DEISA Perspectives

Towards cooperative extreme computing in Europe

Victor Alessandrini

IDRIS - CNRS

va@idris.fr

DEISA objectives

- *To enable Europe's terascale science by the integration of Europe's most powerful supercomputing systems.*

- *Enabling scientific discovery across a broad spectrum of science and technology is the only criterion for success*

- **DEISA is an European Supercomputing Service built on top of existing national services. This service is based on the deployment and operation of a persistent, production quality, distributed supercomputing environment with continental scope.**

- **The integration of national facilities and services, together with innovative operational models, is expected to add substantial value to existing infrastructures.**

- **Main focus is High Performance Computing (HPC).**

The DEISA Supercomputing Environment

- **IBM AIX Super-cluster**
  - **FZJ-Julich, 1214 processors, 6,8 teraflops peak**
  - **RZG – Garching, 748 processors, 3,8 teraflops peak**
  - **IDRIS, 1024 processors, 6.7 teraflops peak**
  - **CINECA, 512 processors, 2,6 teraflops peak**
  - **CSC, 512 processors, 2,6 teraflops peak**
  - **ECMWF, 2 systems of 2276 processors each, 33 teraflops peak**

- **BSC, IBM PowerPC Linux system (MareNostrum) 4864 processeurs, 40 teraflops peak**

- **SARA, SGI ALTIX Linux system, 1024 processors, 7 teraflops peak**

- **LRZ, Linux cluster (2.7 teraflops) moving to SGI ALTIX system (5120 processors and 33 teraflops peak in 2006, 70 teraflops peak in 2007)**

- **HLRS, NEC SX8 vector system, 646 processors, 12,7 teraflops peak.**

AIX SUPER-CLUSTER, September 2005
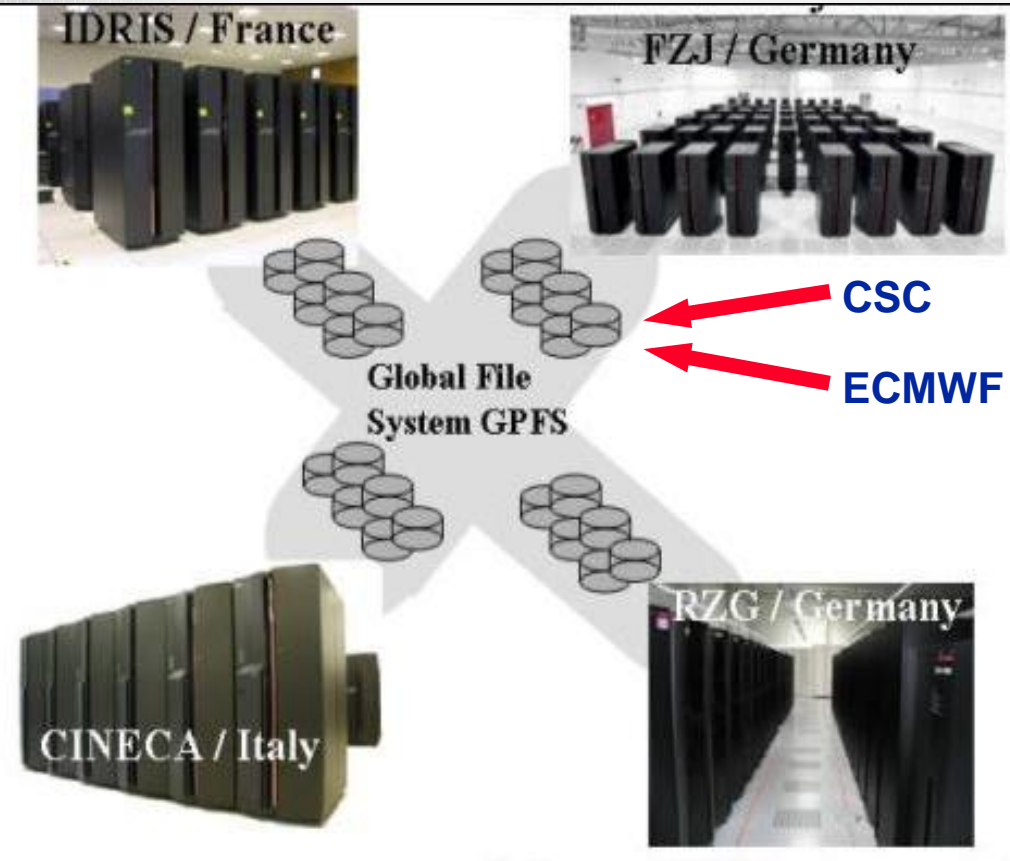
Services:

