

DEISA overview



Users & Applications: Advancement of Science by Extreme Computing



Evolution of Supercomputing Resources

DEISA partners' resources at project start in 2004:
~ **30 TF** aggregated Peak performance

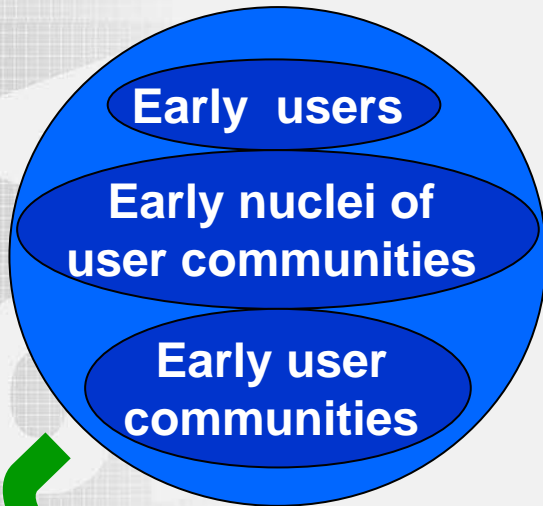
DEISA partners' resources in mid 2008:
Close to **1 PF** aggregated Peak performance
on state-of-the art supercomputers

Cray XT4, Linux
IBM Power5, Power6, AIX / Linux
IBM BlueGene/P, Linux (frontend)
IBM PowerPC, Linux (MareNostrum)
SGI ALTIX 4700 (Itanium2 Montecito), Linux
NEC SX8 vector system, Super UX

**Systems interconnected with dedicated 10Gb/s
DEISA network provided by GEANT2 and NRENs
Fixed fractions of resources dedicated to DEISA usage**

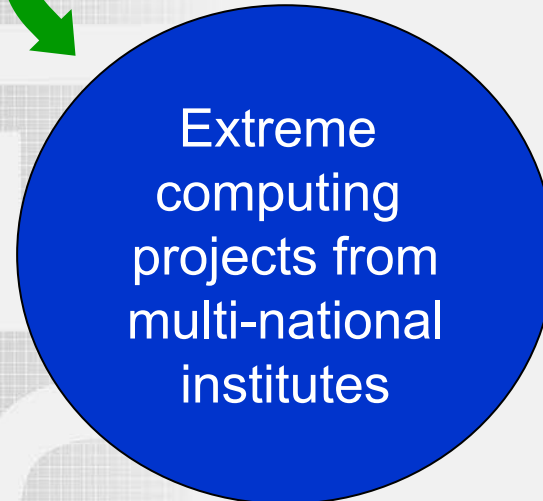


DEISA - Users & Application Support



supported
by

Joint Research Activities
JRA1: Materials Science
JRA2: Cosmology
JRA3: Plasma Physics
JRA4: Life Sciences
JRA5: Industry / CFD
JRA6: Coupled Applications
+
Service Activity SA4
User & Application Support



supported
by

Applications Task Force
ATASKF
+ Service Activity SA4
User & Application Support
+ Operation



JRA1 in Materials Science

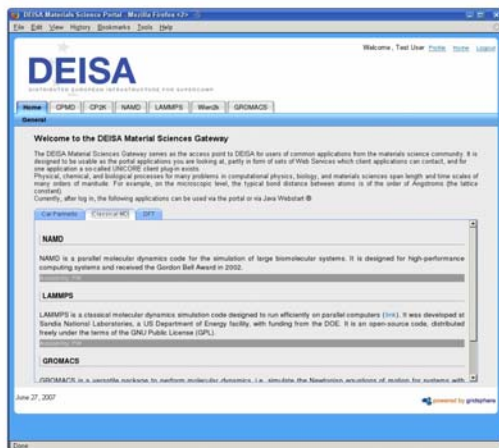
- Support and deployment of important materials science simulation codes for simple and efficient usage within the DEISA environment
- Development of a dedicated portal for materials science that offers a straightforward access to DEISA resources.

