

JURECA - First Experiences

At 10:00 on Monday, 13 July 2015, the first phase of the JURECA system, consisting of 260 compute nodes with dual socket Haswell CPUs and 128 GiB main memory, went into production. The system was well received by users who had waited eagerly for the launch of the new system after the shutdown of JUROPA. Within a few hours the system utilization skyrocketed and has stayed at a constantly high level since then. The launch happened just in time for the International Supercomputing Conference ISC15 in Frankfurt, Germany, where JURECA was proudly presented at the JSC and T-Platforms booths and received much attention from exhibition visitors.

Users were able to prepare their jobs for the new architecture using the test system JUROPATEST, thus reducing the time required to start simulations on JURECA. Nevertheless, while the first phase of JURECA is close to its predecessor in terms of peak performance, the increased core count per node and architectural changes require the adaptation of workflows and optimization of applications. JSC is actively working with users to better adapt their jobs to JURECA. The JUROPATEST test system has been decommissioned and refurbished for a new purpose and is no longer available for JURECA users.

Over the last few weeks, JURECA has shown very satisfactory reliability despite its cutting-edge technology, such as the brand new Mellanox EDR InfiniBand. The tuning and optimization of the system software and hardware is continuing after the

start of production, and maintenance sessions are scheduled as needed to further improve the system. In parallel, work on the second JURECA phase, which could only be started after JUROPA had been decommissioned, is progressing. It is planned to make the full JURECA system with its 1,884 compute nodes in various configurations available to users in September.

(Contact: Dr. Dorian Krause,
d.krause@fz-juelich.de)

Decrypting Complex Brain Signals

Yury V. Zaytsev from the Simulation Laboratory Neuroscience has developed a new method of analysis for understanding the networks formed by hundreds or even thousands of nerve cells in the brain. The synaptic organization of neuronal networks and neural information processing is the basis of all higher-level cognitive brain functions such as vision or speech. Using multi-electrode array technology, neuronal activity in the form of electric pulses produced during the firing of neurons can be recorded, but these signals do not include any direct information about the topological structure of the associated brain region. The standard statistical method used to reconstruct neuronal networks based on generalized linear models can be used to decode networks consisting of some dozens of neurons. Zaytsev's algorithm is less computationally intensive than the above-mentioned method and thus allows the reconstruction of networks consisting of thousands of cells. This new approach uses the

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maximum-likelihood method and has an accuracy of more than 99% under ideal conditions, as has been shown in simulations. The analysis of these larger networks makes such demands on compute resources that it can only be performed on supercomputers. The detailed results are available in the Journal of Computational Neuroscience (<http://dx.doi.org/10.1007/s10827-015-0565-5>). (Contact: Prof. Abigail Morrison, slns@fz-juelich.de)

BaSiGo Project Successfully Completed

In June 2015, the BMBF-funded project "BaSiGo – Bausteine für die Sicherheit von Großveranstaltungen" ended after a duration of 40 months. Universities, research institutes as well as industry partners and safety authorities were involved in this civil security project.

The main motivation for this project was the tragic incident at the 2010 Loveparade in Duisburg, where 21 visitors died and more than 500 people in the crowd were injured. The major collaborative result is a manual, which has just been released to the public (<http://www.basigo.de/handbuch>). It will help to plan and implement future large-scale events. The partners have agreed to continuously expand and update the manual in form of a non-profit association.

Within BaSiGo, JSC's department "Civil Security and Traffic" (CST) performed laboratory experiments with a total of about 2,000 participants. In these experiments, densities of up to six people per square metre were realized, where each individual was automatically tracked by a camera system. Additionally, anonymized properties such as age, sex and height can be linked to each participant. Various geometric set-ups were investigated, such as crossings, bottlenecks and bi-directional flows. The first results of the experiments were included in the BaSiGo manual and are currently being prepared for publication in scientific journals. The large amount of data gathered in the experiments will provide the basis for further in-depth analysis in the coming years. The full dataset will be made publicly available thus allowing the whole community to perform independent analyses. Further information on BaSiGo can be found at <http://www.basigo.de/>.

(Contact: Prof. Armin Seyfried, a.seyfried@fz-juelich.de)

Lattice Practices 2015 at JSC in October

The Workshop "Lattice Practices", taking place from 14-16 October 2015 at JSC, will provide training in state-of-the-art numerical techniques and the use of information technologies for research in lattice quantum chromodynamics (LQCD). Organized by the joint SimLab "Nuclear and Particle Physics", it is primarily aimed at PhD students, but may also be of interest to postdocs and other LQCD researchers, who actively use high-performance computing (HPC) for their work. This year's workshop features lectures

and exercises on data analysis, solvers, and HPC architectures and performance optimization, with two advanced talks on valence techniques and finite temperature LQCD. A total of 30 students can participate in the workshop. For more details on schedule and registration please visit <http://www.fz-juelich.de/ias/jsc/lap15>.

(Contact: Dr. Stefan Krieg, s.krieg@fz-juelich.de)

New Team for Coordination of Computing Time Allocation at JSC

Two new members have joined the team coordinating computing time allocation:

The new head of the NIC Coordination Bureau is Dr. Florian Janetzko. Florian Janetzko studied Chemistry at the University of Hannover. He received his PhD in Theoretical Chemistry in 2003. After post-doctoral stays at CINVESTAV (Mexico City, Mexico), University of Calgary (Canada) and University of Bonn (Germany), he joined JSC's Application Support division in 2008 as a member of the Cross-Sectional Team Application Optimization. He has been involved, among other things, in support and teaching activities as well as in the European Projects DEISA and PRACE as the person locally responsible for the DECI calls.

Dr. Alexander Schnurpfeil is the designated successor of Dr. Manfred Kremer, who will retire from his position as Scientific Secretary of the John von Neumann Institute for Computing (NIC) at the end of March 2016. Alexander Schnurpfeil studied Chemistry at the universities of Leipzig, Bonn and Siegen and received his PhD in Theoretical Chemistry from the University of Cologne in 2006. After a post-doctoral stay at the University of Cologne, he worked as a software developer and teacher. He joined JSC in 2008, also in the Application Support division, where he was, among other duties, responsible for user support for the HPC-FF cluster and was local coordinator of the PRACE Preparatory Access Calls.

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

Calls for Computing Time Applications

New calls for computing time applications were issued on 27 July 2015. Please follow the links to the different types:

Regular simulation projects on JUQUEEN and JURECA: <http://www.fz-juelich.de/ias/jsc/computingtime>

Large-scale projects on supercomputers of the Gauss Centre for Supercomputing (GCS): <http://www.gauss-centre.eu/large-scale-application>

Computing time on the **JARA-HPC Partition**: <http://www.jara.org/de/research/jara-hpc/partition/>

All applications should be submitted by Friday, 28 August 2015, 17:00 at the latest.

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

Editor: Dr. Sabine Höfler-Thierfeldt, ext. 6765