High performance datagrid via GPFS
**Access to remote files use the full
available network bandwidth**

Job migration across sites
**Used to load balance the global workflow
when a huge partition is allocated to a
DEISA project in one site**

Common Production Environment

- **Full production status of dedicated (reserved bandwidth) 1 Gb/s network**
- **GPFS : Full production at FZJ, RZG, IDRIS, CINECA; CSC and ECMWF to follow**
- **JOB MIGRATION: test status in all sites, production expected in November 2005.**

HPC and Grid computing

- Grid computing is not always HPC.

- Message Passing latencies are boosted in WANs from a few microseconds to millisecond, because the speed of light is not big enough.

- Deploying tightly coupled parallel applications in large scale grids may not be compatible with high performance requirements

- Direct Grid computing works best for (almost) embarasingly parallel applications, or coupled softwere modules with limited real time communications.

- It is better to run large, tightly coupled parallel applications in a single platform.

- DEISA implements this resuirement by rerouting jobs and balancing the computational workload at a European scale.

- A co-scheduling service will enable deployment of **weakly coupled** parallel applications on several platforms

Heterogeneous Grid services roadmap
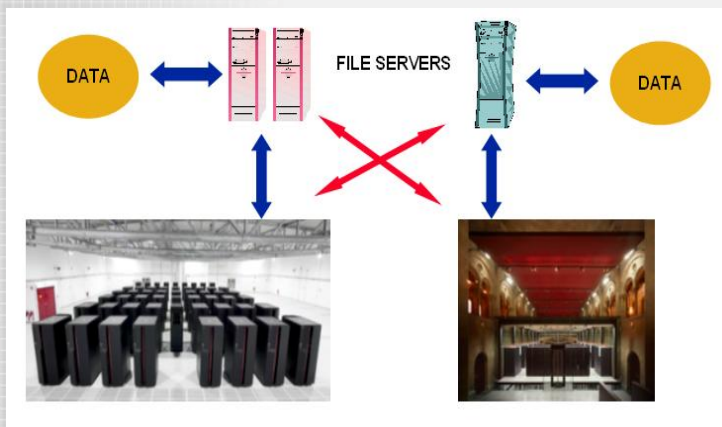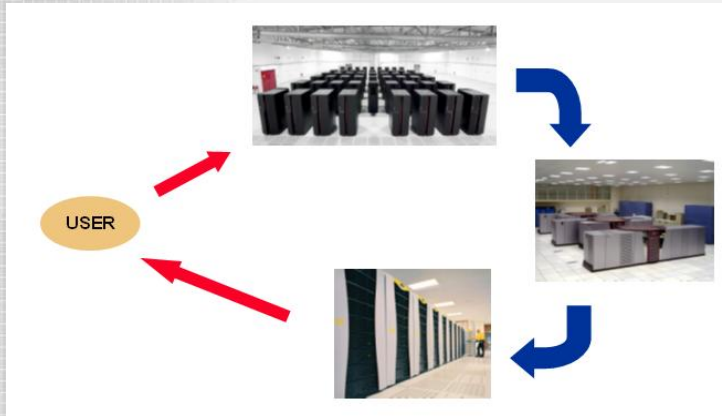
- **Extension of GPFS to non-AIX Linus systems.** GPFS will work also on the extended Grid. Extensions to SGI Altix is validated. MareNostrum can also be integrated in DEISA's GPFS

- **Workflow applications**. Based on UNICORE plus further extensions coming from EU funded projects. Available today.

- **Co-allocation**. Needed to support Grid applications running on the heterogeneous environment. First generation co-allocation service to be implemented by Platform Computing

- **Global data management**. Implementing access to distributed data, fast data transfers across sites, hierarchical data management at a continental scale. First services expected in 2006

- **Science Gateways and Portals**; Specific Internet interfaces to hade complex supercomputing environments from end users, and facilitate the access of new, non traditional users communities.

