

JSCNews

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Centre

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Jülich Becomes CECAM Node

Forschungszentrum Jülich has joined the Centre Européen de Calcul Atomique et Moléculaire (CECAM) as an active node. CECAM is an international organization, which traditionally promotes activities in the fields of atomistic simulations, e.g. quantum ab initio calculations and molecular dynamics via workshops, tutorials or visitor programmes. When the CECAM headquarters moved from Lyon to Lausanne in 2008, the structure of CECAM was transformed into an international multi-site structure, where nodes were established in different European countries, supporting the activities and running their own programmes.

Up to now, eight nodes have been set up in Ireland, France, the UK, Germany, the Netherlands and Italy, all having their own distinct thematic foci. The nodes promote and establish leading research activities in the fields of molecular simulations, multi-scale modelling and algorithms. They form a network structure, working together towards a European software and knowledge base. For more information, see <http://www.cecama.org/>.

Jülich has been a supporting member of CECAM for many years and is already represented on the Council. This year, Forschungszentrum Jülich signed an agreement to establish an active CECAM node in Jülich with the focus on scientific computing in the fields of soft matter and materials science. The Institute for Advanced Simulation will be in charge of organizing and running CECAM-specific activi-

ties, such as workshops, tutorials, schools and visitor programmes. Dr. Godehard Sutmann from JSC has been appointed director of the Jülich node and will coordinate local and international activities. For 2011, a workshop on soft matter, tutorials on DFT and fast algorithms in molecular simulations as well as an international guest student programme will be organized in Jülich as CECAM activities.

(Contact: Dr. Godehard Sutmann, ext. 6746).

SC10 in Retrospect

Supercomputing 2010, the premier international conference and exhibition on high-performance computing and networking, took place in New Orleans, Louisiana, USA, from 13 - 19 November 2010. Conference attendance at this year's event was about 10% higher than the previous year's record. JSC participated in the conference and exhibition for the twelfth time in succession.

The new TOP500 list issued during SC10 ranked Jülich's petaflop supercomputer JUGENE second in Europe and ninth worldwide. Jülich's general purpose supercomputer JUROPA is ranked fifth in Europe and 23rd worldwide.

Several JSC staff members contributed actively to the conference's programme, to tutorials and to various special interest meetings. In particular, Markus Geimer presented a tutorial on "Parallel Application Performance Engineering", Bernd Mohr

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acted as chair of the committee on "Technical Papers: Performance", and David Boehme presented a poster on "Critical Path Analysis for Large-Scale MPI Programs".

JSC highlighted its role as one of the leading European high-performance computing centres at the exhibition, where a record 338 exhibitors, research institutions as well as hardware and software companies, were represented. At its booth, JSC presented its broad spectrum of activities in the form of displays, movies, animated presentations, live talks, and individual consultations.

Particular emphasis was placed on JSC's community-oriented approach to support for scientific computing, the Simulation Laboratories, whose capabilities were demonstrated in talks given at the JSC and the KIT booth. Furthermore, tools developed by JSC for the performance analysis of parallel programs and Grid activities were presented in demonstrations and talks. LLview, the interactive monitoring software for supercomputers, was presented in live demonstrations on the JSC systems JUGENE and JUROPA and drew an extraordinarily large response from the visitors.

Together with CSC (Finland), JSC staff members also organized the PRACE booth and a special interest meeting.

Further information is available at:

<http://www.fz-juelich.de/jsc/news/sc10/>

(Contact: Dr. Walter Nadler, ext. 2324).

Bernd Mohr Now on SC Steering Committee

At the Supercomputing Conference in New Orleans, JSC staff member Dr. Bernd Mohr was elected to the SC Steering Committee. He is the first European member of this governing body for the largest and most important conference in the field of supercomputing. The SC Steering Committee determines the future conference sites and the respective conference chair, and has overall control of the conference budget. JSC congratulates Bernd on this well-deserved success!

Double Honour for MATSEs

On 19 November 2010, two students from Forschungszentrum Jülich received a plaque of honour from Aachen University of Applied Sciences (FH Aachen). In a ceremony at Aachen's historic town hall, Prof. Baumann, rector of FH Aachen, honoured Anna Jakobs (IFF) and Carsten Karbach (JSC) as the best graduates of the bachelor's course Scientific Programming.

The Association of German Chambers of Industry and Commerce (DIHK) has invited Carsten Karbach as the best German trainee mathematical-technical software developer (MATSE) of 2010 to a ceremony which will take place in Berlin on 13 December. He passed his examination with marks of 100 percent. The Federal Minister for Labour

and Social Affairs, Ursula von der Leyen, will congratulate Carsten and the other top German trainees on their excellent examination performances.

(Contact: Prof. Paul Jansen, ext. 6430)

H4H Project Launched

The European ITEA2 project "Hybrid Programming for Heterogeneous Architectures" (H4H), partly funded by the Federal Ministry of Education and Research (BMBF) in Germany, was launched on 1 October 2010. The objective of this project is to provide compute-intensive application developers with a highly efficient hybrid programming environment for heterogeneous computing clusters composed of a mix of classical processors and hardware accelerators such as GPUs.

To meet this challenge, the project will leverage and consistently advance the state of the art in several key software areas: programming models and associated run-time systems, performance measurement and correctness tools, smart translation in particular from OpenMP to CUDA or OpenCL, combined use of MPI and OpenMP, dynamic automatic tuning, and prediction of the execution time of a parallel application on different platforms. To achieve its objective, this project has attracted 25 project partners from France, Germany, Spain and Sweden, including a wide range of HPC users to validate the proposed technology in applications from various domains. The project will run for three years and has a total volume of € 15.6 million.

(Contact: Dr. Bernd Mohr, ext. 3218)

End of Year Colloquium 2010

Date: Thursday, 16 December 2010, 9:30 - 16:00 h

Venue: Hörsaal, JSC

Most talks will be given in German.

Programme:

- 09:30 Thomas Lippert: Begrüßung
- 09:45 Norbert Attig: JUGENE wird europäisch – oder wie verhilft man PRACE-Anwendungen zum erfolgreichen Start
- 10:45 Robert Speck: Viel Wirbel im Nichts?
- 11:15 Ivo Kabadshow: Supersize Me! – Gazillion particles experience the FMM
- 11:45 Jochen Kreutz, Georg Schwarz: Rallye Monte Carlo – Black-Scholes-Modell auf Beschleunigern
- 14:00 Mohcine Chraibi: Von einem, der auszog das Laufen zu lernen
- 14:30 Kristel Michielsen: The mysterious and the beautiful: What if Newton had had a computer?
- 15:00 Lukas Arnold: Heiß oder kalt? – Eingefrorene Magnetfelder auf der Sonne
- 15:30 Thomas Lippert: Who's Afraid of Amdahl's Law?

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