Partnership for Advanced Computing in Europe

The European Projects

Achim Bachem, Forschungszentrum Jülich
Paris, June 3 2008, Ter@tec

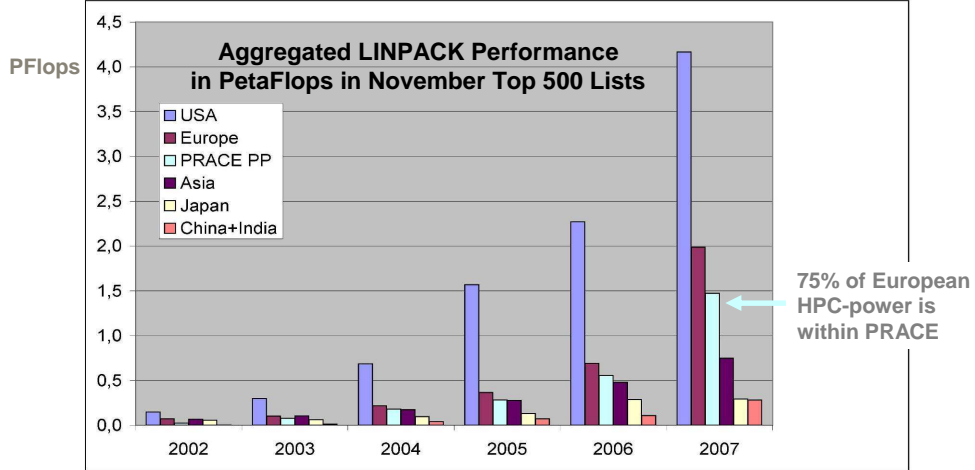---

HPC is a "Key Technology"

- Supercomputers are *the* tool for solving most challenging problems through simulations
- Access to capability computers of leadership class is essential for international competiveness in science and engineering
- Providing competitive HPC services is a continuous endeavor
- This has been acknowledged by leading industry nations such as USA and Japan since the 1990'ies
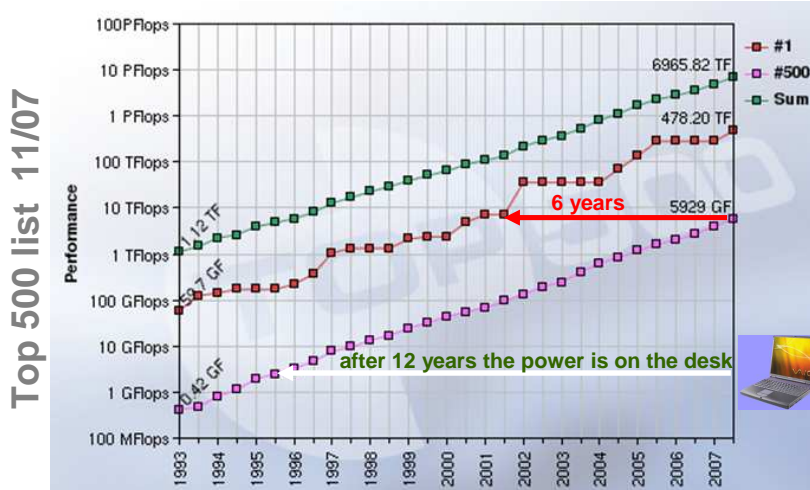- And in Europe ?

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Europe's current position in HPC

Aggregated LINPACK Performance
in PetaFlops in November Top 500 Lists

PFlops

USA
Europe
PRACE PP
Asia
Japan
China+India

75% of European
HPC-power is
within PRACE

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PRACE: The European Access to HPC-Technology

tier 0

finance

aerospace

automotive

virtual power
plant

European Ecosystem

4

6 years technolgy advantage with a #1 system

Top 500 list 11/07

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Computational science infrastructure in Europe

The European Roadmap for Research Infrastructures is the first comprehensive definition at the European level

Research Infrastructures are one of the crucial pillars of the European Research Area

A European HPC service – impact foreseen:
- strategic competitiveness
- attractiveness for researchers
- supporting industrial development

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The ESFRI Vision for a European HPC service

