

First regular PRACE HPC Access Grants for Research Projects

Since August 1, 2010 the Partnership for Advanced Computing in Europe (PRACE) is offering supercomputing resources on the highest level (Tier-0) to European researchers. Jülich Supercomputing Centre (JSC), as one of the three members of the Gauss Centre for Supercomputing (GCS), is dedicating a 35% share of its Blue Gene/P system JUGENE. This is the first Petascale High Performance Computing system available to researchers through PRACE.

Shortly after finishing the "PRACE Early Access Call" reported about in the last issue of inSiDE, proposals for the first regular research projects on JUGENE were solicited in the first Project Access Call, released by PRACE on June 15, with the deadline August 15, 2010. Project Access is intended for individual researchers and research groups, including multinational research groups, and has a one year duration. 59 applications with a volume of about

2,300 Million compute core hours were submitted. After strict technical and scientific evaluation and prioritization, nine research projects have been awarded about 360 Million compute core hours. Two of those research projects are from Germany, two from Spain, and one each from France, Hungary, the Netherlands, Portugal and the UK. Four research projects are from the field of Engineering and Energy, three from Fundamental Physics and one each from Chemistry and Materials and from Medicine and Life Sciences.

More details can be found via the PRACE web pages <http://www.prace-ri.eu/PRACE-1st-Regular-Call>

Calls for Proposals for Project Access are issued twice yearly (May and November). The next PRACE call will open on May 2, 2011 with a deadline of June 30, 2011.

Jülich established as CECAM Node

Forschungszentrum Jülich has joined the Centre Européen de Calcul Atomique et Moléculaire (CECAM) as an active Node. Traditionally CECAM is known as a European organization, which promotes activities in the fields of atomistic simulations, e.g. quantum ab initio calculations or molecular dynamics, and development of methods and algorithms for bridging time and length scales in simulations via organizing workshops, tutorials or visitor programs. When 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 activities and running official CECAM programs. Up to now, nodes were established in 7 European countries, i.e. Ireland (Atlantic Centre for Atomistic Modeling), France (Ile de France, Rhône-Alpes), United Kingdom (Hartree Centre Daresbury), Spain (ZCAM Zaragoza), Germany (multi-site node in Berlin-Bremen-Frankfurt-Halle as well as in Berlin - Freie Universität), Netherlands (Amsterdam-Leiden) and Italy (Trieste-Bologna, Pisa), which all have their different thematic focus. Besides promoting and establishing leading research activities in the fields of molecular simulations, multi-scale modeling, and algorithms, the nodes form a network structure, working together towards a European software and knowledge base.

Forschungszentrum Jülich has been a supporting member of CECAM since years and is represented in its Scientific Council. In July 2010, Forschungszentrum Jülich signed an agreement to establish an active CECAM node in Jülich with a thematic focus on Soft Matter Physics, Materials Science, and Computational Science. The Institute for Advanced Simulation is in charge of organizing and running CECAM specific activities like workshops, tutorials, schools, and visitor programs, which all are approved by the CECAM Council and Scientific Advisory Board. Dr. Godehard Sutmann from JSC was appointed director of the Jülich Node and will coordinate local and international activities. This year a workshop on Soft Matter, tutorials on DFT methods and fast algorithms in molecular simulations as well as an international guest student program on scientific computing are organized in Jülich as CECAM activities. In the future, also a limited number of workshops in the field of scientific computing from external groups is envisioned. For further information, please visit the CECAM web pages:

www.cecaml.org,
<http://www2.fz-juelich.de/jsc/cecaml>

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