

# DEISA Extreme Computing



DEISA PRACE Symposium 2010

Hermann Lederer, Max Planck Society

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RI-222919

# DEISA

**DEISA's fast continental  
file system built on  
GEANT2**

*Six years of operation*

*Most powerful  
European Supercomputers  
for most challenging projects*

*Grand Challenge  
projects performed  
on a regular basis*

*Top-level Europe-wide  
application enabling*

*Virtual Science Community  
Support*

 DEISA 10 Gb/s network infrastructure 



15 partners, 10 countries

## TOP Sites List Generator

The ranking is determined using the sum of the Rmax share of every site in every list since 1993. For example:

Total Rmax in 1993 was 1.12 TFlops and Los Alamos National Laboratory had a total of 7 systems with a combined Rmax of 86.34 GFlops, thus, the share of LANL for June 1993 would be approx. 0.077. We then add those shares per site and rank the sites using the sum of the shares then we divide the sum by the number of the lists since June 1993.

Rank	Site	Country	% in all lists
1	ECMWF	United Kingdom	1.02
2	Forschungszentrum Juelich (FZJ)	Germany	0.87
3	United Kingdom Meteorological Office	United Kingdom	0.66
4	Commissariat a l'Energie Atomique (CEA)	France	0.58
5	HWW/Universitaet Stuttgart	Germany	0.57
6	Leibniz Rechenzentrum	Germany	0.51
7	Max-Planck-Gesellschaft MPI/IPP	Germany	0.49
8	University of Edinburgh	United Kingdom	0.46
9	Deutscher Wetterdienst	Germany	0.44
10	CINECA	Italy	0.36
11	IDRIS	France	0.35
12	Barcelona Supercomputing Center	Spain	0.33
13	CSAR at the University of Manchester	United Kingdom	0.31
14	CSC (Center for Scientific Computing)	Finland	0.30
15	Atomic Weapons Establishment	United Kingdom	0.28
16	Commissariat a l'Energie Atomique (CEA)	France	0.26
17	SARA (Stichting Academisch Rekencentrum)	Netherlands	0.26
18	Ecole Polytechnique Federale de Lausanne	Switzerland	0.26
19	BMW AG	Germany	0.25
20	Swiss Scientific Computing Center (CSCS)	Switzerland	0.22