Supported applications:

CPMD, CP2K, GROMACS, LAMPPS, NAMD, WIEN2K

Threefold access strategy:

- Rich internet application based access independent of the location of the user
- Web Services, enabling integration into the user's own applications
- UNICORE Client with application-specific plug-ins

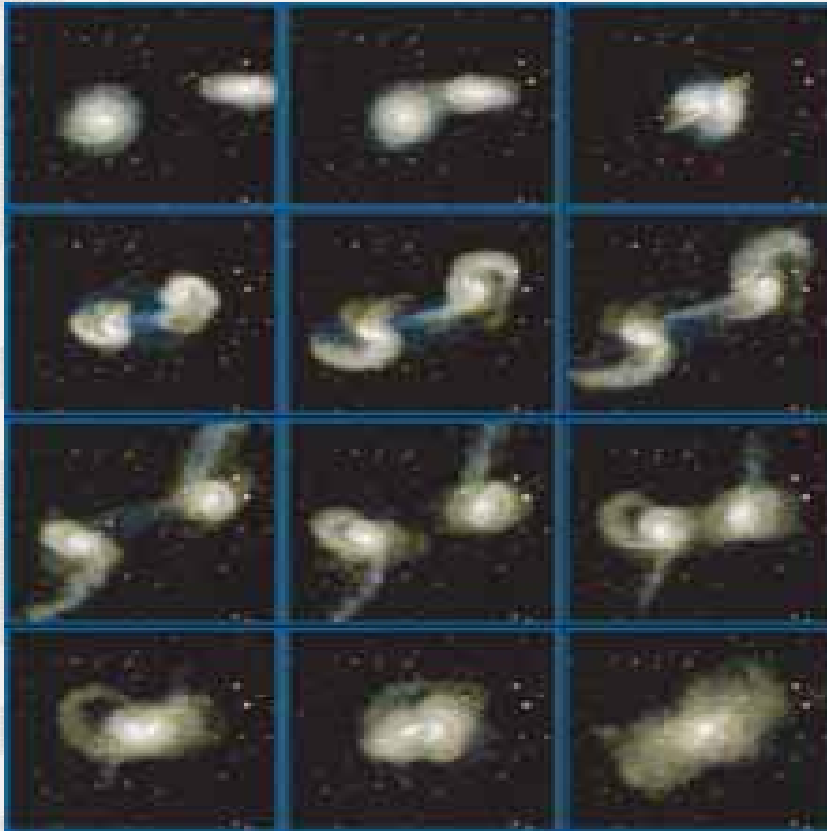


**DEISA
Materials Science Portal**



JRA2 in Cosmology

Application support for the VIRGO consortium
and their application portfolio (including pre- and post- processing)
in the heterogeneous DEISA environment



The Virgo Consortium

formed 1995, is a large international collaboration of astrophysicists dedicated to carrying out the largest and most precise simulations of the formation of cosmic structure.

Codes supported &
DEISA optimized:

Gadget

Flash

+ Pre-processing

+ Post-processing

Unicore and DESHL enabled



JRA3 in Plasma Physics

DEISA Fusion Simulation Suite:

application enabled and optimized for usage on the massively parallel state-of-the-art DEISA hardware

Simulation Codes

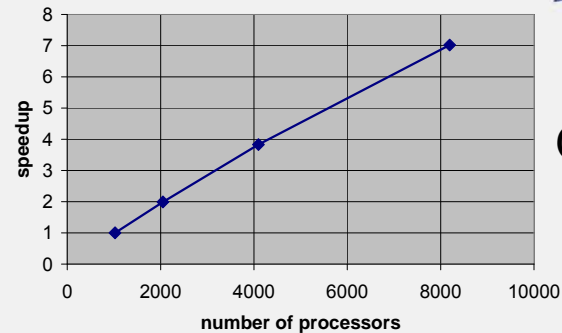
TORB / ORB5 GENE,
EUTERPE GEM GYGLES

High relevance for the European fusion community

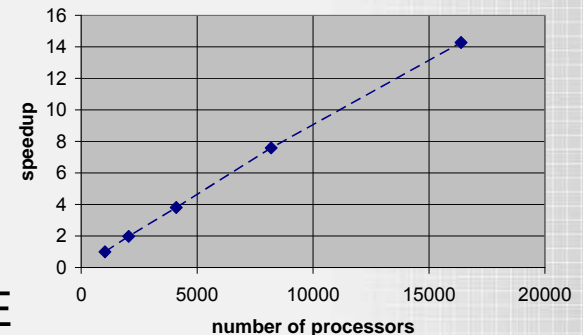
Significant improvements of both the single processor performance and the scalability of the codes

After successful enabling, all codes run efficiently in the range of 512 up to 32,000 processor-cores.

