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Workshop on Supercomputing for Neuroscientists

Neuroscience today is tackling problems of increasing complexity and scale as exemplified by projects such as the Human Brain Project. To fulfil the requirements of computationally intensive simulations and analyses of large data sets, applications suitable for high-performance computing (HPC) systems need to be newly developed or adapted from algorithms originally designed for PCs and small clusters.

With the aim of bringing together neuroscientists interested in using HPC technology for their projects with experts from JSC's Simulation Laboratory Neuroscience, JSC is organizing a workshop "Supercomputing for Neuroscientists" on 3 November 2015. Participants will learn about HPC and how it can be used as an instrument for neuroscience. The SimLab will present some current projects and collaborations as examples of how neuroscience can benefit from using supercomputers. Examples include brain modelling and simulation, and the processing and analysis of brain imaging data. Experts from JSC will explain how to obtain access to Jülich's JUQUEEN and JURECA supercomputers and how the SimLab can support neuroscience groups using these systems. While this part of the workshop is primarily intended for scientists whose affiliation is in Germany and who may therefore apply for computing time on the Jülich supercomputers through the national GCS and NIC calls, it will also touch on how European supercomputing resources, including those at Jülich, may be accessed by scientists from outside Germany through the European PRACE access schemes. Further information can be found at *http://www.fz-juelich.de/ias/jsc/scn*.
(Contact: Dr. Boris Orth, *b.orth@fz-juelich.de*)

Both Sides of PRACE "Summer of HPC"

For the second time, JSC participated in the PRACE "Summer of HPC". This programme offers summer placements for undergraduate and postgraduate students at HPC centres across Europe. Twenty candidates were selected from a pool of highly skilled and motivated applicants from all over Europe. The successful students then participated in on-going research projects at ten different HPC centres, in the period from 1 July to 31 August 2015. Travel and accommodation costs, as well as a grant towards expenses, were provided by PRACE to all successful applicants.

However, it was not only the interested students who had to apply for the programme, also the hosting HPC centres had to undergo a competitive selection process. This year, there were two applications from JSC: one as a host for students with a strong interest in learning how to optimize code for our supercomputers, and a second one from JSC master student Jana Boltersdorf, who applied to spend the summer outside Germany at a different HPC site.

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Both our applications were successful. While Sarah Jenkins (UK) and Albert Garcia (Spain) joined JSC for the summer to gain first-hand experience in day-to-day research, Jana Boltersdorf went to Edinburgh, where she worked on parallelizing a fluctuating finite element analysis (FFEA) tool via MPI. Albert and Sarah were supervised by Andreas Beckmann and Stefan Krieg, working on a molecular dynamics code based on the fast multipole method (FMM) and on optimizing compute kernels from lattice quantum chromodynamics (LQCD). Details on the "Summer of HPC" projects with blogs and videos by the participants can be found at *https://summerofhpc.prace-ri.eu/*.
(Contact: Dr. Ivo Kabadshow, *i.kabadshow@fz-juelich.de*)

MAXI - Multi-system Application Extreme-scaling Imperative

JSC organized the mini-symposium MAXI from 3-4 September 2015 as part of this year's International Conference on Parallel Computing (ParCo) 2015 in Edinburgh. The goal was to encourage users to report about scaling their applications on more than one HPC system. Various contributions from fields such as engineering, neuroscience, and earth modelling were presented. The researchers explained their codes and results gained on systems such as Tianhe-2 (TOP500 ranking #1), large Blue Gene/Q installations (#3, #5, and #9), K computer (#4), SuperMUC Phase 1 and Phase 2 (#20 and #21) and other x86 clusters, as well as the latest NEC vector architecture, sometimes even comparing their performance between architectures. Specific node level performance improvements were also presented as well as an update on the 2013 Gordon Bell award winning code. A broader spectrum of applications and system experience was covered by talks on scaling workshops and usage statistics from JUQUEEN, SuperMUC-2, and K computer. Those activities were reported to lead to easy transitions to even bigger scales, to help co-design future HPC systems, and enable production runs on the 28 racks of JUQUEEN or even simulations of bigger problem sizes.

Overall, the mini-symposium was well received and it became clear that more discussion and reports are desirable also covering problems encountered when using larger and larger systems. Not only should outstanding results be recognized but also the efforts required to reach them. Further information is available at *http://www.fz-juelich.de/ias/jsc/MAXI*.
(Contact: Dr. Dirk Brömmel, *d.broemmel@fz-juelich.de*)

MATSE Exams Passed

At the end of August 2015, all 28 MATSE trainees (mathematical-technical software developers) supervised by the JSC education team passed their final examinations. During a ceremony on 4 September 2015, they were warmly congratulated by Gisbert Kurlfinke, Aachen Chamber of Commerce (IHK), Prof. Volker Sander, Aachen University of Applied Sciences (FH Aachen) and Immo Wetcke, Head of the Office of the Board of Directors (FZJ). The best result was achieved by Thomas Rößler (JSC). He achieved 94 percent, which was the second highest mark of all 115 examinees in the district of Aachen. Since 1964, more than 1,050 trainees have successfully completed this course at JSC.

Since they were also enrolled on the bachelor's course in Scientific Programming at Aachen University of Applied Science (FH Aachen) at the same time, 60 % of the MATSE trainees from Forschungszentrum Jülich also graduated with a bachelor's degree, thus finishing their course in the prescribed time.
(Contact: Prof. Paul Jansen, *p.jansen@fz-juelich.de*)

MATSE: New Course Started

On 1 September 2015, 31 new students started the bachelor's course in Scientific Programming at Aachen University of Applied Sciences in combination with a training course as a MATSE at Forschungszentrum Jülich. Of these students, 26 will receive their practical training in various institutes at Forschungszentrum Jülich, while 5 students have been placed with external partners (industrial companies). Both the vocational training and academic studies are designed to take three years. The curriculum and further information can be found at *http://www.fz-juelich.de/matse*.

The application procedure for 2016 has already started.
(Contact: Prof. Paul Jansen, *p.jansen@fz-juelich.de*)

Events

Workshop Lattice Practices 2015
Date: 14-16 October 2015
Venue: Jülich Supercomputing Centre, Rotunda
Registration: *http://www.fz-juelich.de/ias/jsc/lap2015*

Introduction to GPU programming using OpenACC
Instructors: Anke Zitz, Thorsten Hater, Dr. Paul Baumeister, JSC; Jiri Kraus, NVIDIA
Date: 19-20 October 2015, 9:00-16:30
Venue: Jülich Supercomputing Centre, Ausbildungsraum 2
Registration: *t.hater@fz-juelich.de*

Workshop Supercomputing for Neuroscientists
Date: 3 November 2015, 09:00-17:00
Venue: Jülich Supercomputing Centre, Rotunda
Registration: *http://www.fz-juelich.de/ias/jsc/scn*

Data analysis and data mining with Python
Instructors: Dr. Jan Meinke, Dr. Olav Zimmermann, JSC
Date: 9-11 November 2015, 9:00-16:30
Venue: Jülich Supercomputing Centre, Ausbildungsraum 1
Registration: *j.meinke@fz-juelich.de*

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