JSC @ SC20

Due to the coronavirus pandemic, this year's SC is taking place as a virtual conference and exhibition for the first time. JSC, together with its partners ParTec and the Jülich Aachen Research Alliance (JARA), will present its numerous activities in a brand new virtual booth. The key topic of the booth is the concept of the "Modular Supercomputing Architecture" (MSA). This year's highlight will be the recently installed JUWELS Booster module. This module, with its 75 PFLOP/s peak performance, is based on NVIDIA's A100 graphics cards and helps JUWELS to become the fastest supercomputer in Europe. Co-design partner ParTec will present its expertise in the HPC domain and its key contribution to the modular software stack. The topic of MSA will be complemented by the DEEP projects, which will also be presented at the booth.

Another focus will be on the computing infrastructures in which JSC plays a significant role: the Juelich UNified Infrastructure for Quantum Computing (JUNIQ), offering access to different quantum devices, and two infrastructures driven by the Human Brain Project − the EBRAINS research infrastructure and the Fenix infrastructure.

Within JARA, the activities and services in the Center for Simulation and Data Science (CSD) will be highlighted and videos about the developments of, and contributions to, HPC tools shown.

In addition, JSC will demonstrate HPC tools developed in-house such as LLview, SIONlib, JUBE, and Scalasca, while also presenting its support infrastructure. The focus of applications this year will again be the Earth system and climate sciences with Pilot Lab Exascale Earth System Modelling.

As part of the conference programme, JSC employees will co-organise the "ProTools 2020: Workshop on Programming and Performance Visualization Tools", give presentations in the "Practical Hybrid Parallel Application Performance Engineering" tutorial, present talks, and participate in special interest group sessions and panel discussions. For detailed information, please visit https://fz-juelich.de/ias/jsc/sc20.

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

District-Based Coronavirus Forecasts

Neuroinformaticians at Osnabrück University and the Jülich Supercomputing Centre (JSC) are providing new model results for predicting COVID-19 infections on a daily basis. The results include daily updated estimates of reported new infections and a 5-day forecast for each German district. It can be accessed via an interactive dashboard hosted on JSC's OpenStack HDF Cloud. The forecasts are based on data from the Robert Koch Institute that are statistically analyzed on JSC's JUSUF computing cluster using a new, probability-weighted model developed by the Osnabrück neuroinformaticians.

The "COVID-19 Bayesian Modelling for Outbreak Detection", or BSTI model for short, has two essential features that distinguish it from other methods. Firstly, the new method provides a prediction horizon that makes it possible to assess the reliability of the forecasts. Furthermore, it takes into account the influence of the locally adjacent occurrence of infection. This also allows us to evaluate the dynamics of the spread. Furthermore, it is also possible to assess the situation while accounting for statistical uncertainties, which can provide helpful insights even with low case numbers.

Visitors to the website https://covid19-bayesian.fz-juelich.de can interactively view 5-day forecasts for various available districts or compare the current reporting data from the Robert Koch Institute with estimations of actual new infections. Due to delays in data transmission, the reported figures sometimes differ significantly from the actual number of new cases. A so-called "nowcast" aims to first estimate the current figures using statistical analyses. A "forecast" provides an estimate of the development for another five days.

This is one of the projects that has accepted JSC's offer of computing time and support to help advance coronavirus-related research.

Contact: Jens Henrik Göbbert, j.goebbert@fz-juelich.de

New KI:STE Project − AI Strategy for Earth System Data

Artificial intelligence (AI) methods are currently experiencing rapid development and are also being used more and more frequently in the context of environmental data. However, this use is often in the context of isolated solutions. The systematic use of modern AI methods is not yet established in environmental and Earth system sciences. In particular, there is often a discrepancy between the requirements of a solid and technically sound environmental data analysis and the applicability of modern AI methods such as deep learning for researchers.