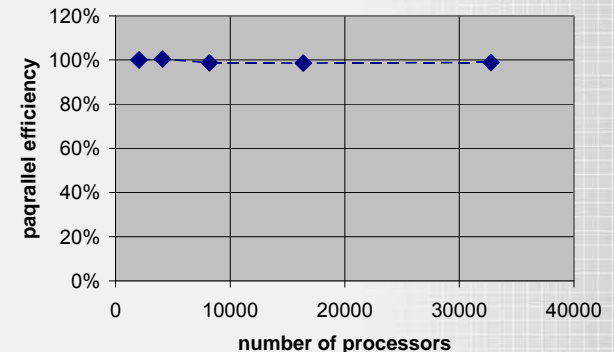
All enabled codes (but the last just finished one) selected for successful projects in the DEISA Extreme Computing Initiative



ORB5

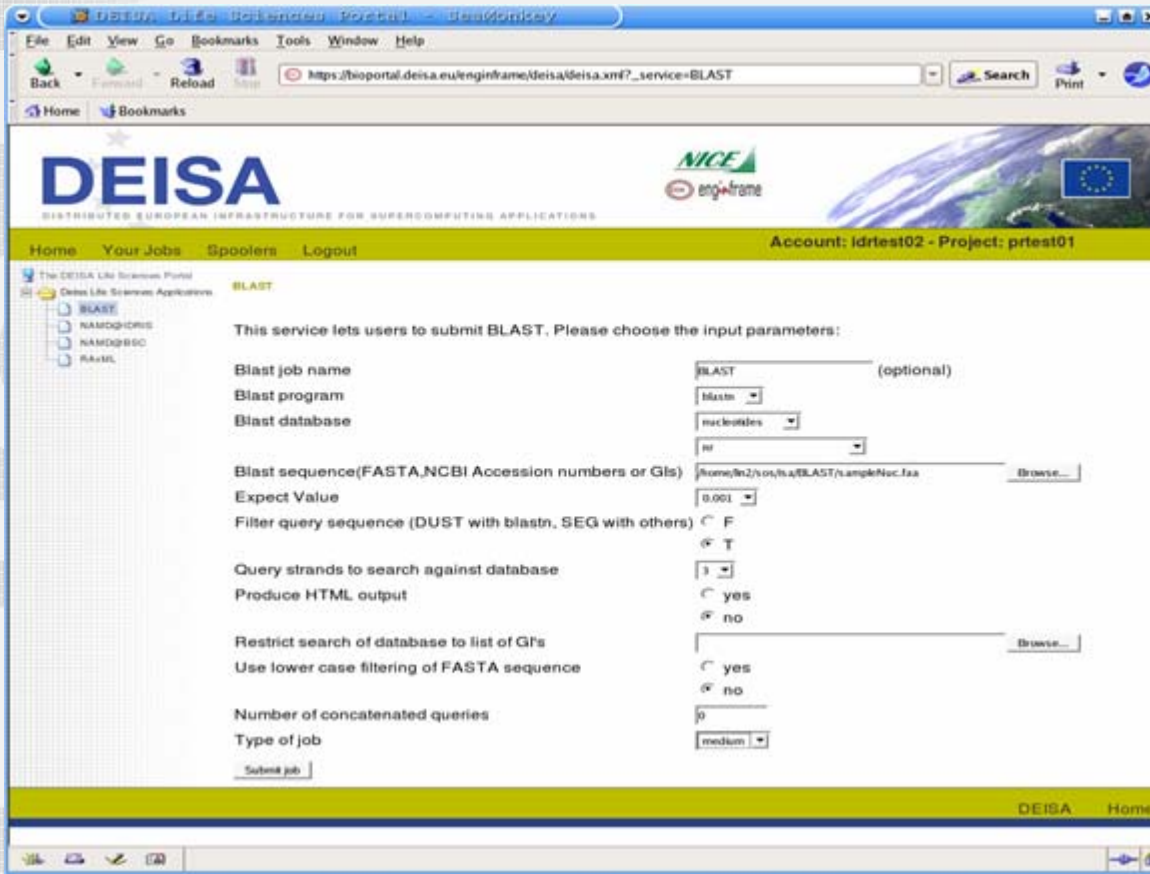


GENE



JRA4 in Life Sciences

Promotion of parallel software in the Life Sciences community



The screenshot shows a web browser window with the URL https://bioportal.deisa.eu/enginframe/deisa/deisa.xml?_service=BLAST. The page header includes the DEISA logo and the text "DISTRIBUTED EUROPEAN INFRASTRUCTURE FOR SUPERCOMPUTING APPLICATIONS". The user is logged in as "Account: ldrtest02 - Project: prtest01". The main content area is titled "BLAST" and contains the following form fields:

- Blast job name: (optional)
- Blast program:
- Blast database:
- Blast sequence (FASTA, NCBI Accession numbers or GIs):
- Expect Value:
- Filter query sequence (DUST with blastn, SEG with others): F T
- Query strands to search against database:
- Produce HTML output: yes no
- Restrict search of database to list of GIs:
- Use lower case filtering of FASTA sequence: yes no
- Number of concatenated queries:
- Type of job:

At the bottom of the form is a button.

