JSC Strengthens Infrastructure for Data Services

In the first half of 2018, the storage infrastructure at JSC underwent a major overhaul and extension in order to address the ever increasing demand for capacity by its supercomputer users.

Since early 2018, a new IBM TS4500 tape library has augmented the two existing libraries for the storage of archive and backup data. The library is equipped with Linear Tape Open (LTO) media and kicks off the transition of JSC's entire tape infrastructure to this storage technology over the coming years. The new library provides a capacity of approximately 170 PB and 6 GB/s bandwidth.

In spring, the fifth generation of the central Jülich Storage Cluster JUST was installed. The system uses the IBM Spectrum Scale and GPFS Native RAID software stack to provide the same functionality and reliability as its predecessor and thus allows an online transition from old to new hardware. Consisting of 22 Lenovo DSS-G storage building blocks with 7,516 disks, JUST now provides a raw capacity of up to 75 PB and up to 500 GB/s bandwidth. Along with the upgrade, a new Ethernet fabric was introduced that scales up to the required multi-terabit/s performance.

The third addition to the storage landscape at JSC is a low-bandwidth, capacity-oriented, multi-purpose storage tier integrated in JUST. The capacity of this new tier, initially 40 PB raw, will be incrementally extended over the next few years. It will enable users to keep large data sets readily accessible for extended periods, store very large raw research data sets that require HPC processing and will also offer new sharing capabilities. To this end, the storage system will be combined with a cloud infrastructure for hosting community data services. JSC will introduce several new service offerings around this storage tier in the course of this autumn and next year.

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Thomas Lippert Elected Chair of PRACE Council

Prof. Dr. Dr. Thomas Lippert, head of the Jülich Supercomputing Centre and member of the board of the Gauss Centre for Supercomputing (GCS), was elected Chair of the PRACE Council during the 30th Council meeting in Amsterdam on 18 June 2018. He will serve a two-year term in this position. The PRACE Council is the highest decision-making body in PRACE, overseeing the research infrastructure and users' access to resources across the PRACE member organizations. Lippert became the German delegate in January 2018, but has long been involved in the creation and guidance of PRACE even before it was officially founded. He served as an advisor to Prof. Dr. Achim Bachem, former Director of Forschungszentrum Jülich and the founding Council Chair of PRACE.

According to Lippert, the challenge ahead for PRACE is to provide true exascale computing capability for science and industry in Europe. As PRACE Council Chair – and together with his colleagues and the scientific and industrial advisors – he is keen to bring the top-level HPC provision and support of PRACE together with the exascale systems of the coming EuroHPC Joint Undertaking.

CECAM Tutorial "Atomistic Monte Carlo Simulations of Bio-molecular Systems"

From 24-28 September 2018, JSC will host for the third time the CECAM tutorial "Atomistic Monte Carlo Simulations of Bio-molecular Systems" organized by SimLab Biology at JSC. Participants will be given an in-depth introduction to the theory and practice of Markov chain Monte Carlo (MCMC) methods as applied to atomistic simulations of proteins and other biomolecules. These ensemble methods offer a computationally efficient alternative to molecular dynamics simulations, in particular for studying processes with long time scales such as protein folding and peptide aggregation.

In contrast to the numerous training courses available for molecular dynamics, students rarely experience useful exposure to Monte Carlo (MC) techniques. CECAM (Centre Européen de Calcul Atomique et Moléculaire) is funding this five-day tutorial for the third time to fill this gap. The open-source protein folding and aggregation package ProFASi developed at SimLab Biology will be used as a demonstration tool for the highly transferable MC techniques. Participants will have access to JURECA for realistic tests of advanced parallel simulation techniques such as replica exchange MC or Wang-Landau. A particular focus of the course is the analysis and interpretation of MCMC simulations. Places are still available for interested researchers, who will find detailed information about the tutorial content on the web page for the CECAM school:
http://www.cecam.org/workshop-1601.html.

