PRACE

Barcelona Supercomputing Center
Centro Nacional de Supercomputación

Portugal, October 12th, 2007

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PRACE Partnership for Advance in Europe

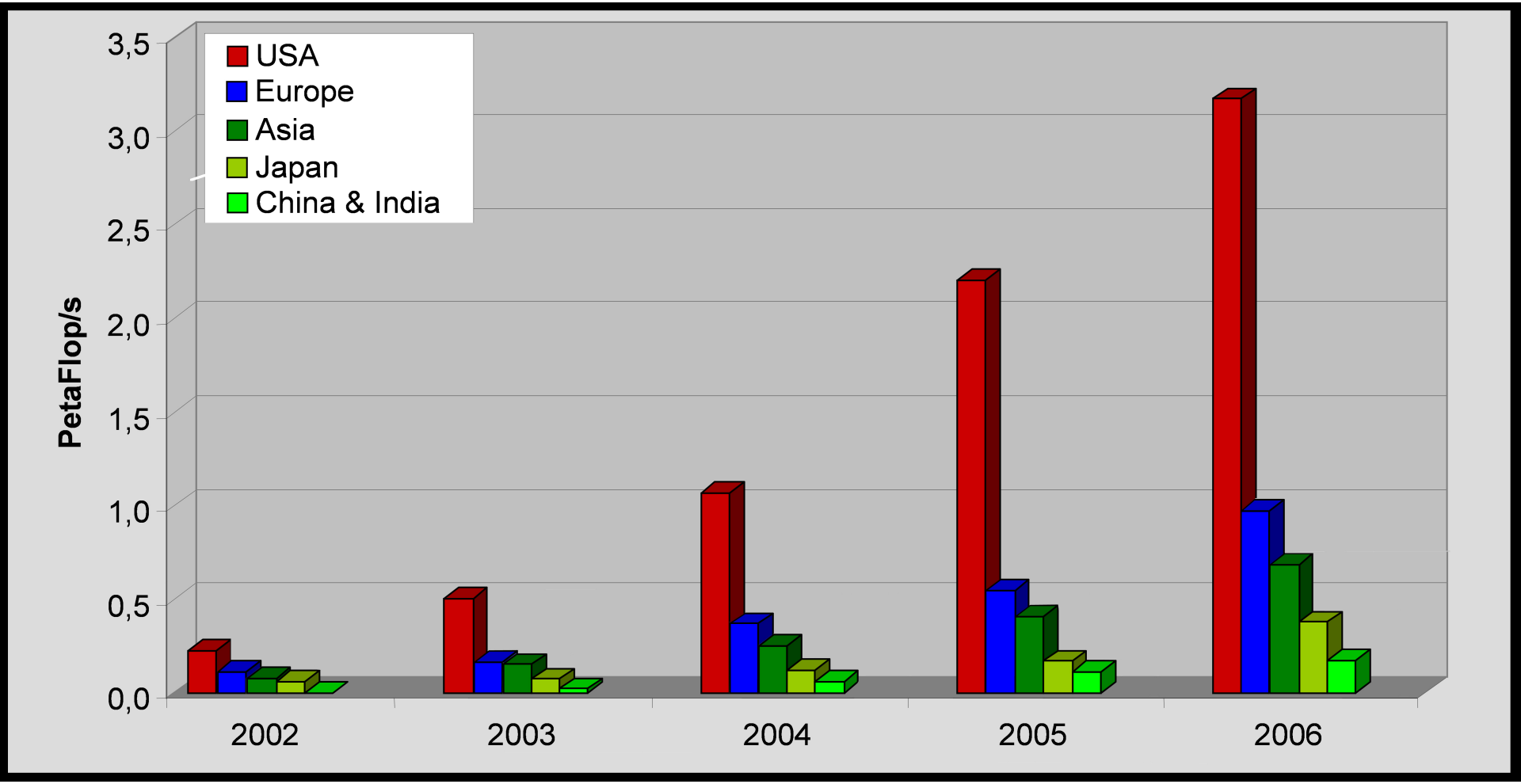
The beginnings

- Informal discussions began in 2004

- High Performance Computing for Europe Initiative (**HPCEUR**) was established (2004 – 2006)

More data.