Running big
simulations
on the DEISA
infrastructure
that couldn't
be done locally

Providing ease
of access to
resources

Application
support for life
science portal

DEISA Life Science Portal



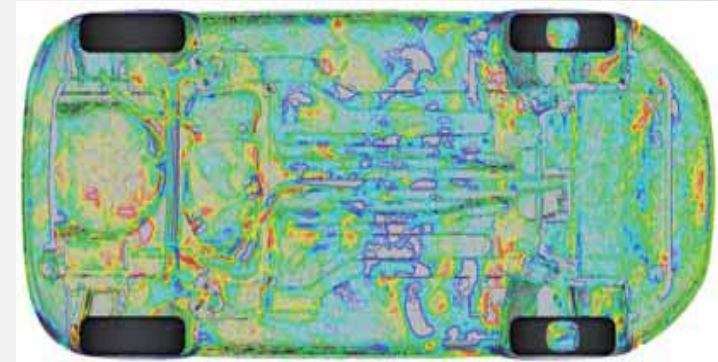
JRA5: Industrial CFD and CAA applications (via CINECA)

Exploit DEISA infrastructure capabilities for the use of industry relevant commercial codes, in order to:

- Demonstrate the use of commercial codes on the DEISA infrastructure
- Raise the limit of industrial simulations capabilities a step forward
- Give hints on how to set up commercial codes ASP service into the DEISA infrastructure
- Give a comprehensive overview on use of distributed grid architecture in the field of CFD and CAA



Focus on CFD
and CAA
applications



JRA6 Coupled Applications

Example:

3D Combustion / Radiation (FOCUS)

- Study the impact of radiative heat transfer (RHT) on the combustion process (3D – more realistic) in DECI context.
- The 2 coupled codes:
 - AVBP solves Navier-Stokes equations and computes the chemical species evolution.
 - DOMASIUM code computes the radiative field coming from the main species.
- **Achievements**
 - Built and optimized 2 large coupled configurations (load balancing)
 - Gas turbine: emphasize to take account of wall properties (sustain: 350 procs. — 288 + 60)
 - 3D diedra: bring out deep changes in the flame behaviour (sustain: 312 procs. — 192 + 120)
 - Changed the coupling technology with PALM without difficulties
- PhD thesis, 2 publications in international reviews.

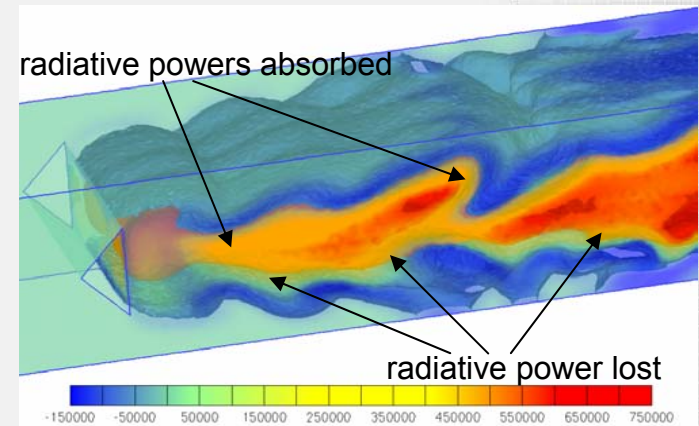


Fig 1: Radiative power in KW.m^{-3}

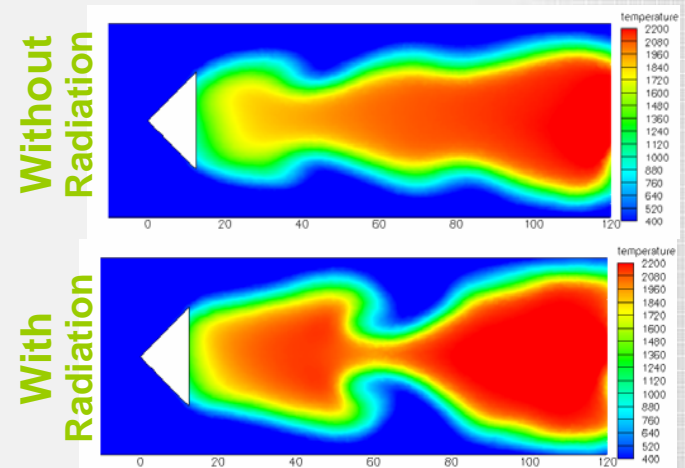


Fig 2: Temperature field in the central plane of the burner ($z = 0$) at $t = 0.55\text{s}$

DEISA Extreme Computing Initiative

DECI



- DECI launched in early 2005 to enhance DEISA's impact on science and technology
- Identification, enabling, deploying and operation of “flagship” applications in selected areas of science and technology
- Complex, demanding, innovative simulations requiring the exceptional capabilities of DEISA
- Multi-national proposals especially encouraged
- Proposals reviewed by national evaluation committees