# DEISA



## Top500 List

## Top Sites since 1993

## Continent: Europe

# DEISA Supercomputers

State-of-the art supercomputers

> 2 PF aggregated peak performance

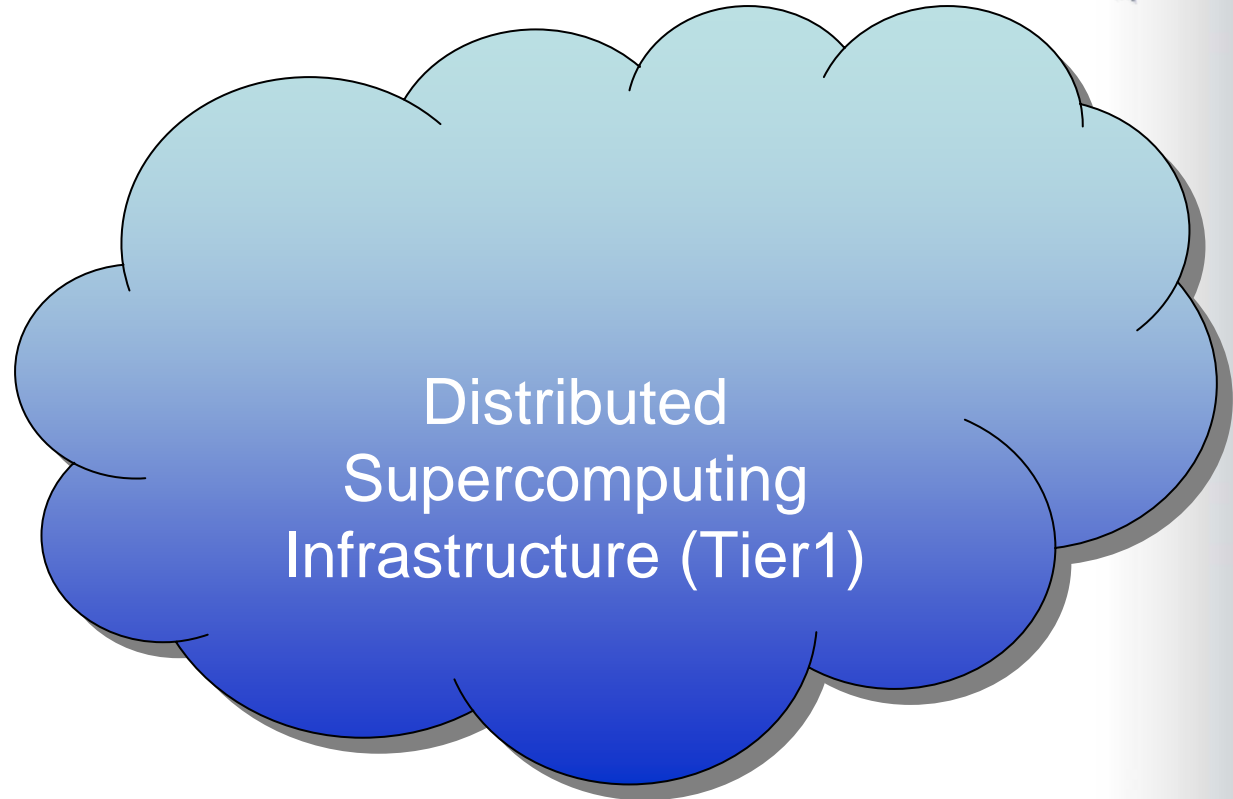
- Cray XT4/5/6, Linux
  - IBM Power6, AIX / Linux
  - IBM BlueGene/P, Linux
  - IBM PowerPC, Linux (MareNostrum)
  - SGI ALTIX 4700, Linux
  - NEC SX9 vector system, Super UX
- 
- Fixed fractions of resources dedicated to DEISA usage
  - Systems interconnected with dedicated 10Gb/s network

# Service Structure

Applications

Users  
(single projects)

Science  
communities



Application  
support team

Operation & user  
support team

Technology  
team

# Distributed Supercomputing Infrastructure (Tier1)

Access via Internet

Single sign-on, secure login

DEISA Common Production Environment

Different Software *Environments*

E(S1) E(S2) E(S3) E(S4) ..... E<sub>2</sub>(S1) E<sub>2</sub>(S2) E<sub>2</sub>(S3)

S1 S2 S3 S4 ..... S1 S2 S3

Different *Supercomputers*

Dedicated 10 Gb/s network – via GEANT2

DEISA highly performant continental global file system

## DECI

# DEISA Extreme Computing Initiative

**2005**

**1st DECI call**

**2006**

**2nd DECI call**

**2007**

**3rd DECI call**

**2008**

**4th DECI call**

**2009**

**5th DECI call**

**2010**

**6th DECI call**

## DECI

# DEISA Extreme Computing Initiative

- Target: Complex, demanding, innovative simulations
- Multi-national proposals especially encouraged
- Review by national evaluation committees
- Selection criteria: innovation potential, scientific excellence, relevance, and national priorities
- Most powerful HPC architectures in Europe available for the most challenging and excellent projects
- Most appropriate supercomputer architecture selected per 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

# DEISA Extreme Computing Initiative



## DECI call 2005

51 proposals, **12** European countries involved, co-investigator from US  
30 mio cpu-h requested  
29 proposals accepted, 12 mio cpu-h awarded (normalized to IBM P4+)

## DECI call 2006

41 proposals, **12** European countries involved  
co-investigators from N + S America, Asia (US, CA, AR, ISRAEL)  
28 mio cpu-h requested  
23 proposals accepted, 12 mio cpu-h awarded (normalized to IBM P4+)