- Sum of peak performance, Top500 lists



The Scientific Case

- The **Scientific case for high-end scientific computing in Europe** was produced (Barcelona 08/05 – Cadarache 04/06)
  - Some statements:

"In the fields of astrophysics, high-energy physics and plasma physics supercomputers are required to support research where real experiments are not possible, too time-consuming or too expensive and where computing systems of lower performance levels are not adequate. They constitute an indispensable tool for top research. In the past few years scientific breakthroughs have been achieved by the use of supercomputers which would not have been possible on computers of lower performance classes."

The Scientific Case

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"In climate research, air quality and meteorology, Europe has been able to establish a scientific community that has played a leadership role and has effectively contributed to international assessments. These have provided the scientific basis for national and international agreements. The European community is already well organised through European projects and collaborative research. The accuracy and details of earth system research and predictions of climate change have been severely limited by the computing resources available to the community."

The Scientific Case

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"For the community in material science, chemistry and nano science, scientific, technological and societal challenges require the acquisition at the European level of capability computers in the 1-10 Petaflop/s range. This would enable simulations of complex systems over the long space and time scales required for quantitatively reliable results and for improved connectivity between experiment and theory. A clear benefit of these developments is the enhanced industrial exploitation potential in a variety of fields relevant to energy production, to electronic and optical communication, and for ceramics for sensors, plastics and complex fluids in the food industry, or hydrogen storage materials. In addition, there are important societal applications that will lead to improvements to cleaner air, sustainable technology, decontamination, nanotechnology and medicine."

The Scientific Case

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"In the life sciences, the emphasis will now be the exploitation of the massive genomic information and its translation to biologically relevant facts. This will increase hugely the need for large computational resources. The first step will be to simulate protein in order to understand the key mechanisms. Then simulations will need to be extended to the duration of the relevant processes, which will increase needs by several orders of magnitudes, in order to reach microsecond and millisecond of simulated time.

Society will benefit from the enhanced modelling and simulation capabilities in several respect: genome annotation will lead to the more effective identification of new drug targets, protein fold recognition and structure prediction are essential to allow the engineering of new proteins, computational biochemistry is a key part of the drug development process."

The Scientific Case

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"In engineering and technological development, modern challenges involve complete systems modelling and possibly optimization. Interactions of different components of the system require modelling from multiple disciplines, dealing with phenomena at multiple scales both in space and time. The examples are compelling: optimized design of aircraft and helicopters, reduced noise and pollution in engines for aircraft and automobiles, fighting forest fires more effectively, the design of new materials required in fuel cells, and more efficient extraction of fossil fuels. Access to high-end supercomputers, and close cooperation with scientists are required to develop the newer models and simulation tools

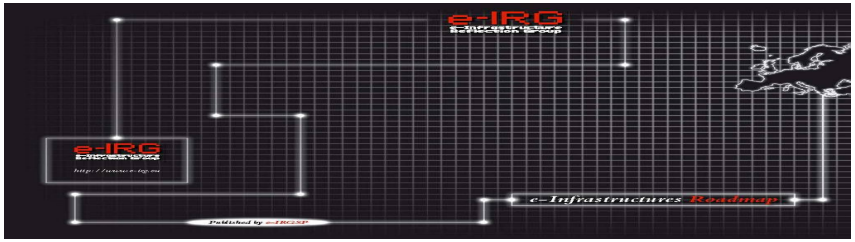
Some interactions

- Interactions with
  - European Commission,

  - European Strategy Forum on Research Infrastructures (**ESFRI**)

ESFRI European Strategy Forum on Research Infrastructures

  - e-Infrastructure Reflection Group (**e-IRG**) expert groups



- Creation of the HPC in Europe Taskforce (**HET**) (2006)