DEISA Extreme Computing Initiative



- Projects chosen on the basis of innovation potential, scientific excellence, relevance criteria, and national priorities
- Most powerful HPC architectures in Europe for the most challenging projects
- Most appropriate supercomputer architecture selected for each project
- Mitigation of the rapid performance decay of a single national supercomputer within its short lifetime cycle of typically about 5 years, as implied by Moore's law



Support Measures

- Application enabling by Applications Task Force (ATASKF), team of leading experts in high performance and grid computing
- DEISA Common Production Environment (DCPE): homogenising the heterogeneous DEISA software environments
- General environment and user related application support
- European team of system operation specialists handling coordination and synchronisation of system services, maintenance measures and failure situations
- Training sessions



Application Enabling and Optimizations

- **Scaling of parallel programs** for efficient usage on thousands of processor-cores challenging, necessary task for state-of-the-art supercomputers
- Support for **data intensive applications**
- Design, deployment and optimization of **workflow applications** to chain several compute tasks (simulation, pre- and post-processing steps)
- **Coupled applications** important e.g. for climate system modelling with separate components for ocean, atmosphere, sea ice, soil, atmospheric chemistry and aerosols
- Adaptation to the DEISA infrastructure
- Optimizations, also architecture dependent optimizations
- Determination of best suited architecture



DEISA Extreme Computing Initiative



Annual Calls for Proposals for challenging supercomputing projects from all areas of science

DECI call 2005

- > 50 proposals, 12 European countries involved, co-investigators from US
- > 30 mio cpu-h requested,
28 projects selected, 12 mio cpu-h awarded

DECI call 2006

- > 40 proposals, 12 European countries involved, co-investigators from N + S America, Asia (US, CA, AR, ISRAEL)
- ~ 30 mio cpu-h requested
23 projects selected, 12 mio cpu-h awarded

DECI call 2007

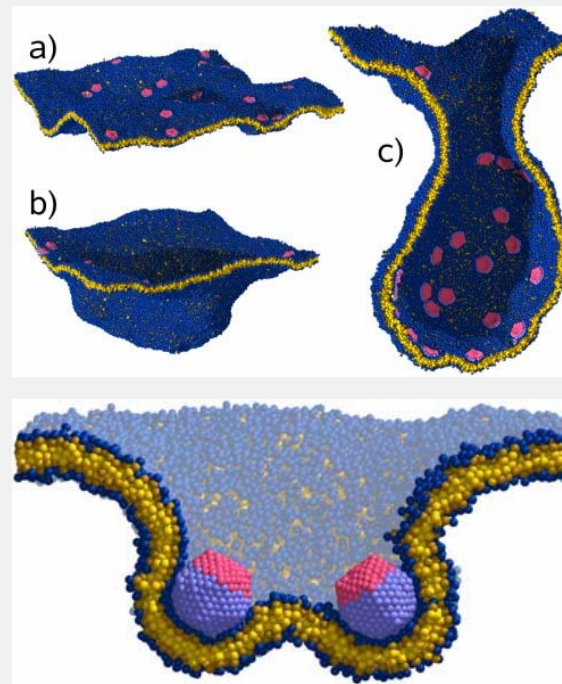
- > 60 proposals, 14 European countries involved, co-investigators from N + S America, Asia, Australia (US, CA, BR, AR, ISRAEL, AUS)
- > 70 mio cpu-h requested
45 projects selected, ~ 30 mio cpu-h awarded



DECI Project POLYRES

Curvy membranes make proteins attractive

Cover story of Nature - May 24, 2007



- a) proteins (red) adhere on a membrane (blue/yellow) and locally bend it;
- b) this triggers a growing invagination.
- c) cross-section through an almost complete vesicle

Benedict J. Reynwar, Gregoria Illya, Vagelis A. Harmandaris, Martin M. Müller, Kurt Kremer & Markus Deserno:
Aggregation and vesiculation of membrane proteins by curvature mediated interactions,
NATURE Vol 447|24 May 2007| doi:10.1038/nature05840



DEISA Extreme Computing Initiative



**Involvements in projects from
DECI calls 2005, 2006 and 2007:**

157 institutes, universities and industry partners

from

15 European countries

Austria

Finland

France

Germany

Hungary

Italy

Netherlands

Poland

Portugal

Romania

Russia

Spain

Sweden

Switzerland

UK

with collaborators from

4 other continents

Asia, Australia, North America, South America



Achievements and Scientific Impact 2008



Summary of DEISA Status (1)

