

DEISA Newsletter

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CONTENTS:

1

First DEISA Extreme Computing Projects started

Second DEISA Symposium, May 4-5, 2006

2

American and European supercomputing infrastructures linked through a common wide-area global file system

3

Major Grid projects' interoperability meeting in Seattle

Achieving high quality results in industrial CFD and CAA simulations

Second DEISA Symposium, May 4-5, 2006

The second DEISA Symposium will be held in Bologna, Italy on May 4 - 5, 2006. The registration for this symposium will open in February at www.deisa.org/symposium. The symposium program will be available there, too.

This Symposium is the second 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 second DEISA Symposium will be held in Aula Magna, Bologna, an ancient church that has been turned into a conference venue.

First DEISA Extreme Computing Projects started

From the 53 proposals received at the spring 2005 call of the DEISA Extreme Computing Initiative, 29 have been retained for operation during the 2005/2006 time frame.

DEISA's Applications Task Force is currently supporting the scientists engaged in this first wave on simulations in the DEISA grid environment. For efficiency reasons, production runs are prepared as much as possible at the user's home sites, whereas the large or collaborative production runs are conducted in the full DEISA grid environment.

Users that need to run workflow applications that visit several computing systems in the grid access the distributed infrastructure with the UNICORE middleware. Some of the projects benefit directly from the common global file system GPFS of the IBM AIX sites, which allows transparent access to remote data inside the AIX super-cluster. Next February, it is expected that the multi-cluster capabilities of the IBM Loadleveler batch system will reach full

production status. This will enable the "job migration" service, which allows re-routing of jobs among the various IBM sites. Depending on the project requirements, the best map onto the DEISA supercomputing Grid is chosen for production runs.

Some of the projects that require exceptional resources at one DEISA site, have already entered production mode. More complex projects that involves complex workflows, sophisticated I/O tuning or hyperscaling to thousands of processors are currently being enabled for operation.

The first projects that have entered or are about to enter production mode on the DEISA grid cover several scientific areas: astrophysics, biophysics and computational biology, climate research, fluid dynamics, lattice gauge theories, materials science, and particle and nuclear physics. The comprehensive project list is available at www.deisa.org/applications/projects2005-2006/.

American and European supercomputing infrastructures linked through a common wide-area global file system



Seattle, Nov 15, 2005. TeraGrid, the US supercomputing cyberinfrastructure, and DEISA, the European supercomputing grid infrastructure, have been linked, for the purposes of a technology demonstration, by a common, scalable, wide-area global file system spanning two continents.

The bridging of communities in the old and the new world were showcased during the Supercomputing Conference SC05 at Seattle. It was shown that any scientist, accessing TeraGrid from any of the participating sites in the US, or accessing DEISA from any of the DEISA sites in France, Germany or Italy, can directly and transparently create or access collaborative data stored in the now linked grid-wide global file systems of TeraGrid and DEISA with one common file address space. The even more important aspect is that the same is true for applications which, executed at any of the participating sites, transparently access data in the common file address space.

High performance wide-area global file systems as GPFS from IBM open totally new modes of operation within grid infrastructures, especially in supercomputing grids with a fairly limited number of participating sites. A common data repository with fast access, transparently accessible both by applications running anywhere in the grid, and by scientists working at any partner site as entry point to the grid, greatly facilitates cooperative scientific work at the continually increasing geographically distributed scientific communities.

Both DEISA and TeraGrid have begun using the high performance wide-area global file system GPFS from IBM in production mode. For the technology demonstration, the dedicated DEISA and TeraGrid networks were interconnected with the help of specialists from GEANT, Abilene/Internet2, and the national

research networks from France, Germany, and Italy (RENATER, DFN, GARR). They established a two continent spanning high performance network between TeraGrid sites at The San Diego Supercomputer Center (SDSC), Chicago, and Indiana, and DEISA sites in several European countries (France, Germany, Italy). Over this dedicated connection, DEISA and TeraGrid global file systems were merged into one common global file system. This network connection between the two infrastructures is expected to become persistent at some time in the future.

The demonstration featured the execution of supercomputing applications of various scientific disciplines which were carried out both as TeraGrid and as DEISA applications. Single site

applications transparently wrote their results to the intercontinental global file system, ready for transparent further processing from other access grid access points.

Featured applications for the demo included a Protein Structure Prediction and a Cosmological Simulation carried out at SDSC, US and a Gyrokinetic Turbulence Simulation and also a Cosmological Simulation carried out at Garching Computing Centre of the Max Planck Society (RZG), Germany.

DEISA at SC05

During SC05 in Seattle DEISA was present as a part of the Dutch booth hosted by SARA, the Dutch DEISA partner. At the booth two screens were made available. On one screen the consortium itself was introduced and the demo was explained. The other display was used for the demonstration itself. According to the response from the visitors the advantages of a real global file system with transparent access to the data were convincing and the live demo, showing that this is already reality, impressing. All in all it was a great success.

