QPACE3 Completely Installed

The installation of both phases of the 3rd generation of QPACE systems has been completed at the Jülich Supercomputing Centre (JSC). The "QCD Parallel Computing Engine (QPACE)" project was started in 2007 by the universities of Regensburg and Wuppertal within the framework of the transregional Collaborative Research Centers SFB/TRR 55. The new system QPACE3 comprises 672 Fujitsu PRIMERGY CX1640 M1 servers with one Intel Xeon Phi 7210 processor each. All 43,008 cores could in theory deliver a performance of 1.79 Pflop/s. The nodes are interconnected using Intel's new Omnipath network technology, which also includes a few storage nodes. The storage can be accessed through a BeeGFS parallel file system.

The compute nodes are directly liquid cooled, which facilitates a very high packaging density. The whole system fits into nine racks that are not even fully populated. The efficiency of the liquid cooling system allows for high temperatures. With an outlet water temperature above 40 °C, most of the heat is removed using power-efficient dry free cooling. JSC is using the experience obtained with QPACE3 to plan for its next large-scale supercomputer, which is going to be installed next year.

QPACE3 is mainly dedicated to simulating the theory for strong interactions, namely quantum chromodynamics, in a version that is discretized on a lattice. The first phase of the system is listed at position 482 of the Top500 list and position 18 of the Green500 list. Further details about QPACE3 can be found at *http://www.fz-juelich.de/ias/jsc/qpace3*.
(Contact: Prof. Dirk Pleiter, *d.pleiter@fz-juelich.de*)

New NIC Research Group "Computational Structural Biology"

The new research group "Computational Structural Biology" of the John von neumann Institute for Computing (NIC) began work at Forschungszentrum Jülich in September 2017. The group is headed by Alexander Schug who studied physics at the University of Dortmund and obtained his doctorate in 2005 at Forschungszentrum Karlsruhe and the University of Dortmund. Afterwards, he worked as a postdoctoral scholar in Kobe (Japan) and San Diego (US) before becoming an assistant professor in chemistry (Umeå, Sweden). In 2011, he returned to Germany to head a Helmholtz Young Investigators Group at the Karlsruhe Institute of Technology. Schug has received multiple awards including a FIZ Chemie Berlin Preis from the German Chemical Society GdCH and a Google Faculty Research Award 2016. His general research interests include theoretical biophysics, biomolecular simulations, and high-performance computing (HPC).

At JSC, his group will leverage the constantly growing capabilities of HPC by integrating data from multiple sources in simulations to gain new insights into e.g. biomolecular structure and dynamics at atomic resolution as well as to understand neural cell tissue growth and differentiation.

As understanding these properties is the key to understanding biological function, this work promises to provide significant new insights with impacts in fields ranging from basic molecular biology to pharmacological and medical research.
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PRACE "Summer of HPC" 2017

For the fourth time, JSC participated in the PRACE "Summer of HPC". The programme offers summer placements for undergraduate and postgraduate students at HPC centres across Europe. Twenty-three candidates were selected from a pool of highly skilled and motivated applicants from all across Europe. The successful students then participated in ongoing research projects at ten different HPC centres within the timeframe from 1 July to 31 August 2017. Travel and accommodation costs as well as a bursary were provided by PRACE to all successful applicants.

This year, Antti Mikkonen (Finland) and Philippos Papaphilippou (Cyprus) joined JSC for the summer to gain firsthand experience in day-to-day research. After a training week for all 23 students in Ostrava at IT4Innovations (Czech Republic), Antti and Philippos started their summer projects at JSC. Antti was supervised by Andreas Beckmann working on a portability layer for fast multipole methods on GPUs, while Philippos was supervised by Stefan Krieg working on developing an auto-tuner for hybrid Monte-Carlo simulations.
(Contact: Dr. Ivo Kabadshow, *i.kabadshow@fz-juelich.de*)

Rhinodiagnost – HPC for Precision Diagnostics of Nasal Cavities

The Rhinodiagnost project prepares the implementation of a NOSE Service Center to deliver new extended possibilities of functional diagnostics to practicing physicians in rhinology and to advance personalized medicine. For a meaningful rhinological diagnosis, advanced rhinomanometry methods and computational fluid dynamics (CFD) are required to evaluate the effectiveness of patient-specific nasal functionalities.

Developments in the field of CFD and high-performance computing (HPC) allow us to individually predict the flow in a patient's human nasal cavity by means of numerical simulations, thereby enabling us to identify anatomical locations of pathologies. Hence, results from CFD and rhinomanometry can be used to *a priori* determine optimal surgery strategies for the individual patient in order to increase the success rate of surgery and to adapt treatment therapies accordingly.

Two German medical device companies, namely Sutter Medizintechnik GmbH and Med Contact GmbH, are joining forces with the Austrian partner Angewandte Informationstechnik Forschungsgesellschaft mbH, and the two research facilities Institute of Aerodynamics (AIA) at RWTH Aachen University and Jülich Supercomputing Centre at Forschungszentrum Jülich to implement the NOSE Service Center.

JSC will develop the software components, making the analysis of the simulation data accessible to the physician interactively and purposefully on modern HPC systems. Beyond this, the possibility of using virtual operations with direct updating and analysis of the flow parameters will be demonstrated in close cooperation with the AIA.

Rhinodiagnost is funded by the Federal Ministry for Economic Affairs and Energy (BMWi) in Germany. The Austrian partner is funded by COIN (Cooperation and Innovation), Federal Ministry of Science, Research and Economy (BMWFW). The project is running under the auspices of IraSME (International research activities by SMEs) for three years beginning in September 2017. Further details can be found at *http://www.rhinodiagnost.eu*.
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News from MATSE education

On 1 September 2017, 32 new students started their bachelor's course in Scientific Programming at Aachen University of Applied Sciences in combination with a training course as a MATSE (mathematical-technical software developer) at Forschungszentrum Jülich. Of these students, 28 will conduct their practical training in various institutes at Forschungszentrum Jülich, while 4 students have been placed with external partners (industrial companies). Both the vocational training and academic studies are designed to last three years. The curriculum and further information can be found at *http://www.fz-juelich.de/matse*. The application procedure for 2018 has already started.

At the end of August 2017, 30 MATSE trainees, who started their vocational training in 2014, passed their final examinations. During a ceremony on 31 August in the auditorium, they were warmly congratulated by Michael Arth from the Aachen Chamber of Commerce (IHK) and Ulrich Ivens from the Vocational Training Centre at Forschungszentrum Jülich. Five of the examinees achieved the best grade of "sehr gut", eighteen more scored the second-best grade "gut". The best result was attained by Steffen Domke (IEK-8), who achieved 95 %. Since 1964, more than 1,110 trainees have successfully completed this course at JSC.

As they were also enrolled on the bachelor's course in Scientific Programming at Aachen University of Applied Science (FH Aachen) at the same time, some of the MATSE trainees from Forschungszentrum Jülich also graduated with a bachelor's degree, thus finishing their course within the prescribed timeframe.
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