The KI:STE project (AI strategy for Earth system data; in German: KI-Strategie für Erdsystemdaten) closes this gap with a sophisticated strategy that combines the development of diverse AI applications on different socially relevant aspects of environmental and Earth system research with a strong training and network concept. It creates the technical prerequisites to make high-performance AI applications on environmental data portable for future users and to establish environmental AI as a key technology.

KI:STE is being funded by the German Federal Ministry for the Environment, Nature Conservation and Nuclear Safety (BMU) for a period of three years. The project will start on 1 November 2020, providing the opportunity to develop an AI platform and compose an Earth science database in collaboration with the University of Cologne, the University of Bonn, RWTH Aachen University, Ambrosys GmbH, 52°North GmbH, and the Institute of Bio- and Geosciences – Agrosphere (IBG-3). JSC is the coordinator of the project and will work on developing a scalable machine learning workflow oriented towards the AI platform. Further information can be found at https://kiste-project.de/home-en/.

Contact: Dr. Scarlet Stadtler, s.stadtler@fz-juelich.de

SEA Projects Selected for Funding by EuroHPC JU

The three members of the new SEA projects family (DEEP-SEA, IO-SEA, and RED-SEA) have been selected for funding in the first research and innovation call for proposals issued in 2019 by the EuroHPC Joint Undertaking (JU). The SEA projects complement each other and together address some of the most critical aspects concerning the operation and use of an exascale supercomputer: programming environment, data management, and interconnects. The projects will start in early 2021 and run for a period of four years.

The goal of **DEEP-SEA** ("DEEP – Software for Exascale Architectures") is to adapt all levels of the software stack to efficiently exploit highly heterogeneous compute and memory configurations, and to allow code optimisation across existing and future architectures and systems. The software stack will enable dynamic resource allocation, application malleability, and programming composability, and include tools to map applications to the Modular Supercomputing Architecture.

IO-SEA ("Input/Output Software for Exascale Architectures") aims to provide a novel data management and storage platform for exascale computing based on hierarchical storage management and the on-demand provisioning of storage services. Efficient management of storage tiers is achieved by removing unnecessary data movements and considering critical aspects of intelligent placement for very large volumes of data.

RED-SEA ("Network Solutions for Exascale Architectures") will pave the way for the next generation of European interconnects. In particular, it will develop the next generation of the Bull eXascale Interconnect, scalable to hundreds of thousands of nodes. New features and efficient network resource management covering congestion resiliency, virtualization, adaptive routing, and collective operations will be implemented.

The SEA projects are driven by a collaborative co-design approach with a selected set of high-impact applications. These representative applications help to formulate requirements that are addressed by software and hardware developers, and are also employed to evaluate the project's results and demonstrate their benefits for users of European computing centres.

JSC participates in all three SEA projects. In addition to leading the DEEP-SEA project and the definition of its software stack, JSC contributes the performance analysis tools Score-P and Scalasca, the monitoring tool LLview, the I/O library SIONlib, and the benchmarking tools Linktest and JUBE. JSC also provides application use cases in the areas of Earth system modelling and quantum chromodynamics. Furthermore, JSC leads the co-design activities in DEEP-SEA and IO-SEA.

Contact: Dr. Estela Suarez, e.suarez@fz-juelich.de

Kristel Michielsen among Falling Walls Finalists

JSC is proud to announce that Prof. Kristel Michielsen from JSC has been accepted as a finalist in this year's Falling Walls and Berlin Science Week (1-10 November 2020). This conference has grown into a World Science Summit to discuss the most recent breakthroughs in science and society. Kristel has been selected as one of 10 winners in the Physical Sciences category. Her project will be highlighted during the virtual Winners Session: Physical Sciences on 6 November, 1.15pm CET, in front of a global audience. Her contribution on "Breaking the Wall to Practical Quantum Computing" can be found at https://www.youtube.com/watch?v=6UyrFJWoruo. Congratulations!