DEISA Newsletter

DISTRIBUTED EUROPEAN INFRASTRUCTURE FOR SUPERCOMPUTING APPLICATIONS

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Distributed European Infrastructure for Supercomputing Applications

DEISA is a consortium of leading national supercomputing centres in Europe aiming to jointly build and operate a distributed terascale supercomputing facility.

Welcome to the DEISA Newsletter

This is the first issue of the DEISA Newsletter, whose purpose is to inform on the activities of the DEISA research infrastructure. DEISA is engaged in the deployment and operation of a persistent, production quality, distributed supercomputing environment with continental scope. As an European supercomputing service built on top of existing national services, DEISA contributes to a significant enhancement of capabilities and capacities of high performance computing (HPC) in Europe. The ultimate purpose of this environment is to enable scientific discovery across a broad spectrum of science and technology.

Scientific impact (enabling new science) is the only criterion for success.

This newsletter is aimed mainly at the scientific community and HPC end users at large, but it will also convey useful information for the Grid technology development community in Europe and the rest of the World. Its purpose is to inform on the major steps in the deployment of the infrastructure, the status of the DEISA services, and, above all, monitor the role of applications in enhancing the scientific impact of the research infrastructure. This Newsletter will also report on recent and forthcoming events.

DEISA Symposium - Perspectives in High Performance Computing

9 - 10 May 2005, Palais des Congrès, Porte Maillot, PARIS, FRANCE

This Symposium is the first of a series that will take place every year in April-May in different locations in Europe. The purpose is to maintain an annual DEISA event dedicated to the discussion of the scientific and strategic challenges in the area of High Performance Computing, and to assess the impact of the DEISA research infrastructure on computational science in Europe. The first Symposium will include the formal inauguration of the Distributed European Infrastructure for Supercomputing Applications – DEISA. The participants are requested to register on www.deisa.org, but there will be no registration fee. The complete program is available there. The registration will close on April 17, 2005.

Scientific topics

The program presents a wide overview of the major computational challenges in all relevant areas of sciences and technology. The scientific areas that will be presented by leading computational scientists include:

• Material Sciences • Climate Modelling • Astrophysics and Cosmology • Bio-Informat-ics • Quantum Chromodynamics • Plasma Physics • Quantum Chemistry • TeraGrid Applications •

Strategic topics

The program deals with general issues concerning national and European scientific policies for HPC, technology assessments, relations of the research infrastructures with the scientific community:

• EInfrastructures in Europe • Trends in HPC in the USA • The DEISA Extreme Computing Initiative •
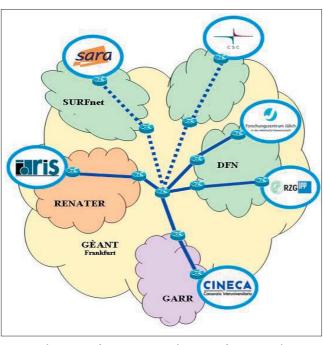
Deployment of the dedicated DEISA network infrastructure

The DEISA project creates a tightly coupled homogeneous super-cluster of leading national high-performance systems - which for all practical purposes appear as an unique European supercomputing platform – as well as an extended heterogeneous supercomputing grid embracing the previous super-cluster and many other leading multi-teraflop supercomputing platforms.

The deployment of the dedicated DEISA network infrastructure will proceed in several steps, following the evolutions of the national and European research network infrastructures, and the adoption of the infrastructure by the user's communities. During the first phase of the project a virtual dedicated 1 Gb/s network infrastructure connecting the four supercomputer systems at CINECA, FZJ, IDRIS and RZG has been implemented. Performance tests have shown that the installed links can be utilized with the full bandwidth capacity available. An extension of the infrastructure to the sites of SARA and CSC is scheduled for Q2 2005.

The current 1 Gb/s infrastructure is expected to operate for a maximum of 18 months. Planning of the "phase 2" infrastructure, that will operate at 10 Gb/s or more, has been started already. The upgrade will be driven primarily by the availability of the next generation GN2 infrastructure and by application needs. This phase will be most challenging, where technological requirements and application needs will challenge the limits that providers can offer to the supercomputer sites. The "phase 2" DEISA network will also be adapted to the deployment of the complete supercomputing grid, incorporating a number of leading heterogeneous platforms in Europe.

A close collaboration between the network teams of DEISA, the NRENs and GEANT guarantees optimum performance of the DEISA network to meet the needs of the user communities and to achieve the highly motivated goals of the project.

Extented DEISA infrastructure to the sites of SARA and CSC

DEISA Extreme Computing Initiative

While the Grid infrastructure is reaching production status smoothly, the DEISA Consortium decided to start acting without further delay in what constitutes the essence of a research infrastructure project, namely, real impact on science and technology.

The Extreme Computing Initiative consists in the identification (by June 2005), the deployment and operation of a number of "flagship" applications of the project, in selected areas of science and technology. These leading, ground breaking applications must deal with complex, demanding, innovative simulations that would not be possible without the DEISA infrastructure, and which would benefit – if accepted – from the exceptional resources from the Consortium.

A European call for proposals addressed to the scientific community is under way. The deadline for submitting expressions of interest to the Consortium is May 30, 2005. The Web server provides further details on the rules for evaluation and selection of proposals, and on the type of application that can be run on the DEISA Grid in the present status of the infrastructure.

DEISA Consortium evolution

DEISA has, from the start, aimed at becoming a privileged vector of integration of High Performance Computing in Europe. In deploying a persistent collaborative environment that engages leading HPC actors, the DEISA partners expect to lay down the seeds of a unique European supercomputing environment that will support future multi-national initiatives for HPC in Europe, whatever these initiatives may be.