- European HPC-facilities at the top of an HPC provisioning pyramid
  - Tier-0: 3-5 European Centres
  - Tier-1: National Centres
  - Tier-2: Regional/University Centres

tier-0 ← PRACE

tier-1 ← DEISA

tier-2

- Creation of a European HPC ecosystem involving all stakeholders
  - HPC service providers on all tiers
  - Grid Infrastructures
  - Scientific and industrial user communities
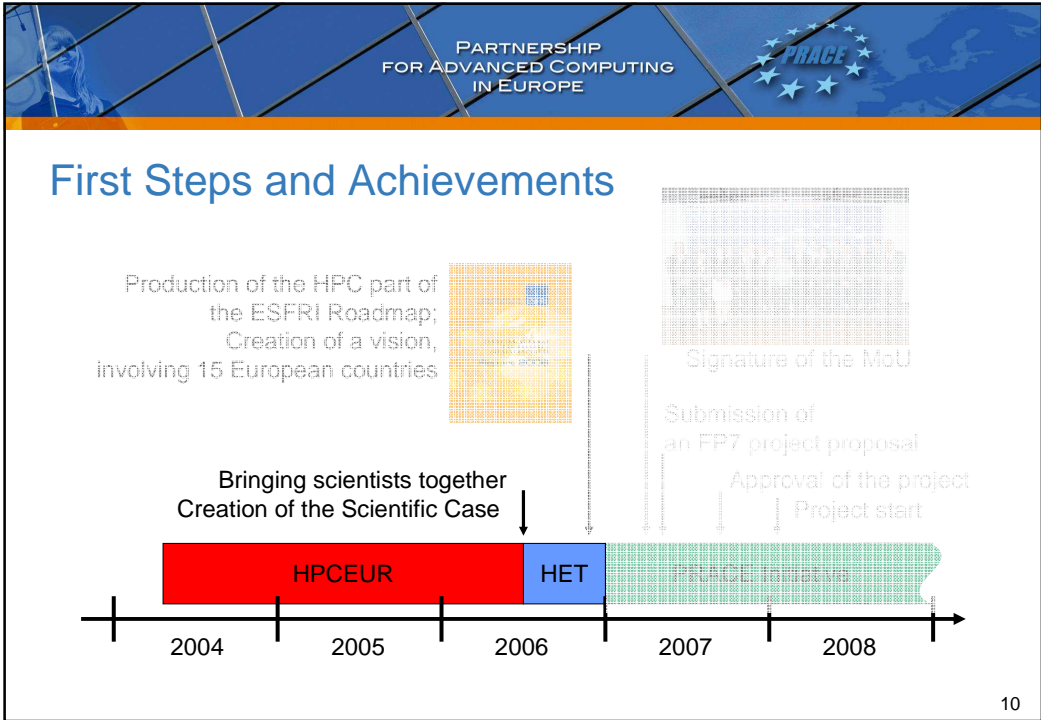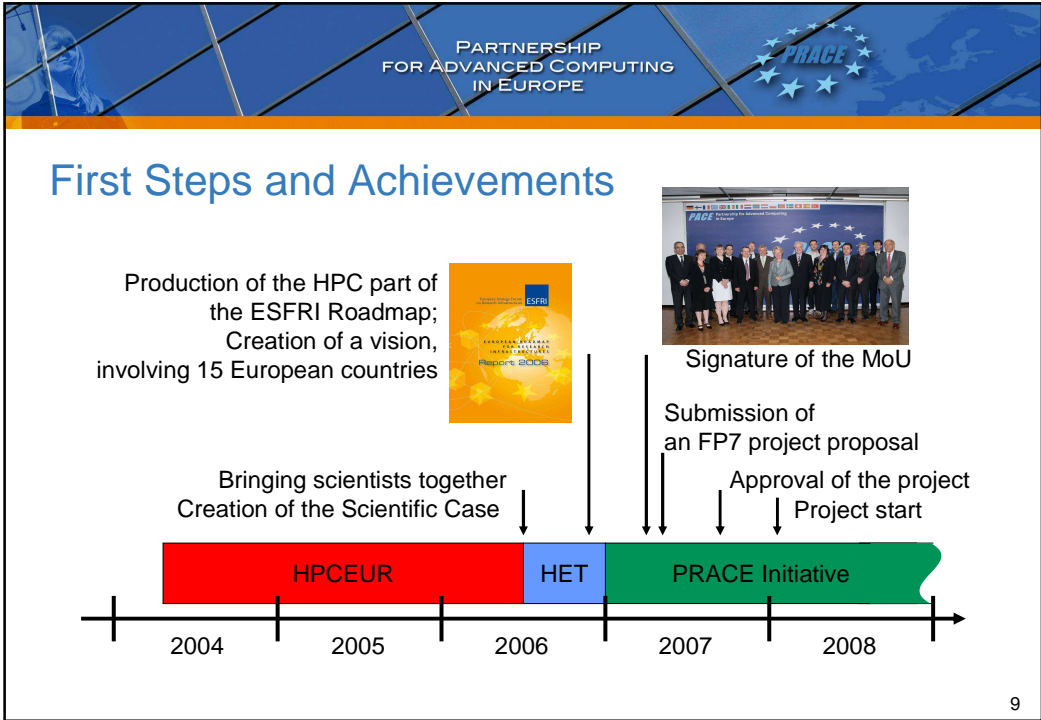 - The European HPC hard- and software industry
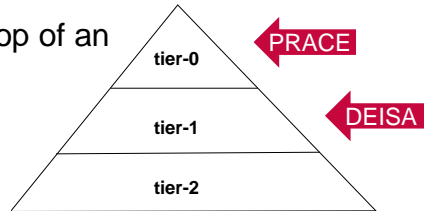
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ESFRI – Estimated costs

