DEISA Continues

The first four years of DEISA (Distributed European Infrastructure for Supercomputing Applications) concluded successfully with the final review on 16 June 2008. The work of all the service activities as well as two technology demonstrations were presented in detail. The major achievement of the four-year project is the deployment and operation of a distributed, heterogeneous infrastructure connecting the eleven national supercomputing centres in Europe. This includes a dedicated 10 Gb/s network (coordinated by JSC), a distributed shared file system, a common security mechanism, a global user management and accounting system, UNICORE as Grid middleware and workflow service, a common set of compilers and libraries (the common production environment CPE) and several other services and technologies. These services are operated on a 24/7 basis by the operations team comprising local administrators and experts from all sites.

In addition to these operational and technology tasks, the application task force performed supercomputing-oriented user- and application-oriented work, including user support, training, documentation, application enabling and enhancing scalability work. The DEISA Extreme Computing Initiative (DECI) made supercomputer time available to the broad European community (over 30 million CPU hours in 2008). Through DECI, access to the supercomputers available in DEISA is granted on a peer-reviewed basis. JSC participated in all technology, operational and application-oriented activities of DEISA.

The achievements of DEISA include creating the foundation for the future European petaflop initiative and the follow-on project DEISA2, which started on 1 May 2008 and runs for three years. Besides management, dissemination and training, the planned work focuses on operations, technologies and applications. With KTH (Sweden), CSCS (Switzerland), CEA (France) and the Joint Supercomputing Centre of the Russian Academy of Sciences, four associated partners will be added to the DEISA infrastructure thus increasing its European scope. Three of these centres are also members of PRACE, hence facilitating the successful DEISA2-PRACE collaboration to boost supercomputing in Europe to a new level.

DEISA2 is coordinated by Rechenzentrum Garching (RZG) of the Max-Planck-Gesellschaft and receives over € 10 million in funding from the 7th Framework Programme of the EU. JSC contributes 5 % of the JUGENE computing cycles as well as 5 % of the future general purpose supercomputer resources. More information about the DEISA infrastructure is available at: *http://www.deisa.eu*
(Contact: Dr. Achim Streit, ext. 6576)

Final Reviews of EU Projects

On 7 - 8 May 2008, the successful final review of the NextGRID project took place. All workpackages and developments as well as the applied business scenarios were presented in full detail to the reviewers and the European Commission.

JSC worked on the UDAP (Universal Dynamic Activity Package) component, which deals with resource and service discovery. The UDAP service is included as an integral sub-component of the CIS (Common Information Service) of UNICORE 6 and thus demonstrates the adoption of NextGRID results.

The OMII Europe project had its final review on 23 May 2008. Besides the non-technical activities, the technical development and integration activities were successfully presented. The implementation of common Grid standards in the middleware technologies gLite, Globus, and UNICORE to achieve interoperability and the adoption of this approach in application use cases was presented and demonstrated in full detail.

JSC worked on all UNICORE-related development activities, in particular adding interfaces for the standards OGSA-BES, OGSA-RUS and SAML-VOMS to UNICORE 6 as well as making GridSphere and OGSA-DAI work with UNICORE 6. Furthermore, JSC led the central infrastructure integration activity, whose objective was to integrate all developments in order to facilitate interoperability and to apply real-world application use cases. The interfaces for OGSA- BES and SAML-based VOMS were integrated in the core components of UNICORE 6 thereby guaranteeing the sustainability of the project work. (Contact: Dr. Achim Streit, ext. 6576)

PROPER 2008 – Workshop on Productivity and Performance

The Virtual Institute - High Productivity Supercomputing (VI-HPS), an international collaboration on HPC programming tools founded by JSC in 2007, is organizing the Workshop on Productivity and Performance PROPER 2008, which will take place in conjunction with the Euro-Par 2008 conference in Las Palmas de Gran Canaria, Spain, on 25 August 2008. The workshop focuses on software tools for the development and optimization of HPC applications. The organizers aim at encouraging younger researchers by offering a number of student grants to support travel and conference participation. For more information, please visit the workshop website at: *http://www.vi-hps.org/proper2008/.*
(Contact: Prof. Dr. Felix Wolf, ext. 1583).

UNICORE Summit 2008

The 4th UNICORE Summit Workshop will be held on 26 August 2008 in conjunction with the Euro-Par 2008 conference in Las Palmas de Gran Canaria, Spain. The international programme committee selected five papers to be presented at the workshop. The papers will be published by Springer in the post-conference workshop proceedings in the LNCS series. As the invited speaker, Emilio Benfenati will talk about

'Grid Approaches for Industrial Chemical and Pharmaceutical Applications'. The programme and more information is available under: *http://www.unicore.eu/summit/2008* (Contact: Dr. Achim Streit, ext. 6576)

NIC Excellence Project Launched

At its meeting in June, the NIC Peer Review Board, strongly supported by the NIC Scientific Council, decided to honour outstanding projects by designating them NIC Excellence Projects of the Year. The first project to receive this distinction for the 2008/9 grant period was submitted by Prof. Dominik Marx from Ruhr-Universität Bochum. It focuses on prebiotic chemical reactions, such as the synthesis of peptides, under extreme conditions which might have been found on the early Earth prior to the emergence of life.

Besides this pleasant duty, the NIC Peer Review Board had to perform a tough selection process: about 50 groups from all over Germany and some applicants from Europe requested more than four times as much computing time than was available for NIC projects on JUGENE, Jülich's leadership-class supercomputer. The demand was even higher for JUMP, Jülich's general purpose supercomputer: 140 groups asked for six times the available resources. All applicants will receive information about assigned computer time grants within the next few days.
(Contact: Dr. Manfred Kremer, ext. 3660)

NIC Workshop "From Computational Biophysics to Systems Biology"

About 120 scientist and students from Germany, Europe and the USA participated in the third annual workshop "From Computational Biophysics to Systems Biology" (CBSB08). The workshop took place from 19 to 21 May 2008 at Forschungszentrum Jülich and was organized by the NIC research group "Computational Biology and Biophysics" headed by Prof. Dr. Ulrich H.E. Hansmann. As in past years, experts from physics, chemistry, biology, and computer science discussed how to bridge the different scales in physics-based simulations of cells. Topics included protein folding and misfolding, aggregation, molecular docking, and the modeling of cardiac contractions. The proceedings of this workshop will be issued as NIC Series Vol. 40 in August. (Contact: Prof. Dr. Ulrich Hansmann, ext. 1526)

Events

Introduction to programming and using the IBM supercomputers
Date: 11 - 12 August 2008, beginning on 11 August, 13:00
Venue: Hörsaal, Jülich Supercomputing Centre
Application: *B.Scheid@fz-juelich.de*, ext. 6402

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