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## Official Inauguration of JUQUEEN

On 14 February 2013, the new supercomputer at JSC, JUQUEEN, was officially inaugurated in the presence of representatives from the German Federal Ministry of Education and Research (BMBF) and the Ministry of Innovation, Science and Research of the state of North Rhine-Westphalia (MIWF). After the last four of the 28 compute racks had been installed in January, JSC was proud to present JUQUEEN in its final configuration to the public.

Prof. Achim Bachem, Chairman of the Board of Directors of Forschungszentrum Jülich, welcomed the guests and thanked the ministries for their financial support provided through the Gauss Centre for Supercomputing (GCS). Prof. Wolf-Dieter Lukas, head of Directorate 5 at BMBF, delivered the official greeting on behalf of the federal minister. He congratulated Forschungszentrum Jülich for being part of the European FET Flagship "Human Brain Project", which will definitely add its share to the scientific simulations running on JUQUEEN. Helmut Dockter, State Secretary at MIWF, addressed JSC in the name of the NRW minister. He expressed his expectation to obtain simulation results relevant to the needs of society in order to facilitate future financial support. Prof. Thomas Lippert, head of JSC, presented a short history of the rapid development in supercomputing, outlined the scientific problems of high complexity that can be tackled with JUQUEEN, and gave an outlook on special simulations suitable to be run on this supercomputer. Following the speeches, the guests were invited to visit JUQUEEN in the machine room, and to toast the computer at a subsequent reception.

In the afternoon, the event continued with a scientific colloquium "Supercomputing in North Rhine-Westphalia". Four renowned top scientists from the fields of brain research, materials science, fluid dynamics and civil security research presented their simulations and gave an outlook on how JUQUEEN will enable new scientific insight for their fields.

(Contact: Dr. Sabine Höfler-Thierfeldt, *s.hoefler-thierfeldt@fz-juelich.de*)

## Guest Student Programme 2013

During summer 2013, JSC will once again be offering a guest student programme. It will be supported by the Centre Européen de Calcul Atomique et Moléculaire (CECAM), the German Research School for Simulation Sciences (GRS) and IBM. Within this programme, students with a major in natural sciences, engineering, computer science or mathematics will have an opportunity to familiarize themselves with different aspects of scientific computing. Together with local scientists, the participants will work on different current topics in research and development. Depending on their previous knowledge and on the participant's interest, the assignments can be taken from different areas. These fields include mathematics, physics, chemistry, software development tools, visualization, distributed computing, operating systems and communication. Special emphasis is placed on the use of supercomputers.

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The participants are expected to have knowledge of and experience in the computer-oriented branches of their subjects. The students should already have completed their first degree but have not yet finished their master's course. Additionally, a letter of recommendation from a university lecturer or professor is required for application.

The programme will last ten weeks and will take place from 5 August to 11 October 2013. Students are encouraged to apply for the programme via email or in writing (English or German). The closing date for applications is 30 April 2013. Further information at *http://www.fz-juelich.de/ias/jsc/gsp/*. (Contact: Dr. Ivo Kabadshow, *jsc-gsp@fz-juelich.de*)

## New DFG Projects GROMEX and CATWALK

Within the DFG priority programme 1648 "Software for Exascale Computing" (SPPEXA), JSC is partner in two new projects GROMEX and CATWALK. Both projects are being funded for a period of three years.

The goal of the **GROMEX project** is to develop a flexible, portable and ultra-scalable solver for potentials and forces within the GROMACS MD code, which is a prerequisite for exascale applications in particle-based simulations with long-range interactions in general. The second challenge is to realistically describe the time-dependent location of (partial) charges, as e.g. the protonation states of the molecules depend on their time-dependent electrostatic environment. Both tightly interlinked challenges are addressed by the implementation and optimization of a unified algorithm for long-range interactions that will account for realistic, dynamic protonation states, and at the same time overcome current scaling limitations.

The project is coordinated by the Max Planck Institute for Biophysical Chemistry in Göttingen with JSC and the Stockholm University as project partners. JSC will provide an implementation of a linear scaling, error-controlled fast multipole method (FMM), which will be ported to the Blue Gene/Q architecture and methodically extended to allow for dynamic protonation states without introducing additional computational overhead. For more information, visit the website *http://www.mpibpc.mpg.de/grubmueller/sppexa* or contact Dr. Holger Dachsel (*h.dachsel@fz-juelich.de*).

The **CATWALK project** deals with the following aspects: The cost of running applications at exascale will be tremendous. Reducing the runtime and energy consumption of a code to a minimum is therefore crucial. Moreover, many existing applications suffer from inherent scalability limitations that will prevent them from running at exascale in the first place. Current tuning practices, which rely on diagnostic experiments, have drawbacks because they detect scalability problems relatively late in the development process when major effort has already been invested in finding an inadequate solution. Furthermore, they incur the extra cost of potentially numerous full-scale experiments.

Analytical performance models, in contrast, allow application developers to address performance issues already during the design or prototyping phase. Unfortunately, the difficulties of creating such models combined with the lack of appropriate tool support still render performance modelling an esoteric discipline mastered only by a relatively small community of experts. The project's objective is, therefore, to provide a flexible set of tools to support key activities of the performance modelling process, making this powerful methodology accessible to a wider audience of HPC application developers. The partners are the GRS Aachen, Technische Universität Darmstadt, Goethe Center for Scientific Computing, Swiss Federal Institute of Technology Zurich and JSC. More information can be found at *http://www.vi-hps.org/projects/catwalk* or contact Dr. Bernd Mohr (*b.mohr@fz-juelich.de*).

## NIC Workshop HYBRID 2013

From 4-7 March 2013, the NIC Workshop "Hybrid Particle-Continuum Methods in Computational Materials Physics" was held at JSC. It was organized jointly by the NIC research group "Computational Materials Physics" and the Institute for Advanced Simulation. The goal of the workshop was to foster the exchange of ideas between the communities working on complex fluids and on complex solids. 65 participants learnt about the new developments in hybrid particle-continuum methods from 15 invited and 10 contributed talks as well as from 30 posters.

During the workshop, particular emphasis was placed on continuum-mediated interactions between particles, as well as on the adaptive and non-adaptive coupling between particle-based and continuum-based descriptions of materials. The subjects covered included the modelling of hydrodynamic interactions between particles in complex fluids or environments, through coarse-grained descriptions of biological systems, to the coupling of atomically represented regions with various continuum-based theories for fluids and solids. Special methodological aspects were long time scale properties of systems with slow collective dynamics, the development of efficient adaptive resolution algorithms, and the coupling of quantum-mechanically treated regions with continuum descriptions.

The proceedings of the workshop are available as a PDF file at *http://juser.fz-juelich.de/record/132949*.
(Contact: Prof. Martin Müser, *m.mueser@fz-juelich.de*)

## Events

**GPU Programming**
Instructors: Staff from JSC, GRS and NVIDIA
Date: 15-17 April 2013, 09:00-16:30
Venue: Ausbildungsraum 1, Jülich Supercomputing Centre
Registration: *http://www.fz-juelich.de/ias/jsc/events/gpu*

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