- Unlike other European Research Infrastructures:
  - Tier-0 resources have to be renewed every 2-3 years
  - Construction cost 200 – 400 Mio. € every 2-3 years
  - Annual running cost 100 – 200 Mio. €

- A truly European challenge – also in terms of funding

- PRACE – The Partnership for Advanced Computing in Europe
  - An Initiative created to implement the ESFRI vision of a European HPC service
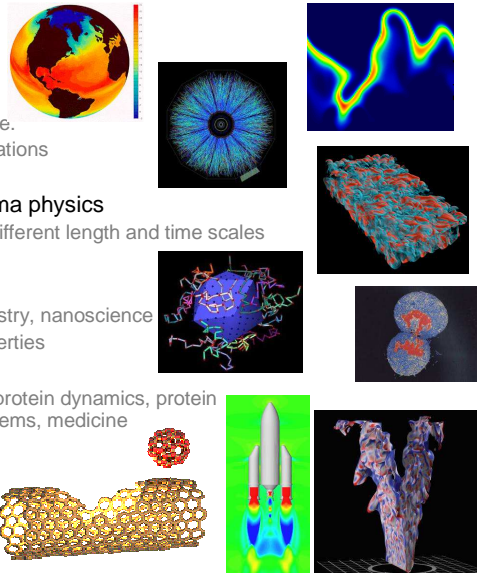
8

First Steps and Achievements

Production of the HPC part of
the ESFRI Roadmap;
Creation of a vision,
involving 15 European countries

Signature of the MoU

Submission of
an FP7 project proposal

Approval of the project
Project start

Bringing scientists together
Creation of the Scientific Case

| HPCEUR | HET | PRACE Initiative |

2004   2005   2006   2007   2008

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HET: The Scientific Case

- Weather, Climatology, Earth Science
  - degree of warming, scenarios for our future climate.
  - understand and predict ocean properties and variations
  - weather and flood events
- Astrophysics, Elementary particle physics, Plasma physics
  - systems, structures which span a large range of different length and time scales
  - quantum field theories like QCD, ITER
- Material Science, Chemistry, Nanoscience
  - understanding complex materials, complex chemistry, nanoscience
  - the determination of electronic and transport properties
- Life Science
  - system biology, chromatin dynamics, large scale protein dynamics, protein association and aggregation, supramolecular systems, medicine
- Engineering
  - complex helicopter simulation, biomedical flows, gas turbines and internal combustion engines, forest fires, green aircraft,
  - virtual power plant