ESFRI

- European HPC infrastructure need was recognized in the **ESFRI** Roadmap (2006)

- Estimated construction cost of 200-400 M€
- Indicative running cost of 100–200 M€ / year

MoU signature

- April, 27th 2007: MoU signature in Berlin

EU-FP7project

- May 2th, 2007: 16 "Legal Entities" from 14 European countries applied EU-FP7-Call
- For the construction of new infrastructures - preparatory phase
- FP7-INFRASTRUCTURES-2007-1

  INFSO: Supercomputing in Call 2007.2.2.1
- Budget: 19 M€

PRACE's Vision & Mission

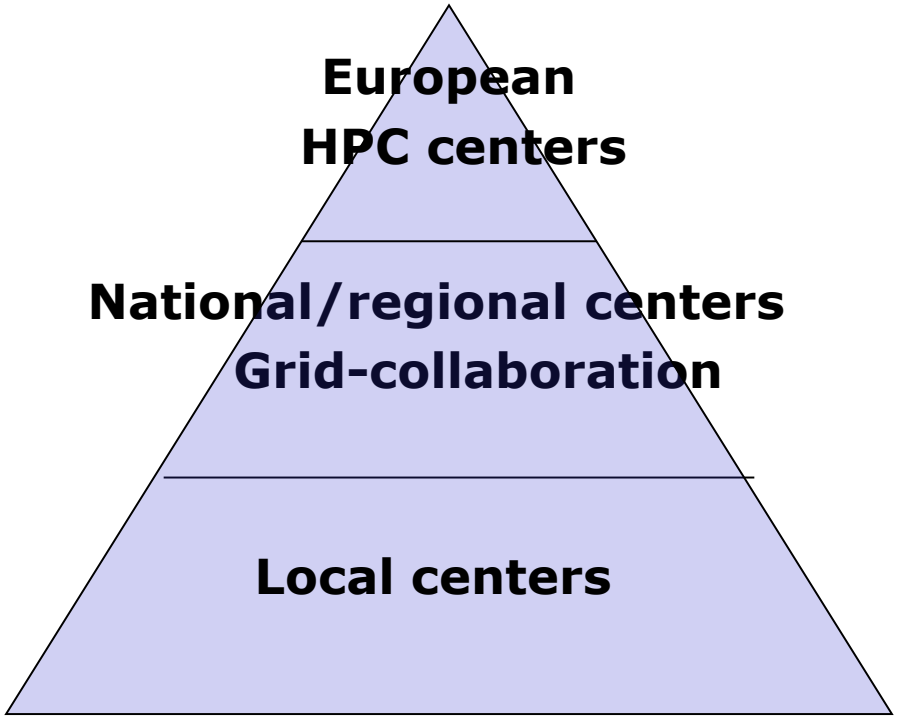
The Vision:

- From cooperative High Performance Computing in Europe to leadership class **European HPC facilities** integrated in a High Performance Computing European Consortium.

The Mission:

- Creation of a persistent pan-European HPC service, consisting of few tier-0 centres providing European researchers with access to capability computers and forming the top level of the European HPC ecosystem.