It is therefore natural that the Consortium searches to integrate in its activities as many leading organizations as possible. A major step was taken at the end of last year, with the incorporation of tree distinguished supercomputing centres as full partners: BSC (Barcelona Supercomputing Centre) in Spain, and LRZ (Leibniz Computing Centre Munich) and HLRS (High Performance Computing Centre Stuttgart) in Germany. These new partners are integrating in the DEISA Grid leading world class systems that are among the most powerful in the world.
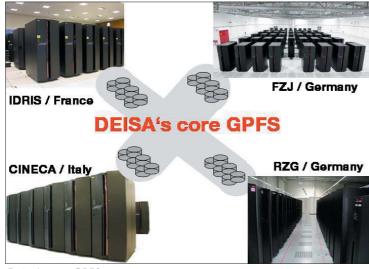
In contributing three architectures (IBM Linux on PowerPC systems, SGI Linux on Itanium systems, NEC vector supercomputers) which are different from the ones previously present in the infrastructure, the new partners definitely reinforced the Heterogeneous Supercomputing Grid concept. This evolution led the Consortium to enhance and refine the definition of the DEISA Grid architecture, to precisely define the services to be deployed and to establish a roadmap for their deployment with well defined priorities. Four fundamental lines of action were identified: workflow application services, global data management services, co-allocation services and, last but not least, portals and Web interfaces aiming at hiding complex supercomputing environment from end users. Further details on the DEISA Grid architecture can be found in the Web server.

The Consortium is currently incorporating several other organizations (supercomputing centres, leading industrial users) as Associate Partners.

More information about the DEISA Consortium is available at www.deisa.org/organisation

DEISA's Global File System reaches network speed across Europe

Global file systems are the key technology for DEISA's data management. Among the four DEISA core sites, CINECA (Italy), FZJ (Germany), IDRIS (France) and RZG (Germany), IBM's Multi-Cluster (MC) Global Parallel File System (GPFS) has been set up, the world's first real production deployment of this file system. Each site provides its own GPFS file system which is exported to all the other sites as part of the common "global" file system. First functionality and I/O tests have been very promising and helped to discriminate between potential configuration options.

Deisa's core GPFS

At present, the current wide area network bandwidth of 1 Gbit/s among the DEISA core sites can be fully exploited by the global file system. The only limiting factors left are the 1 Gbit/s network connection and disk I/O bandwidth.

This could be confirmed by several benchmarks, which showed I/O rates of more than 100 Mbytes/s, thus hitting the theoretical limit of the network connection.

Production-grade functionality and performance of the new global parallel file system could be successfully demonstrated with a real application. A resource demanding plasma physics turbulence simulation code was executed at the different core sites, using direct I/O to the MC-GPFS, the disks physically located hundreds of kilometres away from the compute nodes.

More information available at www.deisa.org/organisation/global_filesystems.php

Primer now available

The DEISA Primer is the basic documentation of the infrastructure. It includes all the information needed by users to access and execute applications in the DEISA supercomputing environment. One of the first tasks of the Users Support Team was to deploy a Common Production Environment across all sites, to enable the migration and redeployment of applications on different platforms of the infrastructure. The Common Production Environment is the common software basis (shells, compilers, libraries, tools and applications) available on each site, managed in a coherent way by all the partners. It also offers to users a powerful and flexible way to define which software resources they really need to run his current applications.

Besides the Common Production Environment, the DEISA Primer contains information on the DEISA hardware infrastructure, scientific resource management, access to DEISA resources, security issues, DEISA local and distributed file systems, workflow applications management with Unicore, and many other subjects. An accompanying FAQ (Frequently Asked Questions) provides an easy and alternative way to find quickly answers to some common questions, from some general topics to the meaning of some special terms and solutions to some frequent problems.

DEISA Primer was published in March 2005. It is available at www.deisa.org/userscorner/primer.php

Notes from GGF 13

The Global Grid Forum (GGF) held its 13th international meeting in Seoul, Korea, from March 13 to 16, 2005. Over 425 Grid experts from 26 countries met to advance the state of the art in over 50 working and research group sessions, workshops and general keynotes. A special session was held on European Grid Strategies, chaired by Mr Ulf Dahlsten, director of Emerging Technologies and Infrastructures at the EU. This session included presentations of EU policies by leading EU officials, as well as the presentation of four leading FP6 projects (EGEE, DEISA, NextGrid, CoreGrid).

During his opening keynote Mark Liensch, the new GGF chairman, presented GGF's strategy for the future and the proposed operational changes to implement the strategy. Mark stated that fulfilling GGF's mission "Lead the pervasive adoption of grid computing for research and industry" is achieved by focusing on Communities, Standards, and Operations. The Community areas enable active participation and growth for existing research communities. They pro-actively explore, develop and establish new industry communities. They increase community focused GGF events and publish community driven requirements and best practices.

In the Standards area GGF will publish a standards road map, initially OGSA v1.5. GGF will develop and support publication of important Grid specification and manage liaisons with standards organisations.

In the operations area GGF will improve its marketing, event organisation, and sponsorship activities to achieve better satisfaction and financial return for the GGF participants.

The new activities require enhanced structures in the Board of Directors, the Grid Forum Steering Group (GFSG) and also realignment of Working and Research Groups. These changes are documented under the title "Global Grid Forum – Changes to GGF Operating Model". The proposed structure and the open positions have to be reviewed by the membership and finally approved by GFSG. A unique opportunity exits now to become part of the new leadership team of GGF during 2005. The GGF Nominations Committee is chaired by Dietmar Erwin, which, besides his deep involvement in UNICORE, is also a member of the DEISA Executive Committee. Further information on the GGF Nominations Committee can be found at www.ggf.org.