Status and Requirements, e.g.: German Case
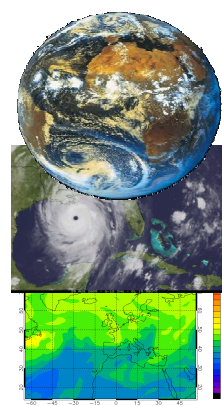
Scientific Field (numbers in TeraFlop/s)	2005-2007	2007-2009	2010
Climate and Earth System Research	20	50-100	>500
Geophysics	1	10-100	>1000
Nanostructure Physics	1	10-50	>200
Solid-State Physics	1	50-100	>1000
Computational Fluid Dynamics	2.5	25-100	>1000
Astrophysics	10	50-100	>500
Elementary Particle Physics and Physics of Hadrons and Nuclei	30	100	>1000
Materials Science	10	50-100	>500
Theoretical Chemistry	3	25-125	>300
Soft Matter	3	30	>200
Biophysics and Bioinformatics	3	15-80	>1000
Plasma Physics	10	50	>500

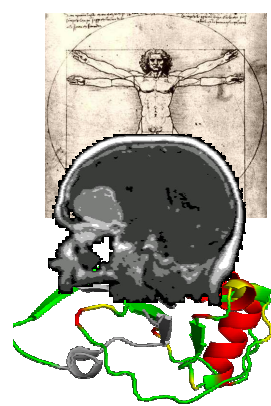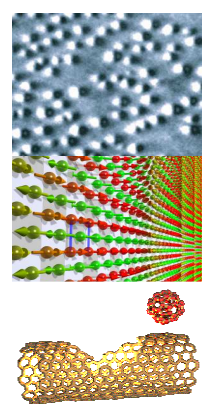A. Bode, W. Hillebrandt, and Th. Lippert: German Scientific Case for the BMBF, 8/2005

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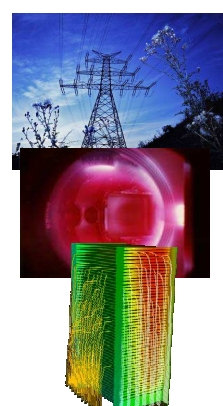Supercomputing Drives Science through Simulation

Environment
Weather/ Climatology
Pollution / Ozone Hole

Ageing Society
Medicine
Biology

Materials/ Inf. Tech
Spintronics
Nano-science

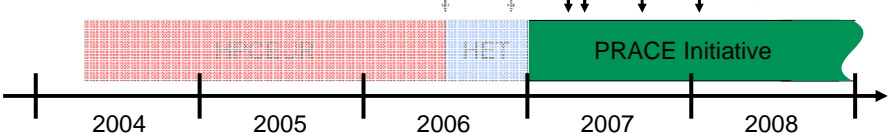**Energy**
Plasma Physics
Fuel Cells

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HPC-EUR   HET   PRACE Initiative

2004   2005   2006   2007   2008

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PARTNERSHIP
FOR ADVANCED COMPUTING
IN EUROPE

PRACE – Project Facts

- Objectives of the PRACE Project:
  - Prepare the contracts to establish the PRACE permanent Research Infrastructure as a single Legal Entity in 2010 including governance, funding, procurement, and usage strategies.
  - Perform the technical work to prepare operation of the Tier-0 systems in 2009/2010 including deployment and benchmarking of prototypes for Petaflops systems and porting, optimising, peta-scaling of applications
- Project facts:
  - Partners: 16 Legal Entities from 14 countries
  - Project duration: January 2008 – December 2009
  - Project budget: 20 M € ,   EC funding: 10 M €

PRACE is funded in part by the EC
under the FP7 Capacities programme
grant agreement INFSO-RI-211528

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PARTNERSHIP
FOR ADVANCED COMPUTING
IN EUROPE

PRACE – Project Consortium

Principal Partners

tier 0

tier 1

General Partners

New Partners - since May 2008 - of the PRACE Initiative :

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The next tasks (I/II):

… growing into a persistent Research Infrastructure

- Define the legal form and governance
- Secure initial and continuous funding
- Prepare procurement and installation of the first Petaflops systems
- Establish the peer review process for academic usage
- Promote Europe wide collaboration between scientific communities using leading edge scientific simulation
- Encourage new projects to increase software and simulation competence
- Provide training and education and disseminate results

