

JSCNews

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Start of the Exascale Projects DEEP-ER and Mont-Blanc 2

The EU-funded Exascale projects DEEP Extended Reach, DEEP-ER for short, and Mont-Blanc 2 started in October 2013. They will run in parallel for three years and are the extensions of the DEEP and Mont-Blanc projects, respectively.

The goal of DEEP-ER, which is coordinated by JSC, is to update the Cluster-Booster architecture introduced by the DEEP project and extend it with additional parallel I/O and resiliency capabilities. In DEEP-ER, Cluster and Booster nodes will be connected to a uniform network. Novel non-volatile memory technology will be tested at different architecture levels, building up a multi-level storage hierarchy. A software environment for parallel I/O and resiliency will be built upon this storage infrastructure. To recover applications after hardware failures, a multi-level checkpoint/restart mechanism using the available memory devices and a task-based recovery mechanism based on the OmpSs programming environment will be set up.

The design and development of the DEEP-ER extensions will be driven by the requirements and results obtained from seven scientific applications, representative of today's HPC applications portfolio. These applications will be ported to the DEEP-ER prototype demonstrating its usability and its scalability towards Exascale.

Fourteen European partners constitute the DEEP-ER consortium. Amongst other activities, JSC is participating in the archi-

tectural (both hardware and software) design, the development of the I/O and resiliency software layers, guidance and support for the application developers, and the installation of the DEEP-ER prototype at Jülich. Detailed information can be found at <http://www.deep-er.eu>.

In the Mont-Blanc 2 project, JSC's contribution focuses on the adaptation of the performance analysis tool Scalasca to the available hardware prototypes, based on energy-efficient processors from the cell phone and tablet market. For further information, see

<http://www.montblanc-project.eu>.

(Contact: Estela Suarez,
e.suarez@fz-juelich.de)

Kick-Off Meeting of Simulation Laboratory "Ab Initio Methods"

On 8 November 2013, the first workshop held by the JARA-HPC Simulation Laboratory "Ab Initio Methods in Chemistry and Physics" took place at JSC. The workshop was designed to introduce the Sim-Lab to the local solid-state physics and quantum chemistry communities, bringing together 50 scientists from institutes within the Jülich Aachen Research Alliance (JARA). By sharing their work and scientific expertise, the participants established a platform defining opportunities for mutual collaboration and prioritization of the Sim-Lab's activities. Short informal talks were given by speakers from each of the main participating partner institutes and cross-

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

Phone +49 2461 61-6402

jsc@fz-juelich.de
www.fz-juelich.de/jsc

sectional groups, followed by extended constructive discussions between the speakers and the audience.

The new simulation laboratory will provide expertise in the field of ab initio simulations for physics, chemistry, nanoscience and materials science with a special focus on high-performance computing on the Jülich supercomputer facilities. It will also act as a high-level support structure in dedicated projects and will host research projects dealing with fundamental aspects of code development, optimization and performance improvement.

Current activities focus on algorithm development and application, leading to a wide variety of research projects: including the development of eigensolvers for density functional theory (DFT) codes, study of thermal properties of material interfaces, fast tensor contraction kernels applied to quantum chemistry, and benchmarking of DFT codes.

(Contact: Dr. Edoardo Di Napoli, e.di.napoli@fz-juelich.de)

Paul Gibbon Appointed Professor at KU Leuven

Paul Gibbon joined JSC in 2001 as a theoretical plasma physicist specializing in parallel N-body algorithms. In 2009, he took charge of the newly formed Computational Science division, which has since grown into one of the largest at JSC with its eight simulation laboratories, including the Plasma SimLab, which he also supervises. His current research interests focus on the application of high-performance computing to topical challenges in plasma physics, such as laser-driven particle acceleration and tokamak edge physics.

Recently he was appointed Associate Professor at the Katholieke Universiteit Leuven (KUL), Department of Mathematics, where he will spend part of his time teaching courses on computational methods. The Jülich-Leuven connection will also be supported by a Helmholtz International Research Group grant on scalable kinetic simulation methods awarded to Prof. Gibbon earlier this year, which will be used to finance jointly supervised PhD and master's students between JSC and his affiliated group within the Centre for Mathematical Plasma Astrophysics at KUL. Further information about the group can be found at

<http://www.fz-juelich.de/ias/jsc/slpp>.

JSC wishes Paul all the best for his new position!

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 SuperMUC (LRZ). Projects are classified as large-scale if they require more than 35 million core hours.

At its October meeting at JSC, the GCS Peer Review Board decided to award the status of a large-scale project to thirteen projects. Two projects were granted a total of 82 million compute core hours on SuperMUC, another two projects were granted a total of 165 million compute core hours on HERMIT, and the other nine projects were granted a total of about 506 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)

NIC Excellence Project 2013

At its October meeting at JSC, the NIC Peer Review Board awarded the title of NIC Excellence Project 2013 to a second outstanding simulation project. The goal of the project "Direct Numerical Simulation of Turbulent Mixing in the Planetary Boundary Layer", submitted by Dr. Juan Pedro Melado (Max Planck Institute for Meteorology, Hamburg), is a comprehensive understanding of turbulence in the planetary boundary layer under strong and weak wind conditions, as well as with pure convective forcing. For more details, see

<http://www.fz-juelich.de/nic/Projekte/exzellenz-2013.html>.

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

Awards for Bachelor's and Master's Students

On 8 November 2013, four students from Forschungszentrum Jülich received an award - the Ehrenplakette - from Aachen University of Applied Sciences (FH Aachen). In a ceremony at Aachen's historical town hall, Prof. Baumann, rector of FH Aachen, honoured Patrick Embgenbroich (IBG-2) and Martin Lischewski (S-NS) as the best graduates of the bachelor's course Scientific Programming, and Sebastian Lührs (IEK-8) and Anna Westhoff (JSC) as the best graduates of the master's course Technomathematics. Anna Westhoff's master's thesis has been published and is available at <http://juser.fz-juelich.de/record/138037>.

(Contact: Prof. Dr. Johannes Grotendorst, j.grotendorst@fz-juelich.de)

Events

Open Dialogue on Pre-Commercial Procurement of Innovative HPC Solutions for the Human Brain Project

Date: 18 December 2013, 10:30-16:30

Venue: Sheraton Brussels Airport Hotel

Info: <http://www.fz-juelich.de/ias/jsc/events/hbp-od-pcp>

Further events, talks, and training courses:

<http://www.fz-juelich.de/ias/jsc/events>