DEISA Service Activities roadmap

Distributed European Infrastructure for Supercomputing Applications
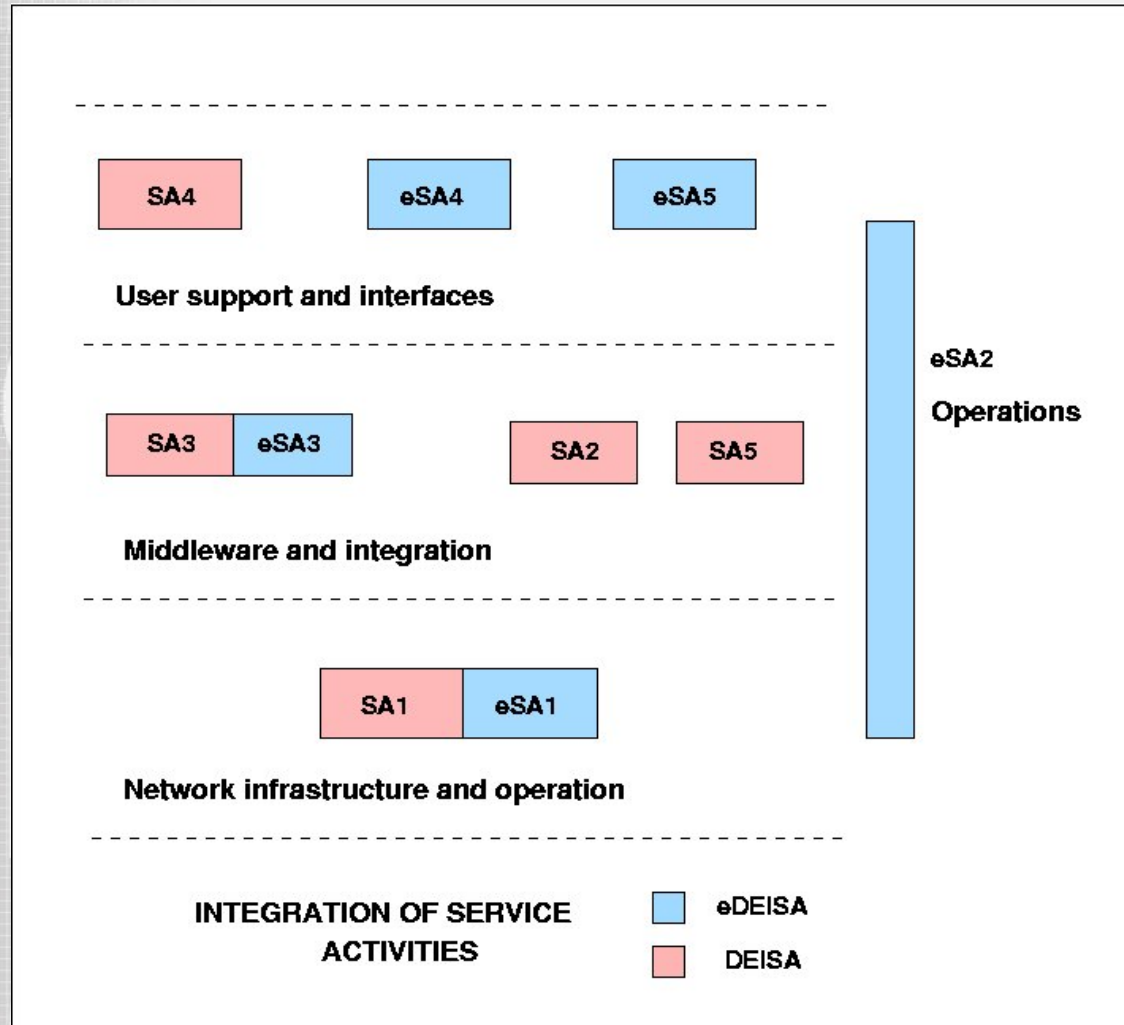
DEISA (existing)

SA1: Networking
SA2: Global File Systems
SA3: Middleware
SA4: User Support
SA5: Security

eDEISA (starting operation, not yet EU funded)

eSA2: Operations
eSA4: Applications Enabling
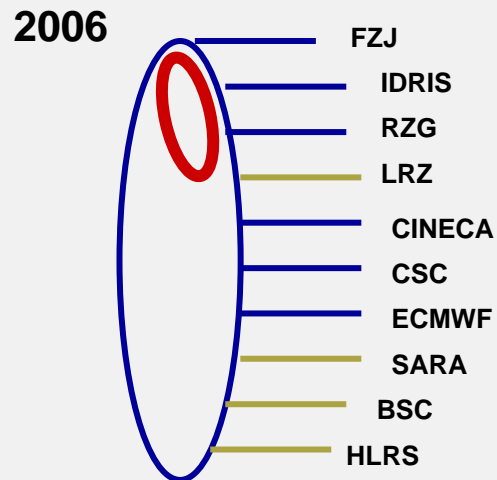**eSA5: Visualization and Portals**