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Project governance – a model for the RI
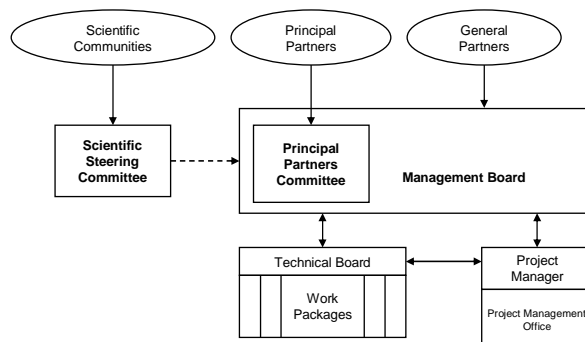
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ERI – A new European Legal Framework

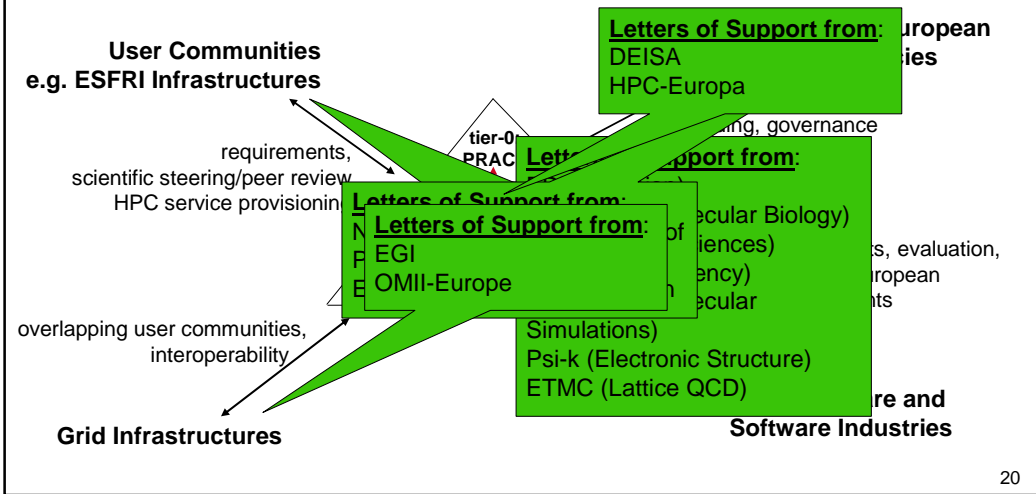- ESFRI roadmap 2006: 35 Research Infrastructures to be established with high priority – 35 new legal entities
  - International Treaties, European Joint undertakings – hard to negotiate in the given timeframe
  - need for a new dedicated legal framework
- ERI – European Research Infrastructure
  - Nature: Scientific non-commercial character, EU flavour
  - Members: states or legal entities designated by them, non-European countries not excluded
  - Status: under construction by EC with involvement of all stakeholders
  - Timetable: Foreseen adoption by the Council by December 2008
- ERI – a promising option for the PRACE legal entity

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HPC Ecosystem Links

Letters of Support from: uropean
DEISA
HPC-Europa

**User Communities
e.g. ESFRI Infrastructures**

tier-0
PRAC

Letters of Support from:

ng, governance

requirements,
scientific steering/peer review
HPC service provisioning

Letters of Support from:
N
P
E

Letters of Support from:
EGI
OMII-Europe

ecular Biology)
iences)
ncy)
ecular

ts, evaluation,
ropean
ts

Simulations)
Psi-k (Electronic Structure)
ETMC (Lattice QCD)

overlapping user communities,
interoperability

re and
Software Industries

Grid Infrastructures

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HPC Services for the European Industry

- Usage of HPC technology in industry is 6-8 years behind technology frontier – as available to top research
- The USA undertakes to boost competitiveness of local industry by shortening this period
  - free-of-charge access to HPC resources through INCITE program
- PRACE is striving towards a similar model
  - Understand industrial needs
  - Raise awareness for competitive advantages of tier-0 HPC usage
  - Design a usage model suited for European industry and SMEs
- 1st PRACE Industrial Seminar: Amsterdam, Sept. 3-4, 2008