## DECI call 2007

63 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 proposals accepted, ~30 mio cpu-h awarded (normalized to IBM P4+)

# DEISA Extreme Computing Initiative



## DECI call 2008

66 proposals, **15** European countries involved, co-investigators from N + S America, Asia, Australia  
134 mio cpu-h requested (normalized to IBM P4+)  
42 proposals accepted, 48 mio cpu-h awarded (normalized to IBM P4+)

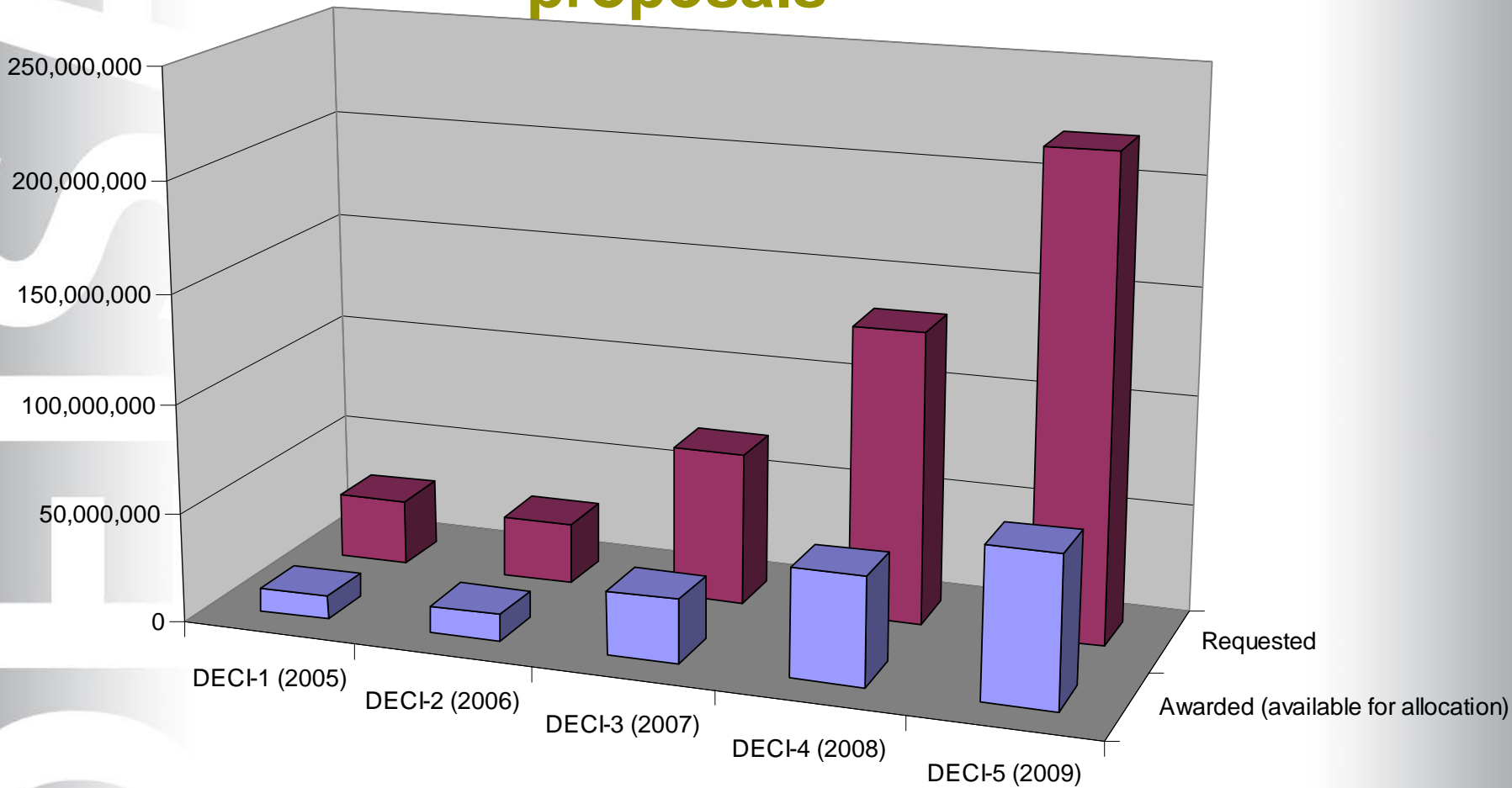
## DECI call 2009

75 proposals, **21** European countries involved, co-investigators from N America, Asia  
220 mio cpu-h requested (normalized to IBM P4+)  
50 proposals accepted, 60 mio cpu-h awarded

