



Jülich Supercomputing Centre

HBP Launches European Research Infrastructure

The Human Brain Project (HBP) is developing a shared European research infrastructure to investigate the human brain using detailed analyses and simulations. For this purpose, the HBP is creating new information technologies such as neuromorphic processors, which are based on the principles governing how the brain works. On 30 March 2016, the HBP released an initial version of the infrastructure, which was built by researchers from 24 countries over the last two-and-a-half years, to users outside the project. With this step, the Human Brain Project is now entering its next phase. The six platforms forming the infrastructure are intended to drive progress not only in neuroscience but also in the European development of HPC and robotics as well as to interconnect researchers through four large European supercomputing and data centres, including JSC.

JSC and CSCS in Lugano, Switzerland, are coordinating the creation and operation of the HBP's High Performance Analytics and Computing Platform. Together with 14 collaboration partners, JSC provides the European neuroscience community with support in using the supercomputers, storage systems, and software. Petabytes of data on the human brain, generated for example by techniques such as polarized light imaging or by simulation, can be stored on the platform and can be analysed and visualized on supercomputers like JURECA using state-of-the-art methods such as deep learning. The research infrastructure can be centrally accessed through the HBP Collaboratory, a web portal where users can also find guidelines, tutorials and information on training seminars, see https://collab.humanbrainproject.eu/. (Contact: Dr. Boris Orth, hbp-hpc-platform@fz-juelich.de)

Big Blue Gene Week

Massive parallelism will be a key quality for tomorrow's supercomputers, and JSC is committed to supporting its users in order to make their applications as scalable as possible. Experiences with scalable applications on the Tier-0/1 parallel supercomputer JUQUEEN acquired through the Extreme Scaling Workshop series and the High-Q Club have encouraged us to maximize the capability of this system by largescale simulations with big jobs.

In order to achieve this goal, JSC plans to schedule a Big Blue Gene Week on JUQUEEN from 14 to 20 June 2016. During this week, job scheduling will be modified so that only jobs with a minimum of four Blue Gene/Q racks, or 65,536 compute cores, will be allowed to run. Smaller jobs will be excluded from execution. This will allow better scheduling and quicker turnaround of jobs requiring four to 28 racks. All projects using JUQUEEN should consider this week in their planning.

Depending on how the Big Blue Gene Week is received by our users and whether there is demand to continue this activity, JSC will consider establishing periods favouring big jobs more frequently. No. 240 • April 2016

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

Phone +49 2461 61-6402

jsc@fz-juelich.de www.fz-juelich.de/jsc Questions and support requests concerning the Big Blue Gene Week should be addressed to *sc@fz-juelich.de*. (Contact: Wolfgang Frings, *w.frings@fz-juelich.de*)

JURECA Porting and Tuning Workshop

In the past few years, JSC has been running Porting and Tuning Workshops on its highly scalable Blue Gene/Q system JUQUEEN. This year's workshop will cover the latest system in Jülich, the new general-purpose cluster JURECA. As the successor to the apparently similar JUROPA system, JURECA is at first as easy to use. The increased complexity of the system, however, requires special attention to multithreading and vectorization to achieve peak performance.

The workshop will take place on 6-8 June 2016. The topics will include best practices for JURECA, possibilities of visualization, and scientific big data analytics. We will also cover efficient I/O and ways to achieve multi-threading and vectorization as well as GPU programming. Special emphasis will be placed on node-level performance and performance analysis.

At the heart of the workshop will be extensive hands-on sessions with the participants' codes, aimed at helping with porting applications to JURECA and understanding performance bottlenecks. After the workshop, participants should have their codes running on JURECA and a clear picture of how to further improve performance. The event will be supervised by members of staff from JSC's Simulation Laboratories and the cross-sectional teams Application Optimization, Performance Analysis, Visualization and Mathematical Methods and Algorithms. Further information can be found at *http://www.fz-juelich.de/ias/jsc/jurecapt16*.

(Contact: Dr. Dirk Brömmel, d.broemmel@fz-juelich.de)

Reaching the Plateau of Enlightenment: GPU Hackathon in Dresden

The first of this year's GPU Hackathons, which are coordinated by ORNL, was jointly organized by TU Dresden and JSC. Six teams came to Dresden from 29 February to 4 March with the goal of accelerating their applications on GPUs focussing on using OpenACC as a programming model.

A team from Charité Berlin worked on GraphVar, a graph theory application to study brain connectivity. A team from JSC came with JuROr, which aims to enable real-time smoke simulations on small computers, while a team from the University of Hannover worked towards large-scale turbulence simulations using PALM. Hunting planets is the goal of a team from the European Southern Observatory. Their application allows them to compare models of planet formation with data from big radio telescopes. The fifth team, from the University of Göttingen, does research on objects at much smaller length scales. Their Monte Carlo simulator enables the physical properties of polymers to be investigated. A local team from MPI for the Physics of Complex Systems intends to simulate bacteria and investigate how they can agglomerate.

Each team received intensive support from at least two tutors. The tutors were provided by PGI, NVIDIA, TU Dresden, JSC, HZDR, MPI and RWTH Aachen University. All the teams appreciated this opportunity of working with so many experts. Hacking for more than 8 hours a day was the usual format, only interrupted by scrum sessions led by Fernanda Foertter (ORNL). All the teams successfully found their way from an initial peak of youthful ignorance through the trough of despair before reaching the slope of hope during the middle of the week. During the final presentations, all the teams confirmed that they had reached the first plateau of enlightenment and left Dresden fired with enthusiasm.

At least three more GPU Hackathons will take place in 2016, including one at CSCS in July. Visit *https://gcoe-dresden.de/?cat=12* and *http://bit.ly/2016GPUHack*. (Contact: Prof. Dirk Pleiter, *d.pleiter@fz-juelich.de*)

Collective Dynamics – a New Open Access Journal

The multidisciplinary journal *Collective Dynamics* focuses on research in the field of pedestrian dynamics, crowds, vehicular traffic and other systems of self-driven particles, such as molecular motors, animal groups or agents. For interdisciplinary research in these areas, it is often difficult to find the appropriate journal and the most suitable audience. Thus the journal aims to be a forum for all researchers working on traffic-like systems, ranging from physicists and computer scientists to psychologists. It welcomes work on fundamental (empirical as well as theoretical) research or concrete applications.

As a peer-reviewed journal, *Collective Dynamics* publishes scientific papers, systematic reviews and other educational articles, e.g. lecture notes. It is an open access journal free of charge and independent of a publishing company. Founded by Prof. Andreas Schadschneider from the University of Cologne and staff members of JSC, *Collective Dynamics* published the first two articles in March 2016. The homepage of the journal can be found at

http://collective-dynamics.eu/.

(Contact: Prof. Armin Seyfried, a.seyfried@fz-juelich.de)

Events

Node-Level Performance Engineering

Instructors: Dr. habil. Georg Hager, Prof. Gerhard Wellein, RRZE/HPC, University of Erlangen Date: 28-29 April 2016, 09:00-17:00 Venue: Jülich Supercomputing Centre, Rotunda Info: http://www.fz-juelich.de/ias/jsc/events/node-level

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