

## JSCNews

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Supercomputing  
Centre

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### Shutdown of JUBL

After the successful launch of the IBM Blue Gene/P system, JUGENE, this February and its general availability to all existing JUBL projects for almost two months, the time has come to shutdown its predecessor system, JUBL. The JUBL job queues will be closed on 28 April 2008. After this date, the system will be decommissioned and shutdown at the end of April 2008.

We would like to ask all of our JUBL users to migrate to JUGENE as soon as possible according to the rules described on the web page <http://www.fz-juelich.de/jsc/jugene/usage/resources> and to move all parts of their projects from JUBL to JUGENE.

JUBL went into operation in summer 2005; initially as a one-rack system before being upgraded to an eight-rack system in January 2006. Its utilisation is a true success story: high-scaling programs from an unexpectedly wide spectrum of research fields, such as lattice quantum chromodynamics, materials science and theoretical chemistry (CPMD, VASP), biophysics and engineering, were able to fully exploit the capacity of this innovative architecture and to tackle challenging problems which were out of reach before. Furthermore, it succeeded in serving as a test system for a future leadership-class supercomputer for capability computing applications. JSC quickly learned how to keep such a system with a limited number of CPU-intensive applications in stable operation mode, and how to support these applications most efficiently

by offering scaling workshops. All in all, JUBL will be remembered as the first step towards petaflop computing in Jülich. (Contact: Klaus Wolkersdorfer, ext. 6579)

### New EU Project "SmartLM"

The SmartLM project started in February 2008. It is partly funded by the European Commission within the 7th Framework Programme and will be completed over a period of 30 months. The objective of the project is to develop Grid-friendly software licensing for location-independent application execution.

The licensing models that currently exist for commercial applications support software used on compute resources within an administrative domain. Licenses are provided on the basis of named users, hostnames, or sometimes as a site license for the administrative domain of an organization. If licensed software is used in a Grid environment, spread across multiple organizations and their administrative domains, things become more complicated. The increasing usage of Grid environments means that these limitations must be addressed and overcome.

SmartLM will provide a generic and flexible licensing virtualization technology. The solution will implement software licenses as Grid services, providing platform-independent access from resources across organizational boundaries. The generic licensing virtualization technology will be integrated into the major Grid middleware solutions UNICORE and Globus.

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A number of widely-used license-protected commercial applications will be adapted to be executed under the control of the new licensing mechanisms.

The project consortium, led by the company Atos Origin, is formed by independent software vendors, business analysts, application service providers, academic partners, and public centres. JSC coordinates the standardization activities of the project and integrates the license technology into the UNICORE Grid middleware. Detailed information can be found on the project's website: <http://www.smartlm.eu/>. (Contact: Daniel Mallmann, ext. 2433)

## Workshop on Visualization of Scientific Data

In March 2008, an informative meeting on the visualization of scientific data took place in the Jülich Supercomputing Centre. About 30 participants from Forschungszentrum Jülich had the opportunity to learn about the existing visualization software and hardware systems installed in JSC.

The first topic was related to the presentation of scientific results with embedded multimedia content, for example video sequences or Adobe Flash animations. A survey of interactive 3D visualization systems followed. The main features and application range of the software packages IDL, AVS/Express and VTK were outlined and compared.

To show the usefulness of stereoscopic visualization displays for scientific applications, a demonstration was also given of the cylindrical three-channel stereo projection screen installed in the VR rotunda of JSC.

Within the framework of the Jülich-Aachen Research Alliance (JARA), interactive 3D projection screens will also be installed as a visualization infrastructure. It is planned to establish a so-called immersive visualization network (ivNET) in order to create a new quality of collaboration between scientists at RWTH Aachen University and Forschungszentrum Jülich.

In the last session of the meeting, two external partners, one from the University of Düsseldorf and one from RWTH Aachen University, presented current developments in the area of interactive virtual reality visualization and the parallel processing and visualization of extremely large scientific data.

The slides of all presentations can be found online at: <http://www.fz-juelich.de/jsc/cv/vislab/infoveranstaltung>

## Upgrade of SoftComp Linux Cluster and SoftComp Workshop

In November 2006, a Linux cluster was established for the user community of SoftComp (Soft Matter Composites). SoftComp is a Network of Excellence aiming to establish a knowledge base for an intelligent design of functional and

nanoscale soft matter composites. The start configuration comprised 66 AMD Opteron compute nodes providing a total peak performance of 1 TFlop/s. Over the course of a year, about 25,000 jobs were run with an overall CPU time consumption of 1.5 million hours.

At the beginning of 2008, a cluster upgrade to 125 compute nodes was accomplished resulting in a peak performance of nearly 2.5 TFlop/s. In addition, a fileservers and an Infini-Band network were introduced allowing parallel programs to be run more efficiently.

In order to mark the SoftComp cluster upgrade, a colloquium has been scheduled at the Jülich Supercomputing Centre on Tuesday 29 April 2008. SoftComp scientists will report on their applications and will have the opportunity to discuss with JSC staff members how programs should be adapted to the new configuration. The detailed programme can be found at: <http://www.fz-juelich.de/jsc/softcomp/colloquium> (Contact: Willi Homberg, ext. 2424)

## X-WiN Access Increased to 5 Gbit/s

At the beginning of 2008, the access bandwidth of Forschungszentrum Jülich to X-WiN, the German Research and Education network, was increased from 2 Gbit/s to 5 Gbit/s. This upgrade was performed within a general cost-neutral doubling of access bandwidth offered by DFN to pass on cost reductions to their customers. At the same time, the central firewall system has been replaced by a CISCO Firewall Service Module and central multi-layer switches have been upgraded to make the increased bandwidth available to the campus network, including the super-computer complex.

## Events

### BlueGene/P Porting, Tuning, and Scaling Workshop

Date: 22 - 24 April 2008

Venue: Jülich Supercomputing Centre

Registration: <http://www.fz-juelich.de/jsc/bg-ws08/>

### DEISA Symposium

Date: 28 - 29 April 2008

Venue: Our Dynamic Earth, Edinburgh

Programme: <http://www.deisa.org/symposium/>

### SoftComp Workshop

Date: 29 April 2008

Venue: Jülich Supercomputing Centre, VR rotunda

Programme: <http://www.fz-juelich.de/jsc/softcomp/colloquium>

### Workshop "From Computational Biophysics to Systems Biology 2008"

Date: 19 - 21 May 2008

Venue: Auditorium, Forschungszentrum Jülich

Registration: <http://www.fz-juelich.de/cbsb08/>

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