## DECI call 2010

122 proposals, **24** European countries involved, co-investigators from N America, Asia  
570 mio cpu-h requested (normalized to IBM P4+)

# CPU requested in DECI proposals



**Demand for CPU increasing at a faster rate than supply**

# DEISA Extreme Computing Initiative



## Projects from DECI calls 2005, 2006, 2007, 2008, 2009:

Involvement of over 180 research institutes and universities from 25 European countries:

Austria	Belgium	Cyprus	Denmark	Finland
France	Germany	Greece	Hungary	Ireland
Italy	Latvia	Norway	Poland	Portugal
Romania	Russia	Slovak Rep.	Spain	Sweden
Switzerland	Netherlands	Turkey	Ukraine	UK

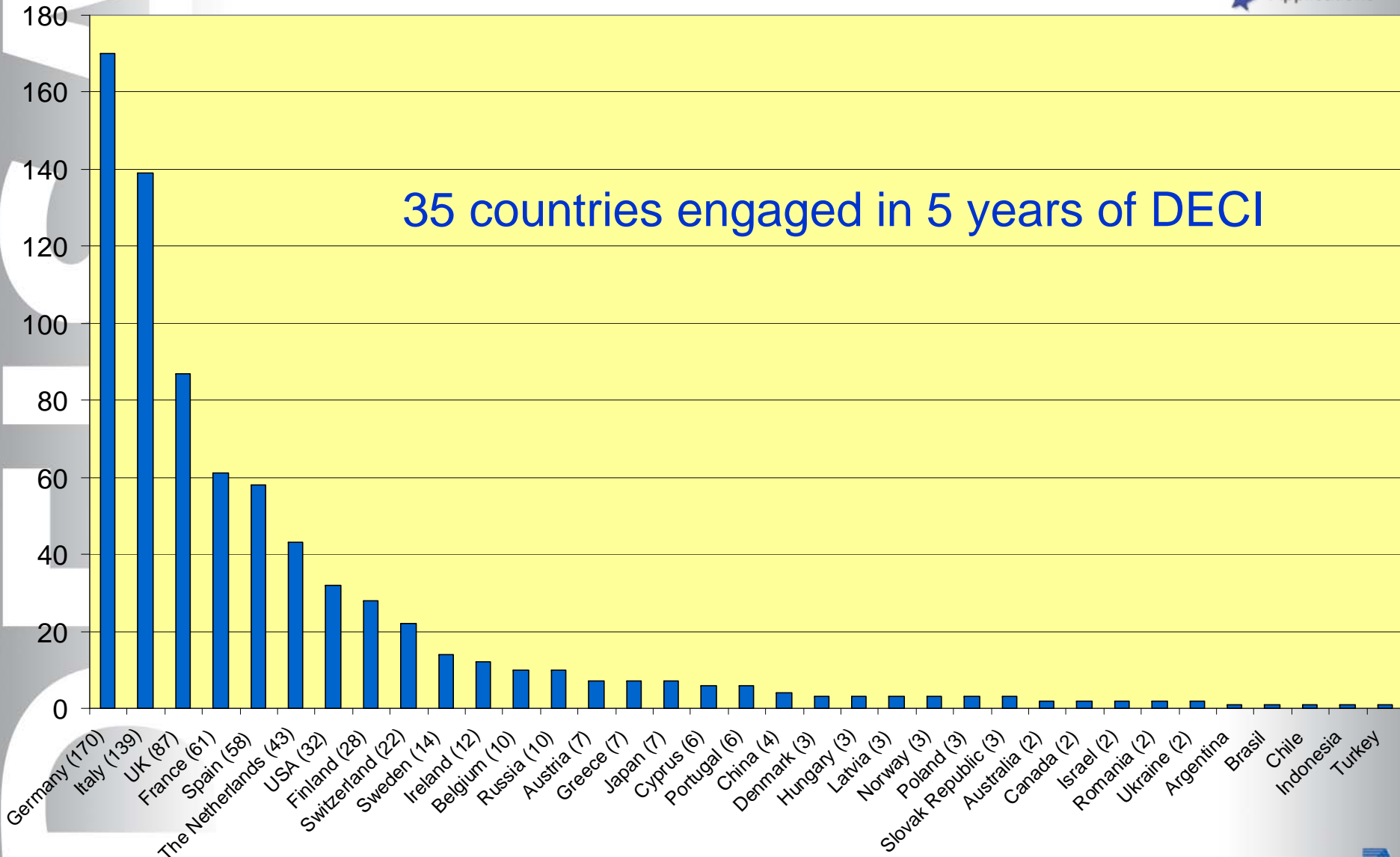
*with collaborators from four other continents*

