JURECA Booster Installation Finalized

Since the announcement of the partnership between JSC, Intel, Dell and ParTec for the deployment of a Booster module for the JURECA system (see JSC News No. 250), the partners – together with the JURECA Cluster module supplier T-Platforms – have been working on installing the system and integrating it with the existing infrastructure. The Booster extends the 1,884-node Cluster with 1,640 additional compute nodes, featuring an Intel Xeon Phi 7250-F (Knights Landing) processor with 96 GiB main memory, interconnected by an Intel Omni-Path Architecture network. JSC and Intel designed the Booster component to complement the Cluster with an architecture focused on capability computing. The Booster is installed in 33 racks side-by-side with the 34 racks of the Cluster system in the JSC facility and shares the same administrative infrastructure, including the log-in partition. Both systems are high-speed interconnected through 198 bridge nodes.

Following the preparation of the facility until the end of August, the installation of the Booster equipment took place in September and October. In late October, JURECA was temporarily taken offline to finalize the integration and stabilization of the whole system. Following system acceptance in November, JSC expects to make the full Booster component available to users at the end of the month. The necessary system software extensions to enable cross-module job scheduling and

execution are currently available at prototype and release-candidate level and are expected to be generally available in early 2018.

Computing time on the JURECA Booster will be made available to members of Forschungszentrum Jülich and RWTH Aachen University through JARA-HPC/VSR calls. Moreover, during an interim period, scientists at German universities and research institutions can request computing time via the John von Neumann Institute of Compute (NIC) calls.
(Contact: Dr. Dorian Krause, *d.krause@fz-juelich.de*)

GAMM Activity Group on CSE Held Workshop at JSC

Together with a long-standing tradition of research on computational mechanics, the fields of mathematical modelling, numerics and scientific computing are key topics of the Gesellschaft für Angewandte Mathematik und Mechanik e.V. (GAMM). They form the basis of modern computational science and engineering (CSE), requiring interdisciplinary and international research collaborations across traditional boundaries.

The 2017 workshop of the GAMM activity group on CSE took place on 19-20 October at JSC. 27 participants from 4 European countries discussed a broad range of CSE-related topics, with a special focus on "coupling" and multi-physics simulations. Finding strategies to efficiently couple models, methods and software to solve for the indi-

vidual physics is a challenging task and a highly active field of research. In particular, with regard to upcoming exascale systems, the scalability of such coupled software solutions is the key to code sustainability and code applicability to solve even more complex multi-physics problems in the future.

This event was jointly organized by JSC, RWTH Aachen University Profile Area CompSE, and JARA-HPC. The partners will also support this distinguished GAMM activity group in the future. The next workshop is planned for summer 2018 at the University of Siegen. For more information on the recent event, visit
http://www.fz-juelich.de/ias/jsc/gamm-cse-2017.
(Contact: Dr. Robert Speck, *r.speck@fz-juelich.de*)

Antoine Tordeux Appointed Professor at University of Wuppertal

Antoine Tordeux started work at JSC in 2012. Having obtained his PhD in mathematics at Paris-Est University, he undertook research on traffic flow modelling and the estimation of road traffic fuel consumption and pollutant emission and gave lectures in statistics, probability and traffic flow theory in the prestigious French Engineering Schools "École des Ponts et Chaussées" and "École Polytechnique" from 2007 to 2012. At JSC, he has been working in the field of pedestrian and road traffic modelling and simulation with Prof. Seyfried in the Division Civil Security and Traffic. Tordeux was recently appointed junior professor at the Faculty of Mechanical and Safety Engineering of the University of Wuppertal. The professorship in Traffic Safety and Reliability is funded by the Eugen-Otto-Butz-Foundation. His lectures at the University of Wuppertal are about reliability engineering and road traffic safety. His research concerns the development of dynamic tools for the analysis of the reliability of driver assistance systems and autonomous vehicles. Motion planners in automation systems can be described, together with the noisy measurements of vehicle sensors, by stochastic processes for which it is possible to rigorously quantify collision probabilities. Tordeux will also, in collaboration with Dr. Chraibi and Prof. Seyfried at the JSC, develop a research project on the prediction of pedestrian dynamics in complex buildings using machine learning techniques. JSC wishes Antoine all the best in his new position at Wuppertal!

Festive Colloquium Marks the 30th Anniversary of the HLRZ and NIC

On 1 September 2017, JSC hosted a festive colloquium to mark the 30th anniversary celebration of the Höchstleistungsrechenzentrum (HLRZ) together with Prof. Hoßfeld's 80th birthday. The HLRZ is the forerunner of today's John von Neumann Institute for Computing (NIC). The event provided a welcome opportunity to look back on some remark-

able achievements and highlights made possible by simulation on high-performance computers in recent years. After a warm welcome by Prof. Sebastian Schmidt, Prof. Kurt Binder, chairman of the NIC Scientific Council, presented the answers to complex questions arising in the field of soft matter physics – a research area in which supercomputing has provided deep insights. Prof. Wolfgang Nagel from TU Dresden, who was a PhD student of Prof. Hoßfeld and JSC staff member in the 1990s, looked back at the origins of parallel computing. Prof. Thomas Lippert discussed the current state of today's supercomputing, and the evolving possibilities in neural networks and deep learning. Looking to the future, Prof. Hans De Raedt from the University of Groningen gave an outlook on the coming revolution of quantum computing and the associated challenges and opportunities. The staff and users of today's JSC and NIC would like to sincerely thank Prof. Hoßfeld for laying the foundations of these institutions and for all his ground-breaking and pioneering work. We look forward to the coming innovations with excitement and will always fondly remember the first steps into the then new field of HPC.
(Contact: Dr. Alexander Trautmann, *coordination-office@fz-juelich.de*)

End of Year Colloquium 2017

Date: Tuesday, 12 December 2017, 09:00-16:00
Venue: Jülich Supercomputing Centre, Hörsaal
Info: *http://www.fz-juelich.de/ias/jsc/events/eoy-2017*

09:00 Thomas Lippert: Welcome
09:15 Willi Homberg: Kühlkonzepte der Jülicher Supercomputer im Wandel der Zeit
09:40 Philipp Thörnig: Ein Booster für JURECA – Die Installation des ersten modularen Supercomputers für den produktiven Betrieb
10:05 Edoardo di Napoli: Simulating Quantum Materials: goals, obstacles and perspectives in the era of pre-exascale computing
11:00 Christian Feld: SCIPHI – Score-P and Cube extensions for Intel PHI
11:30 David Haensel: Eine Kuh macht Muh, viele Kühe machen Mühe.
12:00 Jette Schumann: Drängeln für die Gerechtigkeit – über die Psychologie in Fußgängerströmen
14:00 Jenia Jitsev: KI-Wandel durch Deep-Learning-Architekturen – von Durchbrüchen zu neuen Herausforderungen
14:30 Alexander Schug: Computersimulationen der molekularen Maschinerie des Lebens: Von der Proteinfaltung bis zur Medikamentenentwicklung
15:00 Holger Gohlke: Was haben Biomakromoleküle mit Stahlbaukonstruktionen gemeinsam?
15:30 Thomas Lippert: Abschlussvortrag