- Network of Cooperation
- Deployment and operation of a continental HPC eInfrastructure
- Unified and seamless access to European supercomputing resources
- Access to most powerful and most adequate supercomputer architectures in Europe
- Portals for transparent access to complex supercomputing environments
- Collaborative Environment and Support
- Establishment of a European Benchmark Suite
- Enabling of cooperative extreme computing in Europe
- Europe-wide support for applications enabling
- Grand Challenge projects performed on a regular basis



Summary of DEISA Status (2)

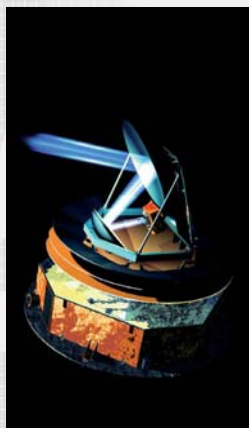
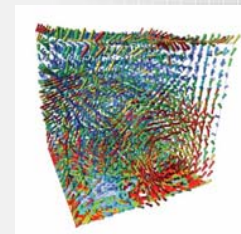
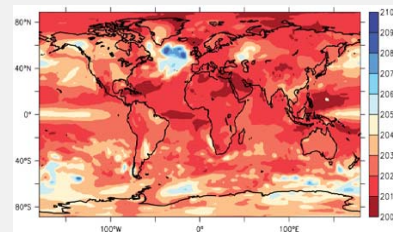
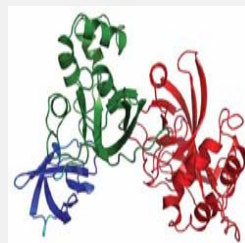
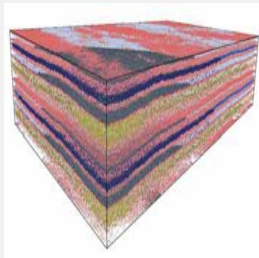
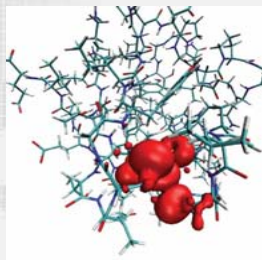
DEISA Benchmark Suite:

Design and development of a European Benchmark Suite

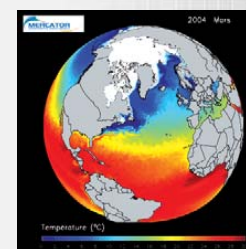
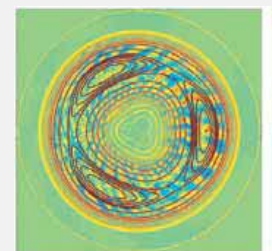
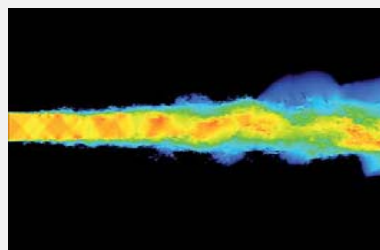
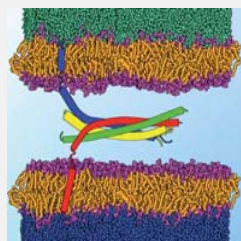
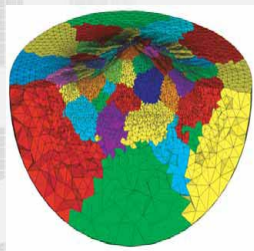
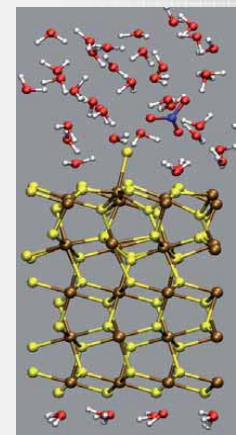
- Applications and datasets from representative scientific fields, complementary in testing essential features of supercomputer architectures under real world conditions
- Set of low-level benchmarks to exercise single important architectural features of a supercomputer
- Porting codes of the Benchmark Suite to DEISA's essential platforms
- Elaboration of a set of rules for vendors
- Contribution to the DEISA performance conversion factors between different architectures



Summary of DEISA Status (3)



**Contribution to the
advancement of
European computational
sciences in the
supercomputing area**



Looking back



“Leading European scientific organisations propose to build a Distributed European Infrastructure for Supercomputing Applications (DEISA) for science and technology. The aim is to provide a seamless and easy to use high performance computing facility, transparently accessible in a standardised way by end users across Europe.”

“The proposed Integrated Project associates national HPC centres, research centres, and technology providers, to build a – hopefully - production quality, distributed, high performance supercomputing environment in Europe.....”