North America, South America, Asia, Australia

# DECI – Investigators by Countries



35 countries engaged in 5 years of DECI



## Cover Story of Nature

### Curvy membranes make proteins attractive

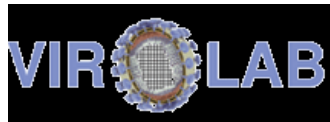


**Nature 447 (2007), 461-464**

*For almost two decades, physicists have been on the track of membrane mediated interactions. Simulations in DEISA have now revealed that curvy membranes make proteins attractive*

# Virtual Community Support

## Life Sciences



[www.virolab.org](http://www.virolab.org)

Virtual laboratory for infectious diseases

EU FP6 project

8 EU countries, 11 EU partners



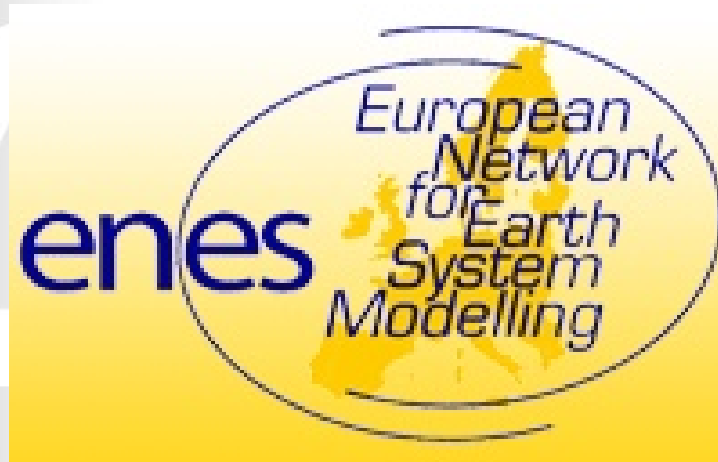
[www.vph-noe.eu](http://www.vph-noe.eu)

EU FP7 project

7 EU countries, 13 EU partners

# Virtual Community Support

## Climate Research



[www.enes.org](http://www.enes.org)

### **European Network for Earth System Modelling operating the IS-ENES Project**

Consortium and international project  
15 EU countries, 44 EU partners, plus USA

# Virtual Community Support

## Space Science



**LFI-PLANCK**

[www.esa.int/SPECIALS/Planck](http://www.esa.int/SPECIALS/Planck)

Planck space mission of European Space Agency  
(Low Frequency Instrument part)

Project of EU organisation  
6 EU countries, 6 EU partners, plus USA

# Virtual Community Support

## Fusion Energy Research:



[www.efda.org](http://www.efda.org)