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HPC in the automotive industry
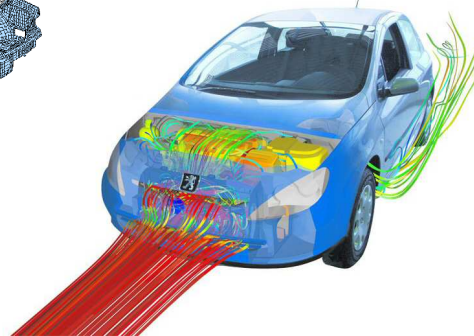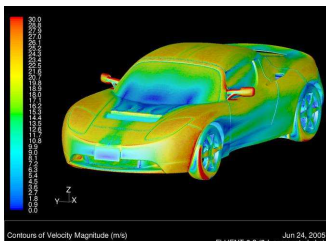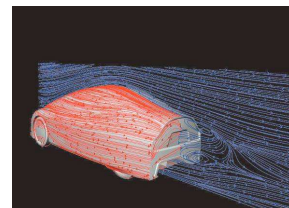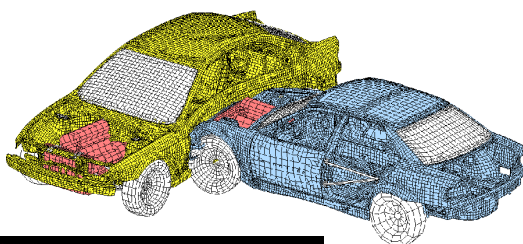
The next tasks (II/II):

… growing into a persistent Research Infrastructure

- Identify architectures and vendors capable of delivering Petaflops systems by 2009/2010
- Install prototypes at partner sites to verify viability
- Define consistent operation models and evaluate management software
- Capture application requirements and create a benchmark suite
- Port, optimize and scale selected applications
- Define an open, permanent procurement process
- Define and implement a strategy for continuous HPC technology evaluation and system evolution within the RI
- Foster the development of components for future multi-petascale systems in cooperation with European and international HPC industry
- ***Start a process of continuous development and cyclic procurement of technology, software and systems for the permanent PRACE Research Infrastructure***

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Fostering European HPC Industry

- Most HPC vendors today are US- or Japan-based
- An independent access to HPC-technology is a strategic issue for Europe
- PRACE will foster European developments by
  - Translating user requirements to architectural specifications for future multi-petascale HPC systems
  - Supporting the creation of consortia of industrial and academic stakeholders to develop future components and systems
    - Europe-based and international companies with R&D activities in Europe
    - European HPC centres
  - Example: PROSPECT INTEL, IBM, QUADRICS, ParTec, BSC, DWD, FZJ, LRZ, …
  - Example: TALOS BULL, CEA, HLRS, INTEL, QUADRICS

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PRACE Roadmap

Creation of the legal entity providing the European Tier-0 HPC service

Procurement of the first tier-0 systems

Legal form, funding, peer review defined

Prototype procurement

PRACE Project

PRACE Research Infrastructure

PRACE Initiative

Beginning of close cooperation

DEISA, eDEISA, DEISA2 Projects

2007 2008 2009 2010 2011

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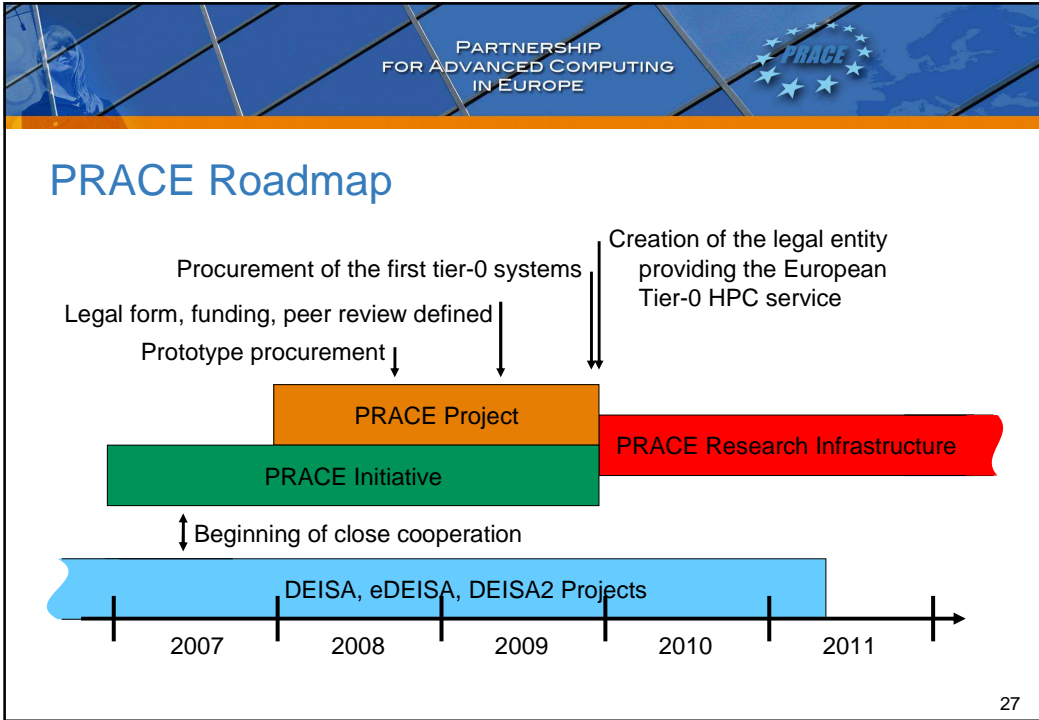
French – German HPC Cooperation