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NIC Excellence Project May 2018

The NIC Peer Review Board regularly awards the title "NIC Excellence Project" to outstanding simulation projects. At its April meeting, the board decided to honour Prof. Simon Trebst (Institute for Theoretical Physics, University of Cologne) for his project "Simulation of quantum-mechanical many-fermion systems". The project, which has been granted computing time on JUWELS, uses different methods to tackle the many-fermion problem. In particular, it employs different numerical approaches, including sign-problem-free quantum Monte Carlo, the pseudo-fermion functional renormalization group and machine learning techniques. For more details, see http://www.john-von-neumann-institut.de/nic/excellence-2018 (in German).

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vfdb Excellence Award for Benjamin Schröder

At this year's general meeting of the vfdb (Vereinigung zur Förderung des Deutschen Brandschutzes e.V.), Benjamin Schröder (formerly JSC) received the excellence award for his doctoral thesis. vfdb, which is the largest community for fire safety engineering in Germany, awards the prize once a year for outstanding scientific work with a crucial impact for fire safety.

Benjamin Schröder's work was part of the ORPHEUS project coordinated by JSC, which aimed at the fire safety of underground stations. The research in his thesis entitled 'Multivariate Methods for Life Safety Analysis in Case of Fire' tackled a holistic analysis of life safety. Two major aspects made the work outstanding: the analysis is based on a large scenario ensemble and it also features a new analysis approach for complex building structures.

In contrast to state-of-the-art analyses using only a few scenarios, the new approach led to more than 8500 scenarios for the underground station investigated. Here, the fire and evacuation dynamics were coupled and the smoke spread data were computed on the supercomputer JURECA. To analyse the large amount of data, a new method based on a spatiotemporally resolved ASET/RSET (available/required safe egress time) map was proposed. This led to the definition of a single scalar value to characterize the criticality of a scenario. Finally, a cluster analysis allowed a few scenarios to be identified which represent the full criticality spectrum. The methods outlined in Benjamin Schröder's thesis are already being applied by practitioners in the German fire safety community. For further information, visit
http://www.fz-juelich.de/ias/jsc/vfdb-award

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Events

Introduction and training "Intel KNL Many-Core - usage and profiling"
Instructors: Representatives of Intel, JSC staff members
Date: 3-6 September 2018
Venue: Jülich Supercomputing Centre, Rotunda
http://www.fz-juelich.de/ias/jsc/events/knl

Training for Maxeler Dataflow Architectures
Instructors: Leading experts from Maxeler
Date: 20-21 September 2018
Venue: Jülich Supercomputing Centre, Rotunda
http://www.fz-juelich.de/ias/jsc/events/maxeler

CECAM tutorial: Atomistic Monte Carlo Simulations of Bio-molecular Systems
Instructors: Dr. Sandipan Mohanty, Dr. Olav Zimmermann, Dr. Jan Meinke, JSC
Date: 24-28 September 2018
Venue: Jülich Supercomputing Centre, Rotunda
http://www.cecam.org/workshop-1601.html

Porting code from Matlab to Python
Instructors: Sandra Diaz, Lekshmi Deepu, Dr. Alexander Peyser, Wouter Klijn, JSC
Date: 8-9 October 2018
Venue: Jülich Supercomputing Centre, Computer Lab 2
http://www.fz-juelich.de/ias/jsc/events/matlab2python

Introduction to Python
Instructors: Martin Lischewski, Sebastian Linner, JSC
Date: 15-17 October 2018
Venue: Jülich Supercomputing Centre, Computer Lab 1
http://www.fz-juelich.de/ias/jsc/events/python

Introduction to GPU programming using OpenACC
Instructors: Dr. Andreas Herten, JSC Jiri Kraus, NVIDIA
Date: 29-30 October 2018
Venue: Jülich Supercomputing Centre, Computer Lab 1
http://www.fz-juelich.de/ias/jsc/events/openacc

For further events, talks, and training courses see
http://www.fz-juelich.de/ias/jsc/events