European Fusion Development Agreement

Legal entity

26 EU countries, 31 EU partners



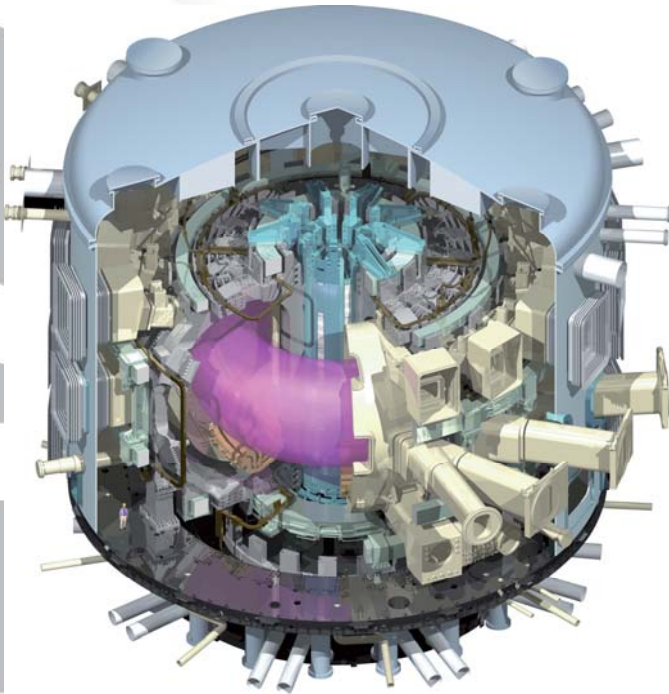
[www.euforia-project.eu](http://www.euforia-project.eu)

EU Fusion fOR Iter Applications (EUFORIA)

EU FP7 project

14 EU countries, 14 EU partners

# Fusion Energy Research



**ITER**

„The fusion community has benefited from over 10 million hours of computer resources under DEISA in the last couple of years, via the different organizations and projects.

This has allowed significant progress to be made in the use of large-scale computer resources for fusion applications.

DEISA facilitates access to a diverse set of computer architectures, which has created new opportunities for the fusion community.“