cea

JÜLICH
FORSCHUNGSZENTRUM

- Strategic Partnership of FZJ and CEA formed
  – MoU signed under patronage of Research Ministers at 3rd French – German Forum on Research in Paris, February 2008
- Supercomputing is a main subject of cooperation
  – Joint research on I/O, petascaling applications, energy efficiency
  – Joint proposal for a prototype of a Petaflops system for 2009/2010 within the PRACE project
  – The centres are willing to host two of the European tier-0 level HPC centres

JÜLICH **participates in PRACE through** GCS
FORSCHUNGSZENTRUM

cea **participates in PRACE through** GENCI

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Opportunities ahead

- PRACE builds upon
  - the HPC expertise of 14 European countries in HPC service provisioning and on projects like DEISA
  - the expressed support of our national governments, the European Commission and many scientific communities
  - an excellent team-spirit grown during the past years of HPCEUR, HET, PRACE and other joint endeavors

- The time is right to
  - boost competitiveness of European research and economy through HPC
  - create services to fulfill the HPC requirements of the upcoming ESFRI infrastructures
  - create and shape the European HPC ecosystem

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PRACE
Kickoff-meeting
January 2008

Back Up - slides

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DEISA - Distributed European Infrastructure for Supercomputing Applications

- DEISA / eDEISA visions and achievements in FP6:
  - To enhance Europe's capability computing and science by the integration of Europe's most powerful supercomputing systems Tier-1 in a European HPC e-infrastructure
  - DEISA built a European Supercomputing Service 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
- DEISA2 objectives in FP7
  - Consolidation of the existing DEISA infrastructure
    - DEISA2 providing a lean and reliable turnkey operational solution for a persistent European HPC ecosystem
  - Evolvement towards a robust and persistent European HPC ecosystem
    - DEISA2 as the vector for the integration of Tier-0 and Tier-1 systems in Europe

[excerpt from DEISA2 presentation by H.Lederer, St. Heinzel et al.] 32

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The basic DEISA infrastructures and services

- Dedicated high speed network infrastructure
- Common AAA infrastructure
- Global data management infrastructure
  - global filesystem and high performance file transfer
- DCPE (DEISA Common Production Environment)
  - job management and science gateways (portals) to supercomputing resources
- Common Operation Environment
  - Common monitoring and Information systems
  - Common system operation
  - Common help desk
- Global Application Support

[excerpt from DEISA2 presentation by H.Lederer, St. Heinzel et al.] 33

PRACE – DEISA Cooperation

- DEISA is
  – operating a distributed infrastructure of national tier-1 HPC resources
  – has huge experience and technology for its operation
  – is the closest to a tier-0 RI in Europe so far
- PRACE and DEISA cooperate closely
  – leverage DEISA results for the future PRACE Research Infrastructure
  – coordinate technical work to avoid duplicate efforts and to achieve optimal resource usage in both projects; current focus is on distributed system management, data management and benchmarks
  – ensure interoperability
  – eventually join into a single initiative

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