



Jülich Supercomputing Centre

Human Brain Project - PCP: Call for Tender

As the leader of the Human Brain Project's High-Performance Computing Platform subproject, Forschungszentrum Jülich is conducting a pre-commercial procurement (PCP) in order to obtain appropriate innovative HPC technology solutions that meet the specific requirements of the project. The HBP PCP will procure research and development services for HPC system components allowing interactive visualization and steering of large-scale and data-intensive brain simulations on a pre-exascale HPC architecture. The tender documents can be downloaded at http://apps.fz-juelich.de/hbp-pcp/ (registration required).

(Contact: Dr. Boris Orth, b.orth@fz-juelich.de)

JSC at ISC'14

The International Supercomputing Conference (ISC) will take place from 23 June to 26 June 2014 in Leipzig. JSC, together with its partners in the Gauss Centre for Supercomputing (GCS), namely HLRS (Stuttgart) and LRZ (Garching), will present its wideranging supercomputing activities at the GCS booth #940.

In particular, JSC will showcase LLview, the comprehensive interactive monitoring software for supercomputers developed inhouse, demonstrating live the operation of various supercomputers worldwide. In addition, JSC will also show the LLview monitoring components of the Eclipse PTP development environment for supercomputing applications. A wide spectrum of scientific results obtained with the supercomputers at Jülich will be presented in videos and animations. Finally, JSC's participation in the Human Brain Project will be another hot topic.

JSC staff will give several presentations at the conference and will also be on hand at the European Exascale Projects (#833), the PRACE (#932), and the UNICORE (#951) booths. Detailed information about JSC's participation can be found at http://www.fz-juelich.de/ias/jsc/isc14. (Contact: Dr. Walter Nadler, w.nadler@fz-juelich.de)

Successful Technology Transfer with Siemens

In a cooperation with the Corporate Technology Multicore Expert Center of Siemens AG, work has started on the RAPID project (Runtime Analysis of Parallel applications for Industrial software Development). In a first step, experts from JSC and Siemens will extend and enhance measurement and analysis support for node-level programming models of JSC's well-known HPC performance toolset Scalasca, as these are the current basis for industrial applications. This includes multi-threading models like POSIX, Windows, ACE, and QT threads as well as task-based models like MTAPI. This will also benefit Scalasca's current HPC users who employ these models in hybrid applications as well.

(Contact: Dr. Bernd Mohr, b.mohr@fz-juelich.de) No. 222 • May 2014

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Computer Simulation Explains Iridescent Colours of a Bird-of-paradise

The silvery neck feathers and the orange-green-blue iridescent breast feathers of the male bird-of-paradise Lawes's parotia form a sharp contrast to their otherwise jet black plumage. The role of these coloured feathers in the mating dance has only recently been unravelled, but their coloration mechanism remained poorly understood. In a recent PNAS article, Kristel Michielsen from JSC and her colleagues from the University of Groningen, the Netherlands, give an explanation for the various optical mechanisms causing the feathers' colours.

The coloration of both feather types is structural: the colour is produced by melanin rodlets arranged in layers, together acting as interference reflectors. The light reflection by the silvery neck feathers is unidirectional and well-described by multilayer theory. The reflection by the richly coloured breast feathers is three-directional and much more complex.

To unravel the reflection properties of the breast feathers, Kristel Michielsen and her colleagues applied finitedifference time-domain (FDTD) modelling. Transmission electron microscopy sections of feather barbules, the smallest branches of feathers, were greyscaled, extended into a three-dimensional simulation volume, and, subsequently, complex refractive index values were assigned to the different greyscale values. The FDTD modelling confirmed and refined the multilayer treatment of the neck feathers, but the modelling approach allowed for the first time a detailed explanation of the multicoloured breast feathers. It thus was found that the boomerang-shape of the barbules of the breast feathers enables the birds to change the colour of their chest plumage abruptly while dancing.

TDME3D, a massively parallel Maxwell equation solver, was used for the simulations, which were performed on the IBM Blue Gene/P of the University of Groningen. The calculation for one structure, one wavelength, one polarization state, and one incidence angle required a memory of approximately 150 GB. More information can be found in the PNAS article (DOI:10.1073/pnas.1323611111).

(Contact: Prof. Kristel Michielsen,

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New GCS Large-Scale Projects

Twice a year, the Gauss Centre for Supercomputing (GCS) issues a call for large-scale projects on its petascale supercomputers JUQUEEN (JSC), HERMIT (HLRS), and Super-MUC (LRZ). Projects are classified as large-scale if they require at least 35 million core hours.

At its April meeting at GSI Helmholtzzentrum für Schwerionenforschung in Darmstadt, the GCS Peer Review Board decided to award the status of a large-scale project to seven projects. One project was granted a total of 70 million compute core hours on HERMIT and the other six projects were granted a total of about 314 million core hours on JUQUEEN. The projects come from the fields of astrophysics, chemistry, high-energy physics, and fluid dynamics. For more details on these projects, see *http://www.gauss-centre.eu/large-scale*.

(Contact: Dr. Walter Nadler, w.nadler@fz-juelich.de)

"Bernstein Network - Simulation Lab Neuroscience" HPC Workshop

Neuroscience today is attacking problems of increasing complexity and scale, as exemplified by projects like the Human Brain Project. The application of large data sets to computationally intensive theoretical simulations and analyses requires the adaptation of software and theory from local clusters to high-performance computing systems (HPC). To bring HPC scientists together with neuroscientists interested in HPC applications, the "Simulation Laboratory Neuroscience – Bernstein Facility for Simulation and Database Technology" at JSC and the "National Bernstein Network Computational Neuroscience" will hold a workshop for scientists interested in collaborating in the development of petascale neuroscience simulations and analyses.

This workshop will be focused on finding ways to make JSC resources available to the neuroscience community by expanding projects to current supercomputer scales, exploring new problems which may be amenable to methods available at this scale, and catalysing collaborations with the Sim-Lab Neuroscience. The SimLab will present currently available resources at the JSC and on-going projects that leverage those resources. Attendees will present current neuroscience problems that they are interested in exploring using the larger computational resources available in Jülich.

The workshop will take place on 4 and 5 June at JSC. Please contact *hpcns-meetings@fz-juelich.de* by 18 May to register. For further information, see

http://www.fz-juelich.de/ias/jsc/events/bernstein-hpc. (Contact: Dr. Alexander Peyser, a.peyser@fz-juelich.de)

Events

Parallel I/O and Portable Data Formats

Instructors: W. Frings, Dr. M. Stephan, Dr. F. Janetzko, JSC Date: 21-23 May 2014, 09:00-16:30 Venue: Ausbildungsraum 1, Jülich Supercomputing Centre

Registration: http://www.fz-juelich.de/ias/jsc/events/parallelio

3rd Workshop on Parallel-in-Time Integration Date: 26-28 May 2014, 09:00-16:30

Venue: Rotunda, Jülich Supercomputing Centre Info: http://www.fz-juelich.de/ias/jsc/pintws2014