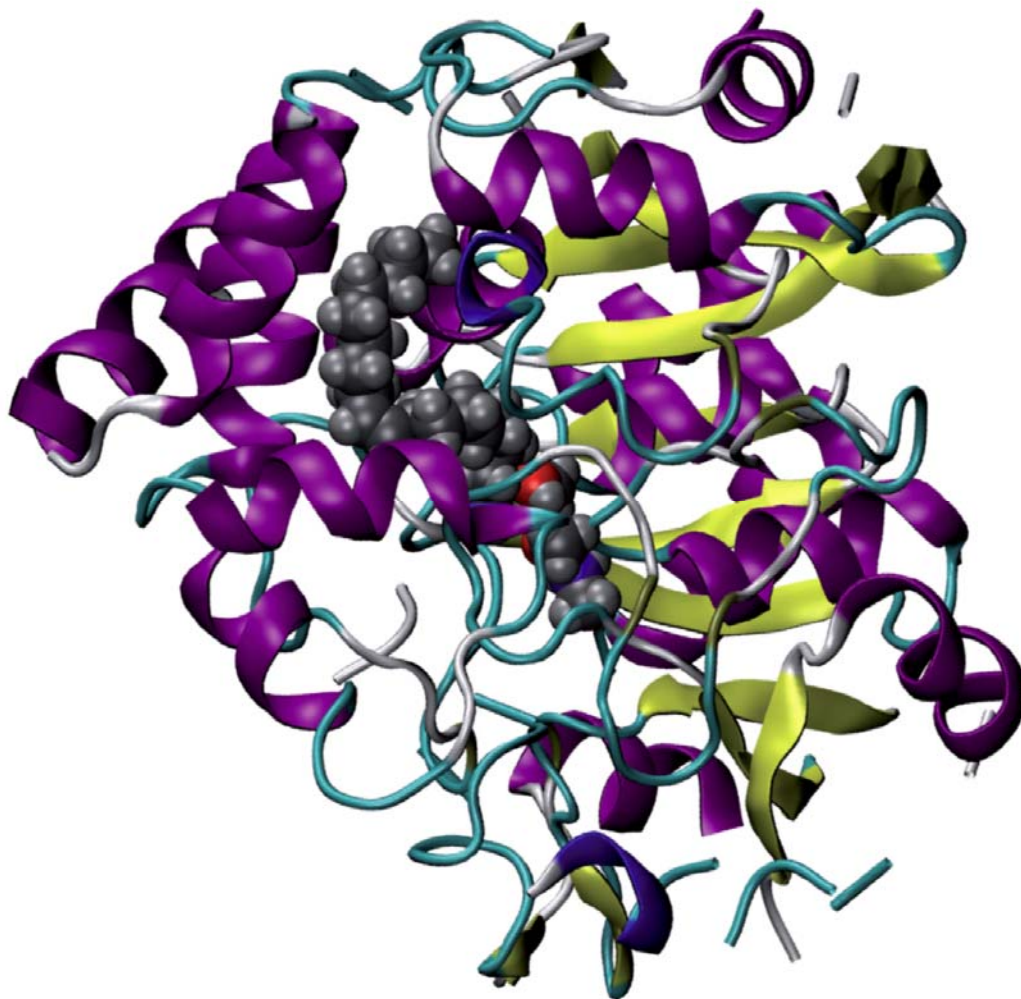
# DECI Project EUQUAKE

## Earthquake scenarios for Europe

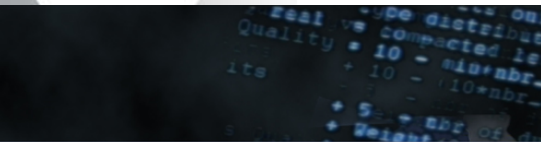


# DECI Project TotalEnz

## Modeling Enzymes: Catalysis of Life



First  
principles  
calculation  
of free  
energy  
barriers of  
enzyme  
catalysed  
reactions

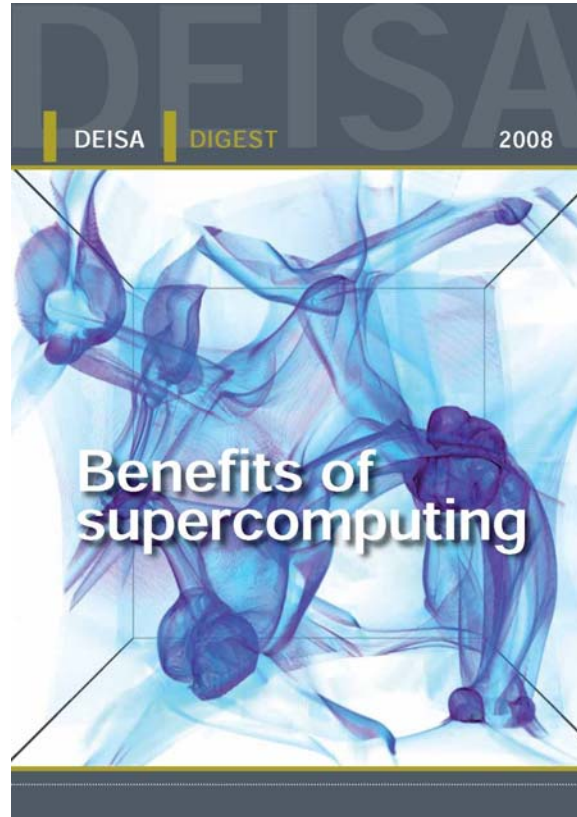


DEISA

TOWARDS A EUROPEAN HIGH-PERFORMANCE-COMPUTING INFRASTRUCTURE

COMBINED POWER FOR FASTER COMPUTATION

# Scientific Impact



Brochures and video can be downloaded from <http://www.deisa.eu/publications/results>