Dedicated network roadmap (secured)

Today

FZJ
IDRIS
RZG
CINECA
LRZ
SARA
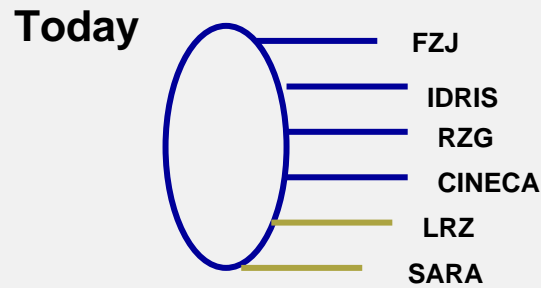
Today:

Six sites connected with dedicated bandwidth at 1 Gb/s

Provided by GEANT and NRENs

2006

FZJ
IDRIS
RZG
LRZ
CINECA
CSC
ECMWF
SARA
BSC
HLRS

2006:

•**Ten sites connected at 1 Gb/s**

•**Four sites connected at 10 Gb/s (proof of concept network platform)**

◯ 1 Gb/s   ── AIX site
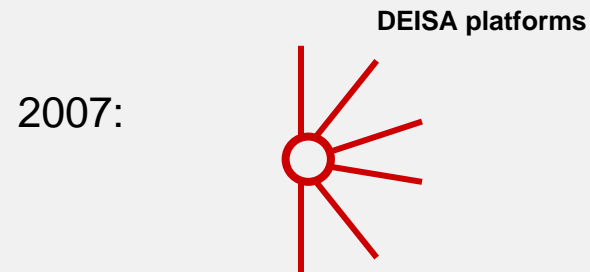
⬭ 10 Gb/s   ── Other OS.

Dedicated network roadmap (planned)

DEISA platforms

2007:

All DEISA computing platforms connected at 10 Gb/s to a central router in Germany.

Provided by GN2 and NRENs

Star topology.

2008 ?

N x 10 Gb/s
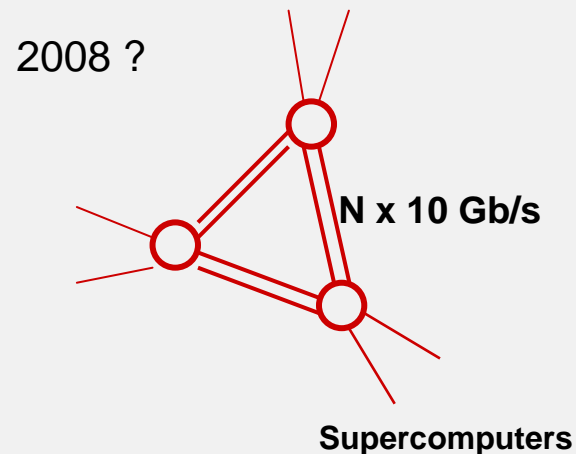
Scalable topology, internal backbone,

Two or three entry pointd for 10 Gb/s links coming from supercomputers.

Supercomputers

Enabling science

- Initially, DEISA had an « early users » program: a number of Joint Research Activities integrated in the project from the start

- As some services in the infrastructure reached production quality, we moved towards « exceptional users »

- **The DEISA Extreme Computing Initiative**: identification, deployment and operation of a number of « flagsjip » applications in selected areas of science and technology.

- Applications are selected on the basis of scientific excellence, innovation potential and relevance criteria (the application must require the extended infrastructure services)

- European call for proposals: April 1st -> May 30, 2005 (to be repeated evey year)

- Evaluation Juin -> September 2005.

- 2005-2006 projects are starting operation.

Adapting applications to the infrastructure: the ATASKF

- Creation, in April 2005, of the Applications Task Force (ATASKF), to support the Extreme Computing Initiative.

- The ATASKF carries out a prospective action with the European Scientific community. It provides guidance to find the best fit betweed the users requirements and the DEISA supercomputing environment.

