

## JSCNews

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### **New World Record in Qubit Simulation on JUQUEEN and Sunway TaihuLight**

The simulation of universal quantum computers (QCs) on classical digital computers is a major challenge. In order to increase the number of qubits of the QC by one, this requires the memory of the digital computer to be doubled. For instance, a computer with slightly more than 0.5 petabytes of memory is needed to accurately simulate the operation of a universal QC with 45 qubits.

There are only a few computers in the world which have the amount of memory, number of compute nodes, and a sufficiently powerful network connecting all the compute nodes to perform such simulations. Computing with such a large amount of memory and processors requires software that can efficiently use the parallel architecture of present-day supercomputers.

Recently, the Quantum Information Processing research group of JSC and the Computational Physics group of the University of Groningen, in collaboration with research groups from the University of Tokyo and Wuhan University, used their software to simulate universal QCs with 45 qubits on the Japanese K and the Chinese SunWay TaihuLight supercomputers.

The software, which was used in 2007 to simulate universal QCs with 36 qubits, set world records in 2010 (42 qubits) and 2012 (43 qubits) using JUGENE and JUQUEEN – the IBM Blue Gene/P and Q computers at JSC – respectively. The scaling of the simulation code is nearly perfect, making the

software a good benchmarking tool for testing very large parallel computers.

The research teams of JSC, Wuhan University, and the University of Groningen have now set a new world record by simulating 46-qubit quantum circuits on JUQUEEN and Sunway TaihuLight. For this breakthrough, an adaptive coding scheme was invented to represent the quantum state in terms of 2-byte instead of 16-byte numbers. Benchmarks including Shor's algorithm, adders, quantum Fourier transforms, and random circuits as well as Hadamard and CNOT operations show that the reduction in memory by a factor of eight has no significant impact on the accuracy of the outcomes. This new version of the simulation software can even be used to simulate a 32-qubit universal QC on a notebook with 16 GB of memory.

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### **NIC Symposium 2018**

The 9th NIC Symposium will be held at Forschungszentrum Jülich from 22 to 23 February 2018. The talks will inform a broad audience of scientists and interested members of the public about the activities and results obtained on the JURECA and JUQUEEN supercomputers at Jülich in the last two years by research projects supported through the John von Neumann Institute for Computing (NIC). Invited talks and a poster session will cover topics in the fields of astrophysics, biophysics, chemistry, elementary particle physics, condensed matter, materials science, soft mat-

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ter science, earth and environmental research, fluid mechanics, plasma physics, and computer science. To accompany the conference, a comprehensive proceedings volume will also be published. It will cover an even wider range of projects than represented by the talks. The detailed programme and the registration form are available at <http://www.john-von-neumann-institut.de/nic/nic-symposium>. (Contact: Dr. A. Trautmann, [a.trautmann@fz-juelich.de](mailto:a.trautmann@fz-juelich.de))

### Third Big Blue Gene Week

From 29 January to 5 February 2018, JSC will make JUQUEEN available for the third Big Blue Gene Week. Once again, it will be possible to run a whole series of massively parallel computations on at least four racks up to the size of the whole machine. Users are encouraged to consider this option in their workflows. If you have any questions, please send an email to [sc@fz-juelich.de](mailto:sc@fz-juelich.de). Further details can be found at <http://www.fz-juelich.de/ias/jsc/events/bbgw3>.

### NIC Excellence Project October 2017

The NIC Peer Review Board regularly awards the title "NIC Excellence Project" to outstanding simulation projects. At its October meeting, the board decided to honour Prof. Michael Moseler (Fraunhofer Institute for Mechanics of Materials, Freiburg) for his project "Ab initio investigation of properties and reactions at interfaces". The project, which has been granted computing time on JURECA, applies quantum mechanical methods to determine the electronic structure at interfaces. Moreover, the same methods are being used to study chemical reactions at interfaces. For more details, see <http://www.john-von-neumann-institut.de/nic/excellence-2017> (in German). (Contact: Dr. A. Trautmann, [a.trautmann@fz-juelich.de](mailto:a.trautmann@fz-juelich.de))

### Svenja Schmidt – Best MATSE in NRW and Germany

Svenja Schmidt from JSC was recognized as the best MATSE (mathematical-technical software developer) trainee in North Rhine-Westphalia (NRW) as well as throughout Germany in 2017 for her outstanding results in the final examinations of the MATSE training course. On 9 November, she was honoured at a large ceremony in Duisburg organized by the regional associations of the German Chambers of Commerce and Industry (IHK) in NRW, which served to highlight the excellent achievements of 240 trainees in all professions.

As the best MATSE graduate in Germany, Svenja Schmidt received an additional award on 4 December in Berlin. The ceremony for the best trainees of all German vocational training courses, which was moderated by Barbara Schöneberger, included a highly motivational speech by Günther H. Oettinger, European Commissioner for Budget & Human

Resources. JSC congratulates Svenja Schmidt on this great success.

Along with her MATSE degree, Ms. Schmidt will graduate with a bachelor's degree in Scientific Programming by completing her thesis on the "Gesture Control of 3D applications with Microsoft Kinect". Svenja Schmidt continues to work at JSC while also undertaking a master's degree in Technomathematics.

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### Awards for Bachelor's and Master's Students

On 8 December 2017, two students from Forschungszentrum Jülich received the Ehrenplakette award from Aachen University of Applied Sciences (FH Aachen). In a ceremony at Aachen's historic town hall, Prof. Baumann, rector of FH Aachen, honoured Gitte Kremling (JSC) as the best graduate from the bachelor's course Scientific Programming, and Thomas Rößler (JSC) as the best graduate from the master's course Technomathematics.

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### Best Paper Awards for ORPHEUS

Three conference contributions of the JSC-coordinated project ORPHEUS have been presented with best paper awards. The BMBF-funded project focuses on public safety in metro stations and will be completed in January 2018.

Two articles describe the experimental and numerical outcomes of underground climate investigations. The contribution of Ruhr University Bochum to the Suppression, Detection and Signaling Research and Applications Conference (SupDet) in September 2017 at Hyattsville, USA, looks at the measurement of the underground climate using fiberoptic communication cables. This experimental paper is accompanied by a paper on numerical simulations of the airflows in underground stations. It was authored by the Bundesanstalt für Materialforschung und -prüfung (BAM) in collaboration with JSC and was presented in September at the International Conference on Automatic Fire Detection (AUBE) in Hyattsville.

In June 2017, JSC's contribution to the International Workshop on Performance Portable Programming Models for Accelerators (P<sup>3</sup>MA) in Frankfurt tackled the performance portability of a real-time smoke spread code. The code, named JuROr, is written in OpenACC and developed from scratch within the ORPHEUS project.

These awards demonstrate the scientific impact of the BMBF-funded project, which has led to a broad range of publications and PhD theses. The ORPHEUS consortium will present its results at a public event in Berlin on 18 January 2018.

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