Slideshow on the demo available at http://www.deisa.org/press/press_releases.php



One featured application for the demo was a Cosmological Simulation carried out at Garching Computing Centre of the Max Planck Society (RZG), Germany.

Major Grid projects' interoperability meeting in Seattle

Many production Grid projects have begun to offer services to end-users during the past several years, with an increasing number of applications projects that require access to resources in multiple grid systems. Most of the production grid projects regularly interact with another grid project in pairs wise fashion, discussing opportunities to collaborate and to work towards interoperation. These bilateral discussions have identified a number of opportunities where, with mi-

nor modifications, specific services offered by multiple grid systems could interoperate.

Directors and Technical leaders from the nine major production grid projects in Europe (EGEE, DEISA, UK eScience), North America (TeraGrid, OSG, Pragma) and Asia-Pacific (NAREGI, K*Grid, APAC) met together on November 17, 2005 during SC05 in Seattle (USA) to discuss these opportunities and to plan for production interoperation, in four specific services within the next year.

The services identified for interoperability discussions are:

- Authorization and identity management
- Resource and Information schema and services
- Job submission, Audit, Tracking
- Data movement and management

Working groups have been established to prepare a first draft of specific actions to be taken. A open discussion will take place during a workshop to be held at the next GGF meeting in Athens, in February 2006.

Achieving high quality results in industrial CFD and CCA simulations



Shape noise measurement in the wind tunnel

The industrial and scientific objective of this joint research activity is to move CFD (Computational Fluid Dynamics) and CAA (Computational Aero Acoustics) simulations a step forward, in order to achieve high quality results from very complex and detailed geometries.

The final goal is to demonstrate the scientific relevance of results coming from simulation of problems that today are investigated by experimental studies and show that time needs for the overall simulation procedures is compliant with time planning of new products design process.

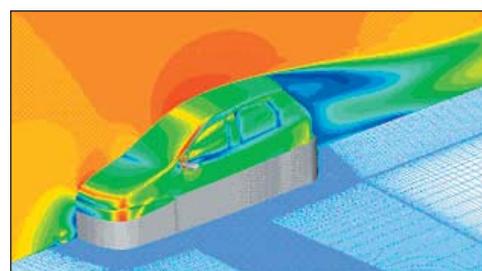
For these purposes four relevant test cases have been defined, each one with degrees of growing complexity, both in term of model dimension and time/frequency resolution.

Focus of simulations performed into first test case is on shape noise generated from a detailed car body, to establish wall pressure fluctuations due to the unsteady flow field around

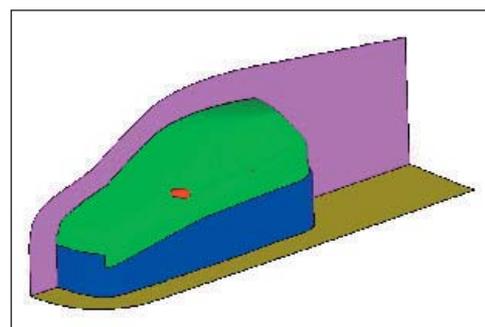
a car at cruising speed. The interest of this simulation relies on the possibility to study different car shapes as they are defined by the style department, many months before any prototype can be ready. The availability of such noise prediction tools is becoming crucial for car manufacturers to meet customers increasing demand for quieter vehicles.

The second test case deals with the simulation of open sunroof buffeting, an extremely annoying noise generated into the passenger compartment when cars move with the sunroof open. This phenomena is a consequence of a feed-back mechanism between velocity fluctuations of the separated shear-layer over the opening, and the acoustic modes of the passenger compartment. State of the art deflectors can only moderate the phenomenon, and new designs will be explored with the availability of DEISA infrastructure.

Computation of noise generated and propagated inside heating and ventilation ducts for passenger compartment constitutes the sub-



CFD simulation of the mean flow around the selected shape: velocity field in the symmetry plane and wall shear stress magnitude over the car.



Computational domain for the NLAS simulation of noise around a complete car

ject for the third test case. Many geometrical and technological constraints drive the designing process of ventilation ducts, and the lack of CAA simulations at this stage may result in a poor aeroacoustic performance that can be disclosed only at the late testing step. The main challenges for this simulation regard the simulation of the sources, mainly located in recirculation zones like curves or turning fins, and wave propagation and resonance through the whole length of the duct.

The last test case deals with shape optimisation of a simplified car body. The potential of this approach would bring to increase aerodynamic efficiency of vehicles in order to achieve fuel savings and performance improvements. Here the challenge is on time needs for hundreds of CFD analysis coming from a matrix that takes into account design variables that are commonly considered.