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FORSCHUNGSZENTRUM

JSCNews
Jülich
Supercomputing
Centre

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The Jülich Supercomputing Centre

Supercomputing is a driving force for the field of simulation sciences, which is the third category of scientific research complementing theory and experiment. The ever increasing complexity of the systems and processes under investigation in science and engineering results at the same time in growing requirements concerning the accessibility of theories to simulation, the accuracy of mathematical modelling, the efficiency of numerical and stochastic methods, and the computational methodology. This includes the performance and scalability of supercomputers, networks, Grid infrastructures, and data centres as well as programming models, software technology and visualisation techniques. Furthermore, due to the generation of complex data flows, future large-scale experimental research presents extraordinary challenges for the storage and processing of huge amounts of experimental data.

The mission of the Jülich Supercomputing Centre (JSC) is to provide large-scale computational resources and infrastructures for German and European science. Under the name *Supercomputing*, JSC's work programme forms part of the Helmholtz Association's research field *Key Technologies*. It is structured into three topics:

- *Supercomputer Facility*, concerning the provision of supercomputer resources of the highest performance and widest scope along with the design and construction of future leadership-class systems in cooperation with European companies.
- *Computational Science and Mathematical Methods*, providing well-qualified support through *Simulation Laboratories*, an innovative community-oriented research and support structure, together with cross-disciplinary scientific support groups.
- *Grid Technologies and Infrastructures*, making Grid technologies available for distributed supercomputing infrastructures, empowering computational scientists and experimentalists to use the European high-performance computing (HPC) infrastructure most effectively.

In the following, we will outline some of the important goals and activities for the near future.

Supercomputer Facility

The prime objective of this topic is the advancement of JSC to a world-class leadership facility. JSC strives to become a European supercomputing centre with petaflop/s capability in 2009/2010. As a member of the Gauss Centre for Supercomputing, JSC heads the European project *Partnership for Advanced Computing in Europe (PRACE)*, which is preparing the creation of a pan-European supercomputing service at the highest performance level, its full integration into the European HPC ecosystem and its sustained operation.

For Jülich, the realisation of such ambitious goals implies the cost-efficient and continuous upgrading of JSC's supercomputers,

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data storage, networking and post-processing capabilities towards a petascale facility, enabling both the highest scalability *and* broadest general purpose flexibility. Only through a continuous dual modernisation process can the sustained provision of supercomputer resources of the highest performance and widest scope be guaranteed.

We can only remain in the forefront of high-performance computing through active research and technological development at the system level. This will be carried out by JSC in close collaboration with leading hardware vendors, software companies and system integrators, embedded in the PRACE initiative. Activities range from the investigation of novel hardware architectures to the design and development of hardware and software for the next generation of leadership-class systems, including cluster computing, networking, security and scientific visualisation systems.

Computational Science and Mathematical Methods

An effective utilisation of leadership-class supercomputing facilities requires both outstanding technical operation and high-level user support at JSC. To this end, JSC is pursuing the realignment of disciplinary research and cross-sectional activities by its innovative concept of Simulation Laboratories. This measure will ensure the long-term critical mass of the existing research teams and will further intensify cooperation with external academic groups. A Simulation Laboratory is a targeted research and support structure focused on a specific scientific community. Each of these consists of a core group located at a supercomputing centre and a number of associated scientists outside. The first Simulation Laboratories for Jülich and regionally based communities will be created in the fields of computational plasma physics, earth sciences, computational biology and nanosciences. They are complemented by cross-sectional research groups on mathematical modelling and methods and on performance analysis tools that play a key role in the scaling of large application codes to future petascale machines. The topic also comprises the work of the Jülich research group at the John von Neumann Institute for Computing, whose current research theme is Computational Biology and Biophysics.

Grid Technologies and Infrastructures

JSC develops and provides Grid technologies for distributed supercomputing infrastructures based on the UNICORE paradigm. The overall objective is to support national and international e-infrastructures, such as the Gauss Centre for Supercomputing, D-Grid, DEISA, and PRACE, forming the future European high-performance computing infrastructure. JSC collaborates with many partners to achieve standards-based interoperability between the various Grid technologies, thus creating seamless user access to a wide range of e-infrastructures. It designs and implements world-class service-oriented architectures according to emerging standards from the Grid Computing and Web Services domain, accompanied by the identification and implementation of new trends in the distributed systems research area. JSC is a major partner in the operation of the heterogeneous environment of the D-Grid and will continue to sustain the Grid infrastructures for the German e-Science community, including high-level user support and training events in order to strengthen the application sector. The topic also includes JSC's research and development of future communications and networking technologies, both at the wide and local area and at the processor interconnect level.

Partnerships and alliances

JSC's work has a distinct interdisciplinary and collaborative character. It has an important bridging function for its user communities as well as for the research fields of the *Helmholtz Association* and partners in national and international science organisations and competence networks.

The simulation activities of JSC are integrated in several formal collaborations, in particular in the newly established *Jülich-Aachen Research Alliance (JARA)*, Section *JARA-SIM*. The long-term activities and experiences of JSC in the teaching and training of young scientists together with the Aachen University of Applied Sciences are strengthened by its firm commitment to the *German Research School for Simulation Sciences* at FZJ and RWTH Aachen University, which will be inaugurated in 2008.

JSC was the first German national supercomputer centre founded in 1987 and has established – together with its partners DESY and GSI within the framework of the *John von Neumann Institute for Computing (NIC)* – a highly regarded peer-review scheme for the provision of supercomputer resources. JSC is a founding member of the European project *Distributed European Infrastructure for Supercomputing Applications (DEISA)*. Together with the national HPC centres *Leibniz-Rechenzentrum* in Garching and *Höchstleistungsrechenzentrum Stuttgart*, JSC founded the *Gauss Centre for Supercomputing (GCS)* in 2006. The GCS e.V. represents Germany as a *single* legal entity in the European supercomputing infrastructure initiative PRACE.

Under its new name, the Jülich Supercomputing Centre will endeavour to continue the internationally recognised work of the Zentralinstitut für Angewandte Mathematik. Prospects of success are very good for the Centre in view of its competence in high-performance computing, its excellent equipment, and its active integration into the European HPC ecosystem.

End of Year Colloquium 2007

Time: Wednesday, 19 December 2007, 9:30 - 16:00 h
Venue: Hörsaal, JSC
Programme: *http://www.fz-juelich.de/jsc/events/eyc-2007*

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