DEISA Vision 2002

in the *Expression of Interest for an “Integrated Project” sent to EC on June 4, 2002*



Distributed European Infrastructure for Supercomputing Applications

Expression of Interest for an “Integrated Project”

June 4, 2002

2002

ESFRI launched



European Commission
Research Directorate-General
Brussels, 25 April 2002

Press release

Research infrastructures: the Commission launches a European Strategy Forum

Key words: Research Infrastructures, European Research Area, Science Policy, Strategy Forum.

2003



eIRG launched

About e-IRG

Meetings

Publications

Minutes

Members

Contact

About e-IRG

The e-Infrastructure Reflection Group (e-IRG) Meeting coordinates on a high-European level the introduction of a (grid based) infrastructure for e-Science.

Mission of the e-IRG

The main objective of the e-IRG is to support on the political, advisory and monitoring level, the creation of a policy and administrative framework for the easy and cost-effective shared use of electronic resources in Europe (focusing on Grid-computing, data storage, and networking resources) across technological, administrative and national domains.

The mission of e-IRG was drafted in Rome on 10 december 2003.

Objectives

- To identify the fundamental fabric, services and resources needed to enable pan-European e-Science

DEISA proposal submitted

2004

FP6 DEISA project started with 8 partners

2005

DEISA extended to 11 partners
DECI started

2006



High-Performance Computing In Europe Taskforce



ESFRI Roadmap Report 2006

FP6 eDEISA project started



ESFRI Report 2006, p. 65

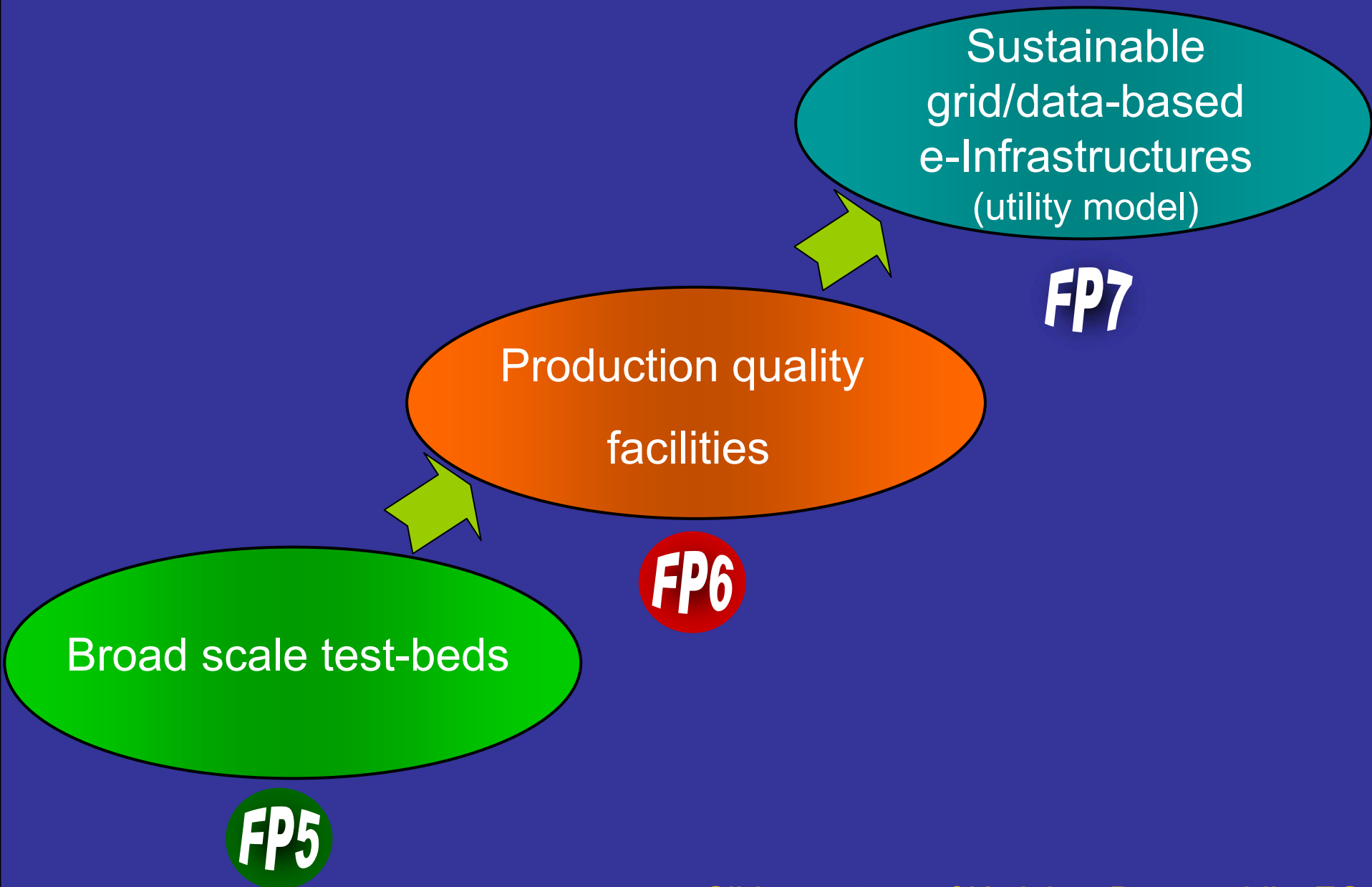
European High-Performance Computing Service