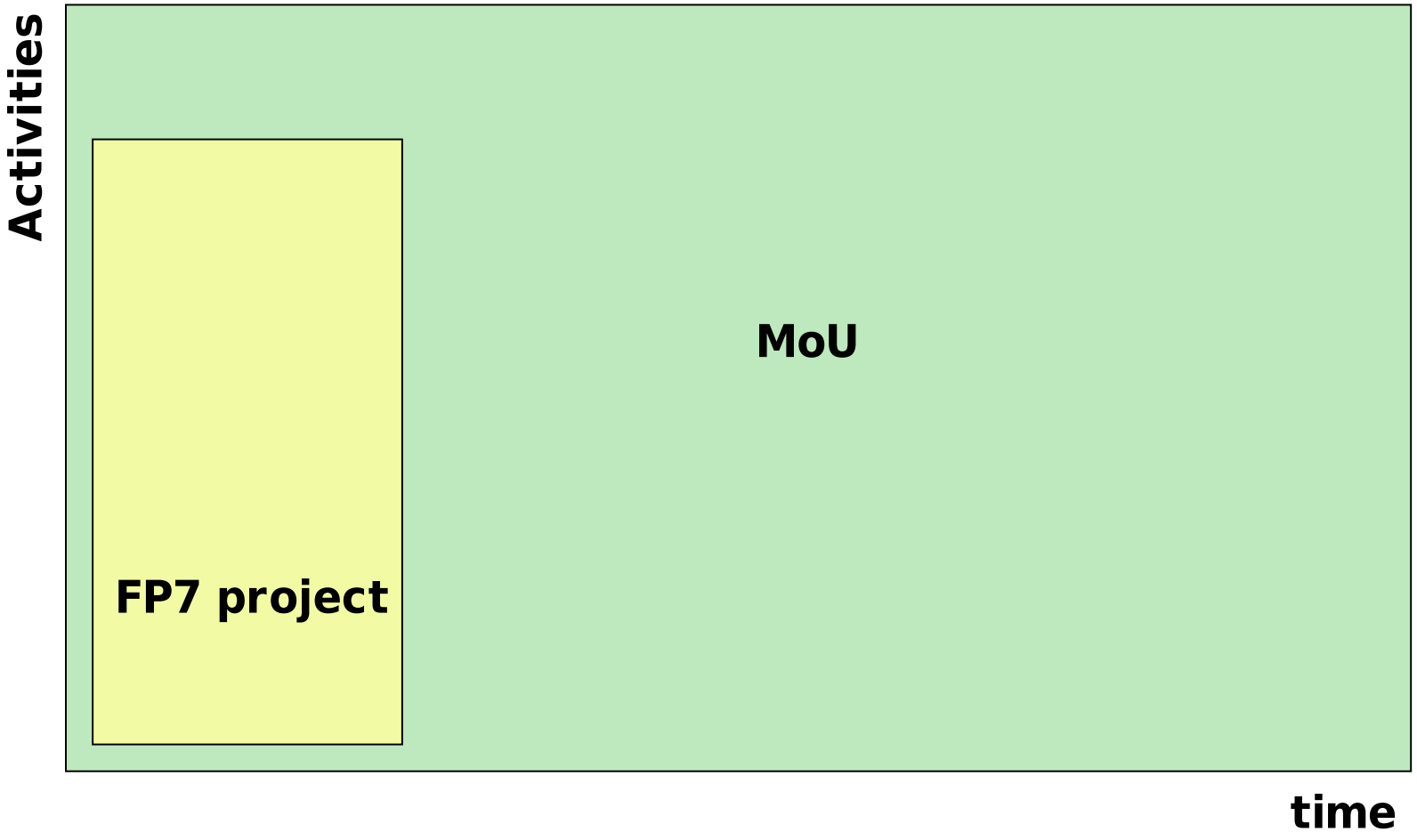
PRACE is embedded in the European Ecosystem



- In addition to providing sufficient resources in each of the Tier-layers, it is important to enable flexible and efficient interoperability

- Critical importance of the European back-bone network (GéANT)

PRACE's MoU & FP7 project



Why do we need a PRACE-MoU?

- Introduce a European governance structure for an European HPC research infrastructure.
- Manage the transition from a cooperative European HPC-Network to a permanent world class tier 0 HPC-Establishment with an European structure (& funding & operating management).
- Provide a smooth insertion in the European HPC-Ecosystem of national and topical centers, networking incl. GEANT and DEISA, user groups and communities.
- Permit joint endeavors, including a FP7 “Preparatory Phase” project.
- Promote European presence and competitiveness in HPC, such as the most effective use of Numerical Simulation at the leading edge.

