New Chairman of GCS Board of Directors

Prof. Thomas Lippert, head of the Jülich Supercomputing Centre, is the new Chairman of the Board of Directors of the Gauss Centre for Supercomputing (GCS). He was elected to this position in mid-April during a GCS assembly in Munich. According to the statutes of GCS, Lippert will hold this post for two years. The position of chairman alternates regularly between the three GCS member centres.

JSC in Four EU-Funded Centres of Excellence

On 8 May 2015, the results were announced of a hotly contested call for new Centres of Excellence within the EU Horizon2020 E-Infrastructures Programme. These new funding instruments are designed to harness computational science and big data expertise in HPC to promote scientific discovery and industrial competitiveness. Out of the 20 submitted proposals, four of the eight projects approved for initial funding will involve JSC participation. These are: EoCoE – an Energy-oriented Centre of Excellence; MaX – Materials Design at the Exascale; E-CAM – an E-infrastructure for Software, Training and Consultancy in Simulation and Modelling; and POP – Performance Optimisation and Productivity.

EoCoE ('echo'), coordinated by the Maison de la Simulation at CEA-Saclay, received the highest grade of the evaluation, and aims to exploit HPC in accelerating the transition to a low-carbon energy supply. It will involve five separate teams from JSC, IEK, and IBG at Forschungszentrum Jülich, as well as over 20 external partners from all over Europe. All four projects plan to start in the autumn of this year.
(Contact: Prof. Paul Gibbon, *p.gibbon@fz-juelich.de*)

15-Year-Old JSC Trainee among Intel ISEF Finalists

The Intel International Science and Engineering Fair (Intel ISEF) is the world's largest international pre-college science competition. Student participants are ninth-through twelfth-graders who earned the right to compete at this annual event by winning a top prize at a local, regional, state, or national science fair. Former JSC trainee Adrian Lenkeit got the opportunity to participate in the 66th ISEF, along with more than 1700 students from over 70 countries, in Pittsburgh, Pennsylvania, from 10 to 15 May 2015.

Adrian qualified for the finals after winning the fourth prize at the German national competition "Jugend forscht 2014" with his own C++/CUDA N-body solver for a GPU. In addition to the computation of the pairwise interactions, he also visualized the trajectories via OpenCL. As a student of the St. Michael-Gymnasium in Bad Münstereifel, he had to complete mandatory two-week training, which he carried out at JSC a few weeks before the science fair. The goal of the hands-on training was to boost the performance of the code and

introduce multi-GPU support via MPI utilizing JSC's own GPU cluster JUDGE for a larger simulation. With the help of the 3D visualization capabilities of JSC's Rotunda and stereoscopic additions to his OpenCL code, he even presented his results to a TV reporter team working for national broadcaster WDR prior to Intel ISEF. After the trip to Pittsburgh, the local newspaper Kölnische Rundschau covered his participation on 20 May: Adrian was ranked fourth as one of the youngest attendees in the Intel ISEF competition and won $ 500.
(Contact: Dr. Ivo Kabadshow, *i.kabadshow@fz-juelich.de*)

New GCS Large-Scale Projects in May 2015

Twice a year, the Gauss Centre for Supercomputing (GCS) issues a call for large-scale projects on its petascale supercomputers, currently JUQUEEN (JSC), HORNET (HLRS), and SuperMUC (LRZ). Projects are classified as large-scale if they require at least 35 million core hours. At its April meeting at DESY in Zeuthen, the GCS Peer Review Board decided to award the status of a large-scale project to 16 projects from various fields of the simulation sciences. Three projects were granted a total of 200 million compute core hours on HORNET, 13 projects were granted a total of about 715 million compute core hours on JUQUEEN (a new record at JSC), and two projects were granted 60 million compute core hours on SuperMUC. For more details on these projects, some of which utilize the resources of several centres, see *http://www.gauss-centre.eu/large-scale*.
(Contact: Dr. Walter Nadler, *w.nadler@fz-juelich.de*)

News from the NIC Scientific Council

The Scientific Council of the John von Neumann Institute for Computing (NIC) held its annual meeting on 16 April 2015 at DESY in Zeuthen. Prof. Kurt Binder, serving his second term as chairman of the NIC-SC since January, chaired the meeting. Dr. Daniela Jacob, director of the Climate Service Center Hamburg, and Prof. Christine Peter, University of Konstanz, were elected as new members and will begin their term in January 2016. New members were also elected to the NIC Peer Review Board: Prof. Wolfgang Wenzel (Karlsruhe Institute of Technology) and Dr. Daniela Jacob (CSC Hamburg). They will begin their term of office at the next meeting of the Peer Review Board in October.
(Contact: Dr. Walter Nadler, *w.nadler@fz-juelich.de*)

NIC Excellence Project 2015

At its April meeting, the NIC Peer Review Board decided to award an outstanding simulation project the title of NIC Excellence Project. The goal of the project entitled "Structure and dynamics of polymer and lipid systems" submitted by Prof. Marcus Müller (Universität Göttingen) is to understand the correlation between the molecular structure and equilibrium thermodynamics as well as the collective dynamics in multi-component, amphiphilic polymer melts and lipid membranes, employing a spectrum of complementary numerical techniques. For more details, see *http://www.john-von-neumann-institut.de/nic/exzellenz-2015* (in German).
(Contact: Dr. Walter Nadler, *w.nadler@fz-juelich.de*)

Supercomputing and Modelling for the Human Brain – General Assembly 2015

A total of 92 scientists from Forschungszentrum Jülich and several partner institutions collaborating within the Helmholtz Portfolio Theme "Supercomputing and Modelling for the Human Brain" (SMHB) met for their annual General Assembly on 30 and 31 March at JSC to present and discuss the progress achieved in 2014 and to agree on the next steps in the project.

The SMHB was launched in January 2013 as one of the Portfolio Themes of the Helmholtz Association and was conceived as a Helmholtz contribution to the European Human Brain Project. Its goal is to achieve a better understanding of the organization and functioning of the human brain by developing a realistic brain model. To meet this challenge, an appropriate infrastructure is necessary for HPC and Big Data analytics. The SMHB work plan therefore integrates a wide range of expertise from fundamental neuroscience, brain modelling and simulation, simulation software technology, HPC, large-scale data management, scientific workflows, and interactive visualization and analysis. The SMHB works closely with JSC's Exascale Labs on the co-design of neuroscience applications and HPC technology.

The SMHB General Assembly 2015 was opened by Prof. Wolfgang Marquardt, Chairman of the Board of Directors of Forschungszentrum Jülich, and by the two project speakers, Prof. Katrin Amunts (INM-1) and Prof. Thomas Lippert (JSC). Many examples were presented of the active and fruitful collaboration between the SMHB partners. Dr. Moritz Helmstaedter from the Max Planck Institute for Brain Research in Frankfurt am Main gave an invited keynote talk on his research in connectomics. A further highlight of this year's meeting was a session in which young scientists introduced their work in short spotlight talks before they went on to discuss it in more depth with interested colleagues in the poster session that followed.
(Contact: Dr. Anne Do Lam Ruschewski, *a.do.lam@fz-juelich.de*)

Events

Scientific workflows & data management with UNICORE
Instructors: B. Hagemeier, M. Rambadt, Dr. B. Schuller, JSC
Date: Tuesday, 16 June 2015, 09:00-15:00
Venue: Jülich Supercomputing Centre, Ausbildungsraum 1
Registration: *b.hagemeier@fz-juelich.de*

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