

JSCNews

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Big Blue Gene Week: Successful and Promising

As announced recently, the Blue Gene/Q supercomputer JUQUEEN at JSC was dedicated exclusively to large-scale massively parallel computations during the week from 14 to 20 June. The response was tremendous, with users taking the opportunity to execute some of their scientifically and computationally most demanding simulations in full parallelism on up to 458,752 compute cores.

More than 77% of the available time was used for true full machine runs, and in total 22 users were able to complete 84 jobs, which amounts to about 70 million core-h. The availability of the system during the week was higher than 93%, thus demonstrating its remarkable reliability. The event served various scientific use cases in topics such as turbulent fluid dynamics, neuroscience, elementary particle physics, molecular dynamics, and complex stencil code development. Among the specific problems addressed were modelling the propagation of polarized light through brain tissue by means of a massively parallel three-dimensional Maxwell solver to enhance the understanding of the structural organization of the human brain, and simulating the mixing of species in a turbulent decaying flow as it occurs in various practical situations.

Due to the positive response, JSC is considering repeating this type of event and encourages all users who have suitable codes and applications to join in and report on their experiences. All users interested in

further information are invited to contact JSC via sc@fz-juelich.de.

(Contact: Dr. Daniel Rohe, d.rohe@fz-juelich.de)

Award of Excellence for ITEA3 H4H Project

At the ITEA Event 2016 on 28 April in Stockholm, the ITEA Board Support Group presented three ITEA Awards of Excellence. These awards recognized high-level technical contributions based on true European collaboration that provide significant results and promote the ITEA programme and its goals. As one of these three projects, H4H received the Award of Excellence in the category "Business impact". The objective of H4H was to provide compute-intensive application developers with a highly efficient hybrid programming environment for heterogeneous computing clusters composed of a mix of classical processors and hardware accelerators. JSC contributed its experience in parallel program optimization and the well-established Score-P/Scalasca toolset for parallel program measurement and analysis to the project, which was funded from 2010 to 2015. JSC's participation in ITEA projects is a real success story: the predecessor project ParMA also received an ITEA Achievement Award in Gold in 2010. More information on the awards and the projects recognized can be found at <https://itea3.org/itea-event-2016/awards-of-excellence.html>.

(Contact: Dr. Bernd Mohr, b.mohr@fz-juelich.de)

Forschungszentrum Jülich GmbH
in der Helmholtz-Gemeinschaft
Jülich Supercomputing Centre
52425 Jülich | Germany

Phone +49 2461 61-6402

jsc@fz-juelich.de
www.fz-juelich.de/jsc

Summer of HPC 2016 - Kick-Off @ JSC

Summer of HPC is a PRACE programme that offers summer placements at HPC centres across Europe to undergraduates and postgraduate students. This year, 21 students from more than 10 different European countries were selected from over 100 applicants to participate. The students will spend two months working on projects related to PRACE scientific or industrial work and eventually prepare a visualization or video as well as a written report of their results.

However, before working together with domain scientists at the hosting sites, participants had to acquire a basic knowledge of HPC. This year's training week took place at JSC from 4 to 8 July and included lectures and hands-on sessions. During the week-long courses, the students learned basic HPC parallelization techniques such as MPI, OpenMP, and CUDA as well as visualization of scientific data. The training also included a high-performance kart race at the nearby Michael Schumacher race track to explain the subtle differences between latency and bandwidth in an experimental setup.

After this challenging and eventful kick-off, two students will remain at JSC for their summer project. Peter Labus from Italy, supervised by Stefan Krieg, will dive into the field of lattice quantum chromodynamics; Johannes Pekkilä from Finland, supervised by Andreas Beckmann, will support the development of fast multipole methods for molecular dynamics simulations on GPUs.

(Contact: Dr. Ivo Kabadshow, i.kabadshow@fz-juelich.de)

Farewell, JUVIS

After more than seven years of successful operation, our visualization cluster JUVIS has reached the end of its lifetime and will finally be shut down by the end of July 2016. After this date, all data stored on the local file system of JUVIS (/home and /viswork) will be deleted. Users who want to save important data are responsible for migrating all files in question to another storage system before the end of July.

The visualization cluster JUVIS was equipped with GPUs and had a direct connection to our GPFS storage system, enabling remote visualization of scientific data without the need to copy large data files to the render cluster itself. From now on, this service will be hosted on dedicated visualization nodes integrated in our JURECA HPC system.

(Contact: Dr. Herwig Zilken, h.zilken@fz-juelich.de)

JURECA Visualization Nodes Available

To perform remote rendering and post-processing of scientific data, 12 GPU-equipped visualization nodes are available as part of our JURECA cluster. Two visualization nodes are configured as login nodes and can be directly accessed via a login to jurecavis.zam.kfa-juelich.de. The remaining

ten visualization nodes are driven by the batch system in the 'vis' partition. We provide ten vis nodes with 512 GB and two with 1 TB main memory.

As a graphical login considerably simplifies access to remote visualization and the data stored on the file system, we support and recommend the use of Virtual Network Computing (VNC) in conjunction with VirtualGL. These tools allow OpenGL commands of visualization software to be directly executed on the GPUs of the JURECA visualization nodes, speeding up the rendering process. To set up a flawless VNC connection to JURECA very easily, we suggest using the utility Strudel developed by the Multi-modal Australian ScienceS Imaging and Visualisation Environment (MASSIVE) at Monash University, Melbourne, Australia. JURECA has been prepared and Strudel updated in recent versions to support our visualization nodes.

All users with an HPC project on JURECA already have access to the JURECA vis nodes via their normal project account. Other users are able to gain access by sending a substantiated request to sc@fz-juelich.de. For further details about how to use the vis nodes of JURECA for remote rendering please refer to the documentation at <http://www.fz-juelich.de/ias/jsc/jureca-visnodes.html>

(Contact: Dr. Herwig Zilken, h.zilken@fz-juelich.de)

Events

Introduction to parallel programming with MPI and OpenMP

Instructors: Dr. Florian Janetzko, Dr. Alex Schnurpfeil, JSC

Date: 09-12 August 2016, 09:00-16:30

Venue: Jülich Supercomputing Centre, Ausbildungsraum 1

Info: <http://www.fz-juelich.de/ias/jsc/events/mpi-gsp>

CECAM Tutorial: Atomistic Monte Carlo Simulations of Bio-molecular Systems

Date: 19-23 September 2016, 09:00-16:30

Venue: Jülich Supercomputing Centre, Rotunda

Info: <http://www.cecama.org/workshop-1339.html>

First JARA-HPC Symposium

Date: 04-05 October 2016

Venue: IT Center, RWTH Aachen University

Info: <http://hpc-symposium.jara.org>

Introduction to GPU programming using OpenACC

Instructors: Anke Zitz, Dr. Andreas Herten, Dr. Paul Baummeister, JSC; Jiri Kraus, NVIDIA

Date: 24-25 October 2016, 09:00-16:30

Venue: Jülich Supercomputing Centre, Ausbildungsraum 1

Info: <http://www.fz-juelich.de/ias/jsc/events/openacc>

If you would like to receive regular information on our events, please send an email to jsc-events-join@fz-juelich.de.

Further events, talks, and training courses:

<http://www.fz-juelich.de/ias/jsc/events>

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