The PRACE MoU stakeholders

- "Principal partner" is a representative of an European country that expressed its interest in hosting (and funding) one of the main Tier0 HPC centers of the target Tier 0 HPC infrastructure.

- "General partner" is a representative of an European state that expressed its interest to collaborate in many aspects related with definition, operation and scientific management. It does not intend to exercise the responsibilities of a principal partner.

- "Associate partner" is a figure that will permit the gradual involvement of scientific communities and industrial users (e.g. climate (ENES), Fusion (EFDA) or Bioinformatics (EBI), ...)

14 countries already joined PRACE

The leadership centers

- The permanent European "*Tier 0 HPC infrastructure*" will be defined during the *preparatory phase* of the "PRACE-project"

- "Tier 0 HPC Center" is a supercomputer centre, part of the European HPC infrastructure, contributing to the European "Capacities" program for Research Infrastructure as defined by the ESFRI roadmap, hosting a capability computer with a computing power significantly larger than the largest supercomputer owned and operated nationally by one of the EC Member States alone.

- It is expected that the cost for the *Tier* 0 HPC center would be in the range of 200-400M€ over 5 years.

Other PRACE MoU stakeholders:

- "The users" are academic and industrial groups and organizations, which require capability computing for performing their scientific tasks or the competitiveness of their products and services.

- "European Commission" is involved as a facilitator and catalyzer by sponsoring ESFRI and eIRG and implementing the "Capacities FP7-programme, by funding several user communities or projects of academic or industrial relevance and by providing key infrastructures (GEANT, DEISA).

- "National funding agencies" will permit part of the funding of the European HPC infrastructure.

Mou Partners

1	Grand Equipement national pour le Calcul I.	GENCI	France
2	GAUSS-Centre for Supercomputing Ass.	GAUSS	Germany
3	Netherlands Computing Facilities Foundation	NCF	Netherlands
4	Barcelona Supercomputing Center	BSC	Spain
5	Engineering & Physical Sciences Research C.	EPSRC	United Kingdom
6	Joh. Kepler Universitaet Linz	GUP	Austria
7	CSC Scientific Computing Ltd.	CSC	Finland
8	Greek Research and Technology Network	GRNET	Greece
9	CINECA Consorzio Interuniversitario	CINECA	Italy
10	UNINETT Sigma AS	SIGMA	Norway
11	Poznan Supercomputing and Networking C.	PSNC	Poland
12	Universidade de Coimbra	UC-LCA	Portugal
13	ETH Zürich - CSCS	ETHZ	Switzerland
14	Swedish National Infrastructure for Comp.	SNIC	Sweden

FP7-Project Partners

1 (Coordinator)	Forschungszentrum Juelich GmbH	FZJ	Germany
2	Universität Stuttgart – HLRS	USTUTT-HLRS	Germany
3	LRZ der Bay. Akademie der Wissenschaften	BADW-LRZ	Germany
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National governmental support

Bundesministerium für Bildung und Forschung	**Germany**	The Federal Ministry of Education and Research supports PRACE and endorses the participation of GAUSS in PRACE, and will participate in the discussions and decisions about financial, organisational, and legal matters
Direction générale de la recherche et l'innovation	**France**	The department for large infrastructures within the French Ministry for higher Education expresses its interest in PRACE and authorizes GENCI to represent France
Ministerio de Educación y Ciencia	**Spain**	The Director-General for Technology Policy, within the Spanish ministry for Education and Science, supports the participation of BSC in PRACE
ICT Research and Innov. Authority	**Netherlands**	The Netherlands ICT Research and Innovation Authority supports the endeavours of NCF, as the responsible funding agency, regarding its participation in PRACE
The Ministry of Education	**Finland**	Within the Finnish Government, the Ministry of Education is responsible for developing educational and science policies and international cooperation in these fields. The Ministry of Education is supporting the participation of CSC Scientific Computing
Ministero dell' Università e della Ricerca	**Italy**	The Ministry of University and Research recognizes the importance of PRACE for world-class research and has nominated CINECA to coordinate the Italian participation.
Ministry of Science and Higher Education	**Poland**	The Ministry of Science and Higher Education in Poland supports the ideas of PRACE and facilitates the participation of PSNC in PRACE
Research Council of Norway	**Norway**	The Division of Science within the Research Council of Norway expresses its support for PRACE and endorses UNINETT Sigma to represent Norway in PRACE
Ministry of Development of the Hellenic Republic	**Greece**	The General Secretariat for Research and Technology is part of the Greek Ministry of Development. It endorses the participation of GRNET in PRACE
Fundacao para a Ciencia e a Tecnologia	**Portugal**	FCT is the funding agency for Science and Technology in Portugal. It endorses and supports the participation of UC-LCA

