and thus directly improve patient care. One goal is to optimize the diagnosis and therapy of intensive care unit (ICU) patients with lung failure. The demand for intensive care medicine will increase over the next 10-15 years. This can be explained by the epidemiological challenges in Germany. Thus, there is a need for improvement that is especially urgent in patients suffering from acute respiratory distress syndrome (ARDS). University Hospital RWTH Aachen, RWTH Aachen University, Bayer AG, and JSC are collaborating in the clinical use case Algorithmic Surveillance of ICU patients (ASIC) within SMITH with a particular focus on ARDS. In order to predict individual disease progression in these patients, ASIC will utilize machine learning as well as established mechanistic systems medicine models, complemented by high-performance computing, and integrated in a hybrid virtual patient model. The ASIC use case will also contribute to the development of an online, rule-based computerized decision-support system. The JSC Cross Sectional Team Deep Learning is supporting the project with deep learning, machine learning, HPC access, and statistical modelling expertise.

(Contact: Prof. Morris Riedel, m.riedel@fz-juelich.de)

New GCS Large-Scale Projects in May 2018

Twice a year, the Gauss Centre for Supercomputing (GCS) issues a call for large-scale projects on its petascale supercomputers - currently Hazel Hen (HLRS), JUWELS (JSC) which recently replaced its predecessor JUQUEEN, and SuperMUC (LRZ). Projects are classified as large-scale if they require at least 35 million compute core hours (Mcore-h). During its April meeting at DESY in Zeuthen, the GCS Peer Review Board decided to award the status of a largescale project to 17 projects from various scientific fields. Eight projects were granted 580 Mcore-h on Hazel Hen, four projects were granted 140 Mcore-h on JUWELS, and five projects were granted 340 Mcore-h on SuperMUC. In total, GCS awarded about 1 billion compute core hours to large-scale projects. For more details on these projects, visit http://www.gauss-centre.eu/large-scale. (Contact: Dr. Alexander Trautmann,

coordination-office@fz-juelich.de)

Bachelor and Master Courses Renamed

In cooperation with Aachen University of Applied Sciences (FH Aachen), JSC offers a dual bachelor's course entitled "Scientific Programming" as well as a subsequent master's course on "Technomathematics". The bachelor's course also integrates vocational training as a "Mathematical Technical Software Developer" (MATSE) at Forschungszentrum Jülich.

The contract partners have agreed that both degree programmes will be renamed "Applied Mathematics and Computer Science" during the re-accreditation in winter semester 2018/19. In addition, the curricula have been extended to include elective lectures from data science. In particular, the master's course introduces a new specialization in data science with lectures on machine learning and tools for data analytics. The changes apply to all students starting their studies in winter semester 2018/19.

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