The facility

A European strategic approach to high-performance computing, concentrating the resources in a limited number of **world top-tier centres** in an overall infrastructure connected with associated national, regional and local centres, forming a scientific computing network to utilise the top-level machines.



Towards sustainable grid-empowered e-Infrastructures



Examples of activities

- Establishing a production-quality scalable, reliable infrastructure, building on the current achievements and being accepted on a global scale
- Addressing issues of an open market for grid services (e.g. implementing incentive-based models for providing grid resources, deploying relevant accounting schemes, etc.)

Expected Outcome

- Providing persistent, cross disciplinary services to pan-European virtual research communities, with increased levels of trust and confidence
- Sharing more computing resources (including distributed supercomputing), scientific instrumentation and data facilities across multiple scientific disciplines
- Promoting open standards and interoperability
- Innovating and consolidating middleware technology
- Adopting robust, reliable and scalable authorisation and authentication schemes
- Implementing attractive mechanisms for the pooling of further resources across a very broad range of user communities
- Evolving towards the adoption of more sustainable organisational models for the provision of services



DEISA – looking forward



In [EU FP7](#) The DEISA Consortium continues to support and further develop the distributed high performance computing infrastructure and its services through the [DEISA2 project](#).

- Continuation and further enhancement of activities and services relevant for

Operation Technologies Applications Enabling

- Extension of the service provisioning model from single project support (DECI) to supporting Virtual European Communities.
- Cooperation with PRACE

Of strategic importance is the cooperation with the PRACE project which is preparing for the installation of a limited number of leadership-class Tier-0 supercomputers in Europe.



DEISA2 in FP7

DEISA2: eInfrastructure project

May 2008 – April 2011

PRACE: design study / preparational project

Jan 2008 - Dec 2009

Goals of DEISA2 and PRACE in-line
with the objective of the ESFRI roadmap

DEISA2 and PRACE will jointly contribute in close
cooperation to building up the European HPC ecosystem

DEISA2-PRACE cooperation group already established



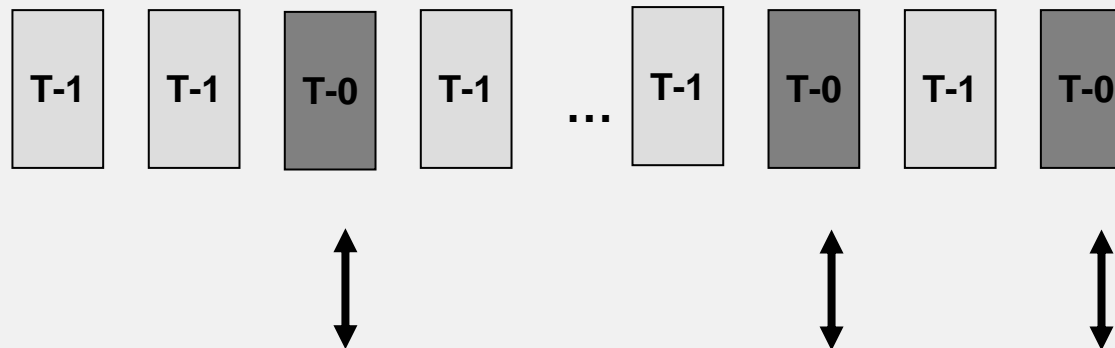
Vision of a European HPC Ecosystem



DEISA2 - The Infrastructure for the European HPC Ecosystem

Deep operational and technological integration of European HPC (T-0 and T-1) centres and systems providing efficient seamless access to shared HPC resources and large data repositories designing and approving an operational model for a large European Virtual HPC Centre.

Providing scientists access to a large distributed HPC environment via integrated services.
DEISA is paving the way to the efficient operation of the T-0 and T-1 ecosystem



PRACE

Building a world-class pan-European High Performance HPC Ecosystem which is operated under the umbrella of an European Legal Entity adopting operational and technological concepts and services designed and approved by DEISA2.



DEISA 2008

Six years of pioneering work towards a European HPC Ecosystem