Support by Research Infrastructures

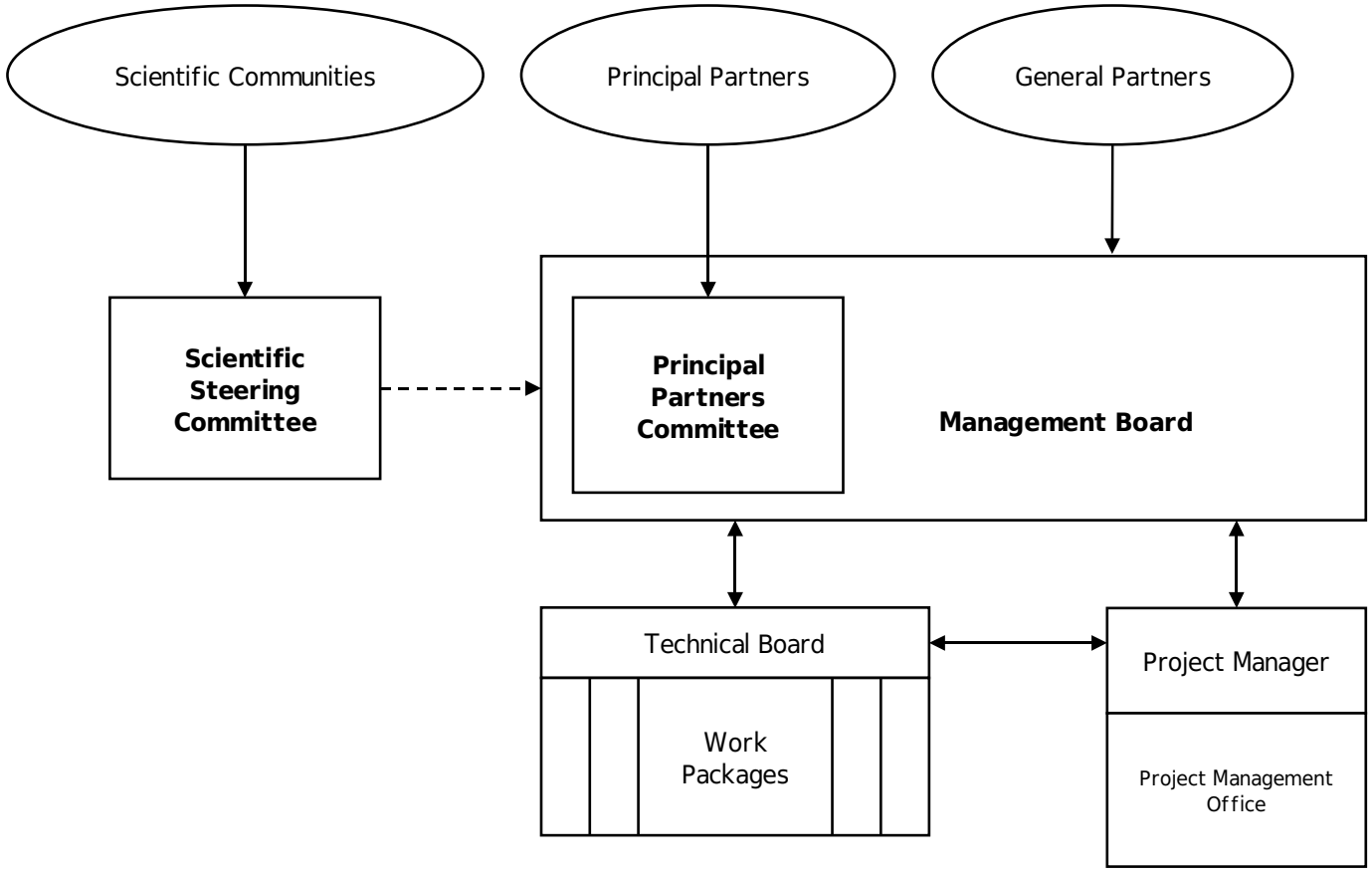
DEISA	**EU-Project**	**DEISA** currently deploys and operates the European Supercomputing Grid infrastructure to enable capability computing across remote computing platforms and data repositories at a continental scale. DEISA considers PRACE as an absolutely necessary and complementary initiative. DEISA offers its services and support for deployment in PRACE.
HPC-Europa	**EU-Project**	**HPC-Europa** is a pan-European Research Infrastructure on HPC providing HPC access and scientific support to researchers in challenging computational activities. HPC-Europa expresses its interest in cooperating in the areas of access technologies and integrated advanced computational services.
OMII-Europe	**EU-Project**	**OMII-Europe** is the interoperability project in Europe providing open standards based interoperability components on top of the four major Grid middleware systems in the world. OMII-Europe is keen to collaborate with PRACE towards provisioning of High end computing resources within Grid computing frameworks.
EGI	**EU-Project**	The consortium of **EGI** aims at establishing a sustainable Grid infrastructure in Europe, coordinating national Grid initiatives. EGI is interested to collaborate with PRACE by receiving requirements from the HPC community towards EGI, concerning governance, legal, and political issues.