- For accepted projects, the ATASKF takes all the actions needed to adapt and optimize the aplications for efficient operation in the DEISA environment

- Most demanded actions are: hyperscaling of parallel applications, data management and improved I/O, workflows.

- We had in 2005 **53 Extreme Computing proposals**.

- **29 projects were retained for operation in 2005-2006**. Full information on DEISA Web server (**www.deisa.org**) after November 8, 2005.

Extreme Computing proposals

- **Bioinformatics**   **4**
- **Biophysics**   **3**
- **Astrophysics**   **11**
- **Fluid Dynamics**   **6**
- **Materials Sciences**   **11**
- **Cosmology**   **3**
- **Climate, Environment**   **5**
- **Quantum Chemistry**   **5**
- **Plasma Physics**   **2**
- **QCD, Quantum computing**   **3**

<u>Profiles of applications in operation in 2005 – 2006</u>

- **Huge parallel applications running in single remote nodes (dominant)**
- **Data Intensive applications of different kinds.**
- **Workflows (about 10%)**

Projects from Plasma Physics

Extreme Gyrokinetic Turbulence Simulations (related to ITER project)
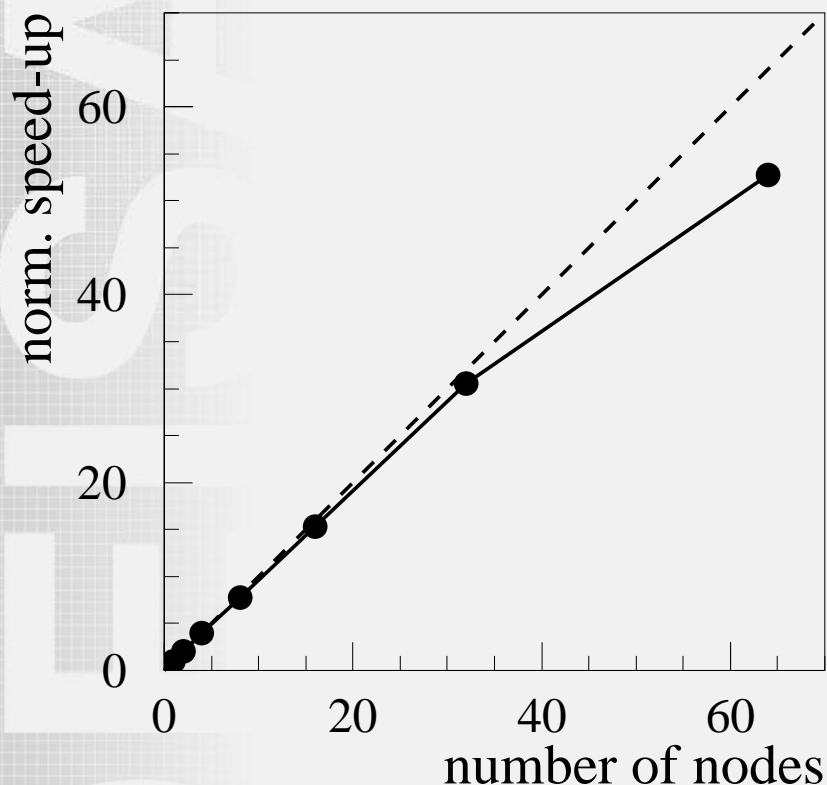
64 nodes = 2048 processors

The nonlinear particle-in-cell code TORB uses a Monte Carlo particle approach to simulate the time evolution of turbulent field structures in fusion plasmas (J. Nuehrenberg, IPP, Greifswald & L. Villard, CRPP, Lausanne)

Within DEISA, TORB has been improved for extreme scalability at IBM system at ECMWF:

On 2048 procs:

Speedup = 1680   Parallel efficiency = 82%
Sustained performance = 1.3 TF

Conclusions

- **DEISA adopts Grid technologies to integrate national supercomputing infrastructures, and to provide an European Supercomputing Service.**

- **Service activities are supported by the coordinated action of the national center's staffs. DEISA operates as a virtual European supercomputing centre.**

- *The big challenge we are facing is enabling new, first class computational science.*

- **DEISA aims at deploying a persistent, basic European infrastructure for general purpose high performance computing.**

- **Interfaced with other grid-enabled complementary infrastructures, DEISA expects to contribute to a global European eInfrastructure for science and technology**

- *Integrating leading supercomputing platforms with Grid technologies may enable new research dimensions in Europe.*