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BEAM-ME – HPC in Energy Systems Modelling

The beginning of this year saw the kick-off meeting for the project BEAM-ME, which is funded by the German Federal Ministry for Economic Affairs and Energy (BMWi) and addresses the need for improved computing power and efficiency in energy systems modelling. With the DLR in Stuttgart as the principal investigator on the modelling side, the project unites various partners with complementary expertise in the fields of algorithms, computing and application development. JSC and HLRS in Stuttgart engage in the task of enabling simulations to run on premier HPC infrastructures; the Zuse Institute Berlin (ZIB) has the task of developing tailor-made parallel algorithms suited for state-of-the-art many-core systems; and GAMS Software GmbH contributes application-level research and development.
(Contact: Dr. Daniel Rohe, *d.rohe@fz-juelich.de*)

HPSC TerrSys Fall School 2016

The Centre for High-Performance Scientific Computing in Terrestrial Systems (Geoverbund ABC/J), together with the JSC SimLab Terrestrial Systems, is organizing an international Fall School on Terrestrial Modelling and High-Performance Scientific Computing (HPSC) from 10 to 14 October 2016. The objective of this applied course is to provide the theoretical and technical context of terrestrial modelling in HPC environments utilizing stand-alone and coupled hydrologic, land surface and atmospheric models. Using the Terrestrial Systems Modelling Platform (TerrSysMP), the course will take a complete tour of terrestrial modelling and HPSC in connection with real-world observations and data assimilation. Topics covered by condensed lectures and hands-on sessions will be model system setup, parallel performance and profiling, coupled models, big data strategies and data assimilation. The course will be held at the University of Bonn with practical afternoon sessions on the JURECA HPC system. The school is intended for master's and PhD students or postdocs with a deep interest in terrestrial modelling. The registration deadline is 30 April 2016. Further information and registration procedures at *http://www.geoverbund-abcj.de/HPSCTerrSys-FallSchool-2016/*
(Contact: Dr. Klaus Görgen, *k.goergen@fz-juelich.de*)

The Centre of Excellence E-CAM

At the end of 2015, the EU-funded Centre of Excellence E-CAM started operation. It strives to establish a software infrastructure in the field of the simulation and modelling of materials and biological processes of industrial and societal relevance. The project consortium comprises 15 partners from 10 European countries connected via the CECAM network structure (*http://www.cecam.org*). The aim is to

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

develop software for scale-bridging problems, which range between electronic and continuum length and time scales.

Work is concentrated within four major work packages focusing on electronic structure calculations, classical molecular dynamics, quantum dynamics and mesoscopic modelling and simulation. JSC plays a central role in software development as well as the management and organization of training events. The software produced in the project will be made publicly available through a software library. Part of the software will be developed in extended software development workshops, which will be organized regularly. Participants will actively contribute to the software stack of the project and will learn program design, documentation, optimization and porting to high-performance computers. A major aspect of the project is networking and cooperating with industrial partners. In collaborations, problem-specific software will be developed and joint schools and tutorials will be organized with the aim of establishing high-performance computing for industrially relevant computations. Further details can be found at *http://www.e-cam2020.eu*.
(Contact: Dr. Godehard Sutmann, *g.sutmann@fz-juelich.de*)

Retrospective of the NIC Symposium 2016

The John von Neumann Institute for Computing (NIC) supports research projects from a broad scientific spectrum including topics from astrophysics, condensed matter and numerical mathematics. The NIC symposium is held biennially in February and provides an overview of the activities and results of projects which were allocated computing time on the supercomputers at Forschungszentrum Jülich by NIC. This year, the NIC symposium had a record number of 200 scientists who attended the conference and poster session.

The participants were welcomed by Forschungszentrum Jülich's Chairman of the Board of Directors, Prof. Wolfgang Marquardt, and director of JSC and NIC, Prof. Thomas Lippert. Prof. Marquardt focused on big data and its significance in scientific simulation. He briefly discussed a selection of emerging key challenges. Prof. Lippert expanded on the challenges of scientific big data analytics in high-performance computing. He also provided an overview of the new general-purpose system JURECA, which has been greatly accepted by the users of the computer facilities at JSC.

Recent results and outcomes were presented in 14 insightful talks and in an overwhelming number of 120 posters. The symposium provided plenty of time for the exchange of ideas and experiences in an interdisciplinary scientific environment. All accompanying materials, including the proceedings, are available at *http://www.john-von-neumann-institut.de/nic/nic-symposium-2016*.
(Contact: Dr. Alexander Schnurpfeil, *nic@fz-juelich.de*)

JUQUEEN Extreme Scaling Workshop 2016

Feedback from last year's very successful workshop motivated the organization of a three-day workshop in February, during which the entire 28-rack JUQUEEN BlueGene/Q system was reserved for over 50 hours. Eight code teams were selected to use this opportunity to investigate and improve their application scalability, assisted by JSC Simulation Laboratory and Cross-sectional Team staff.

The applications **Code_Saturne** from Daresbury Laboratory and **Seven-League Hydro** from HITS (Heidelberg) both displayed strong scalability to 28 racks and thereby become candidates for High-Q Club membership. Existing members, **CIAO** from RWTH-ITV and **iFETI** from University of Cologne and TU Freiberg, showed that they had additional solvers which also scaled acceptably, and in situ visualization was demonstrated with a CIAO/JUSITU/VisIt simulation running on 28 racks. Two adaptive mesh refinement libraries, **p4est** from University of Bonn and **IciMesh** from EC Nantes, showed that they could respectively scale to 917,504 and 458,752 MPI ranks, but both encountered problems loading large meshes. Parallel file I/O limitations also prevented large-scale executions of the IEK-6/Amphos 21 **PFLOTRAN** subsurface flow and reactive transport code; however, an HDF5 import module for **NEST** developed by the EPFL Blue Brain Project could be optimized to use collective MPI file reading calls and enable large-scale data-driven neuronal network simulations.

The optimizations achieved with all codes will be a good basis for running bigger jobs on JUQUEEN in current and future compute time projects. Detailed results for each code provided by the participating application teams appeared in the JSC report FZJ-JSC-IB-2016-01, see *http://juser.fz-juelich.de/record/283461*
(Contact: Dr. Brian Wylie, *b.wylie@fz-juelich.de*)

Events

Introduction to Parallel In Situ Visualization with VisIt
Instructors: Jens Henrik Göbbert, Dr. Herwig Zilken, JSC
Date: 18 April 2016, 09:00-16:30
Venue: Jülich Supercomputing Centre, Ausbildungsraum 2
Registration: *http://www.fz-juelich.de/ias/jsc/events/visit*

GPU programming with CUDA
Instructors: Dr. J. Meinke, J. Kreutz, JSC; J. Kraus, NVIDIA
Date: 25-27 April 2016, 09:00-16:30
Venue: Jülich Supercomputing Centre, Ausbildungsraum 1
Registration: *http://www.fz-juelich.de/ias/jsc/events/cuda*

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