Support by Communities

European Organisations and Research Communities		
EFDA	Europe	The **European Fusion Development Agreement** foresees a huge demand for HPC including tier-0. It is interested in cooperation with PRACE regarding benchmarking and code-scaling and provides the HPC-related requirements for Fusion community.
EMBL-EBI	Europe	The **Euro Bioinformatics Institute** within the **European Molecular Biology Laboratory** foresees huge demands for HPC resources in the future and is interested in investigating access policies to European tier-0 systems for life scientists.
ENES	Europe	The **European Network for Earth System Modeling** has contributed to the scientific case for HPC in Europe and will continue to promote the involvement of the European climate modelling community in PRACE. ENES involvement includes porting of applications on prototype systems of PRACE and defining of facility requirements.
ESA	Europe	ESA is the **European Space Agency**. The Space and in particular Earth Observation communities have very demanding HPC applications. ESA is pleased to collaborate with PRACE on specific applications.
ESF	Europe	The **European Science Foundation** is interested to contribute to PRACE, in particular to peer-review process dissemination activities and computer technologies beyond 2010.
MOLSIMU	Europe	**MOLSIMU,** a COST action on Molecular Simulations to Nanoscale Experiments, is offering its support for PRACE by porting their major applications to the prototype systems installed by PRACE.
Psi-k Network	Europe	The **Psi-k network** is the European Umbrella Network for Electronic Structure Calculations. Several groups within Psi-k are interested to port their ab-initio codes like CPMD, VASP, SIESTA, CASTEP, ABINIT, and Wien 2k on the prototype system of PRACE.

Management structure

PRACE-Project follows the rules of the PRACE-MoU



FP7 Project Work Packages

WP1: Management

Leading participant: Forschungszentrum Juelich GmbH, Germany

Objectives:

- Target oriented, efficient management of the project
- Effective project-internal communication
- Quality control of results and deliverables
- Transparent financial management and control
- Timely communication with the European Commission

FP7 Project Work Packages

WP2: Organizational Concept of the Research Infrastructure

Leading participant: Barcelona Supercomputing Center, Spain

Objectives:

- Definition of the Legal Form of the Research Infrastructure
- Definition of the Governance Structure
- Specification of Funding and Usage strategies
- Establishment of the Peer-Review Process
- Establishing Links with the HPC Ecosystem
- Development of the Operation Model

FP7 Project Work Packages

WP3: Dissemination Outreach and Training

Leading participant: CSC Scientific Computing Ltd., Finland

Objectives:

- Dissemination to the major HPC stakeholders: the European scientific and research communities, Research Infrastructure organizations, Universities and Centres for higher education, and the general public
- Liaise with industrial and business partners as potential HPC users
- Implement an education and training program aiming at scalable computing

FP7 Project Work Packages

WP4: Distributed System Management

Leading participant: ETH Zürich – CSCS, Switzerland

Objectives:

- Deployment of existing solutions on the prototype systems; analysis, evaluation, and deployment of the existing solutions for system management for the future distributed tier-0 systems; provisioning of missing components
- Requirements analysis and uptake of the technologies for the integration with the HPC ecosystem especially with tier-1 including end users' applications
- Planning and design of the necessary solution for distributed system management for the permanent Research Infrastructure

FP7 Project Work Packages

WP5: Deployment of Prototype Systems

Leading participant: Netherlands Computing Facilities Foundation, The Netherlands

Objectives:

- Installation of prototype systems
- Test integration and operation in production environments
- Evaluation of the capabilities
- Benchmarking

FP7 Project Work Packages

WP6: Software Enabling for Petaflop/s Systems

Leading participant:Engineering and Physical Sciences Research Council, UK

Objectives:

- Create an application benchmark suite
- Capture application requirements for petascale systems
- Port, optimise and scale selected applications
- Evaluate application development environments of the prototypes

FP7 Project Work Packages

WP7: Petaflop/s-Systems for 2009/2010

Leading participant:Grand Equipement National pour le Calcul Intensif, France

Objectives:

- Identify architectures and vendors capable of delivering Petaflop/s systems by 2009/2010
- Translate user requirements into architecture and configuration outline
- Define installation requirements for Petaflop/s systems and evaluate consistency with possible installation sites
- Perform a risk analysis and develop mitigation options
- Define technical requirements and evaluation criteria for Petaflop/s systems in 2009/2010
- Define the procurement process for Petaflop/s systems in 2009/2010

FP7 Project Work Packages

WP8: Future Petaflop/s Computer Technologies beyond 2010

Leading participant: Forschungszentrum Juelich GmbH, Germany

Objectives:

- Definition and implementation of a strategy that guarantees a continuous HPC technology evaluation and system evolution within the Research Infrastructure
- Anticipation and evaluation of emerging multi-petascale-technology following the requirements of HPC users
- Fostering the development of components for future multi-petascale production systems in cooperation with European and international HPC industry

The next PRACE tasks

- Recruit and consolidate partnership for financing the infrastructure
- Design the tier 0 service to the user
- Prepare to procure and install the first supercomputers
- Design the peer review process for academic usage
- Promote Europe wide collaboration between HPC based simulation and scientific communities, evaluation and planning organizations
- Improve networking of user communities
- Encourage new projects to increase software and simulation competence for HPC

PRACE Roadmap

- 4Q2007 – 2Q2009: Building the European legal entity
- 1Q2008 – 4Q2009: Building prototypes of Petaflop Computers
- 1Q2010: Starting the production phase with Petaflop computing, servicing the scientific communities

Conclusion

- PRACE gives Europe the unique opportunity to set ambitious goals:

  1. to provide unique tools to the European scientific community

  3. to boost European competitiveness

  5. to position itself strategically at a leading rather than follower role in HPC and its applications

- PRACE is open for new European members