



PACE Partnership for Advanced Computing
in Europe



**An new partnership for creating an integrated European
High Performance Computing Service**

Achim Bachem, Kimmo Koski, Alain Lichnewsky, May 21, 2007

Computational science infrastructure



European Strategy Forum
on Research Infrastructures

ESFRI

EUROPEAN ROADMAP
FOR RESEARCH
INFRASTRUCTURES

Report 2006

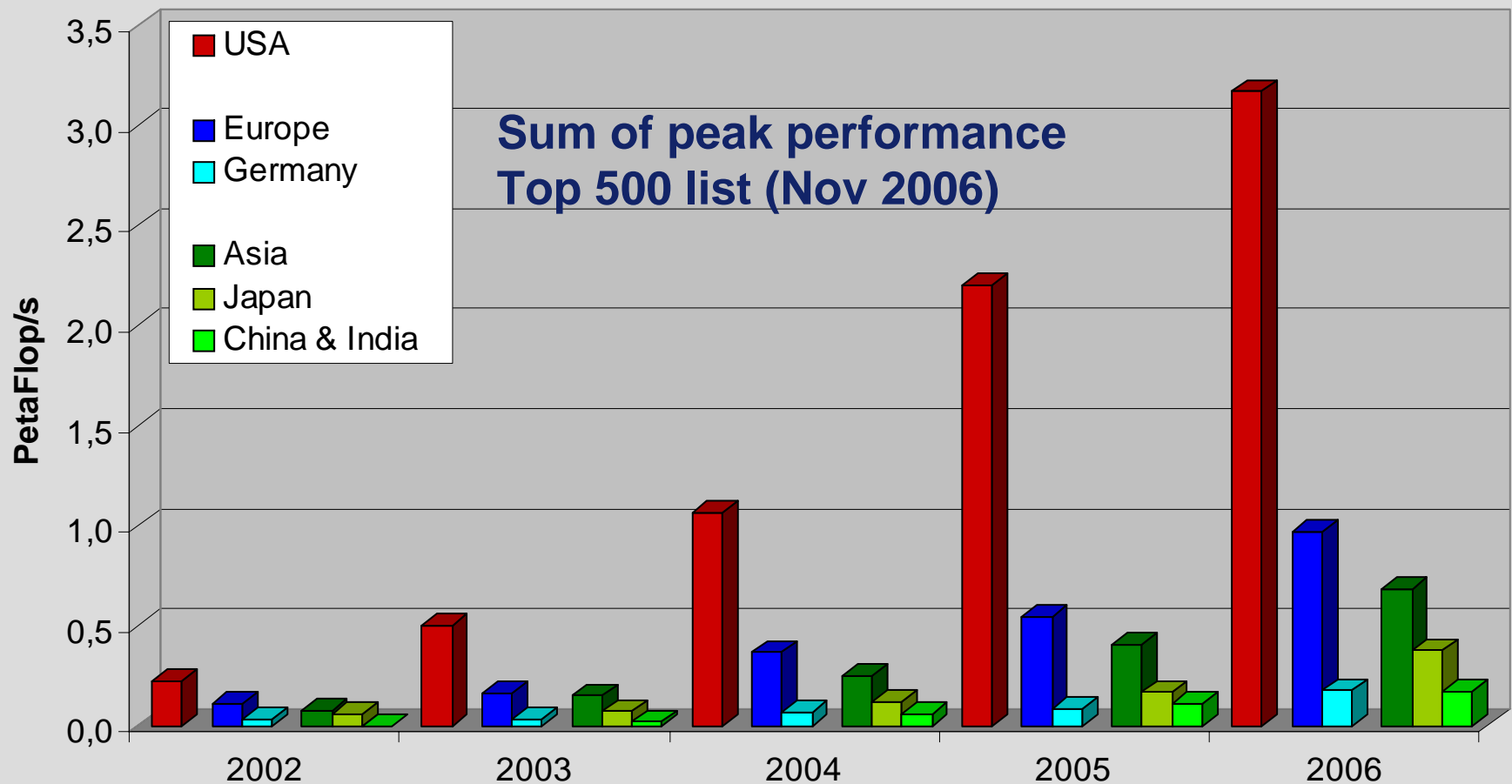
The European roadmap is a first exercise at European level and is the result of wide stakeholder consultation.

1000 high-level experts from all fields of research were involved and consulted in the process of preparing the roadmap, of which 200 were involved in the peer-review.

Research Infrastructures are one of the crucial pillars of the European Research Area, in particular for capacity building.

ESFRI: What's new – impact foreseen

- High-performance computing has a strong impact in terms of maintaining the strategic competitiveness of Europe and increasing its attractiveness for foreign researchers and for supporting industrial development.



ESFRI: What's new – impact foreseen

- The high-end (capability) resources should be implemented every 2-3 years
- Construction cost 200-400 Mio. €, Running cost 100 – 200 Mio. €, i.e. about 1,6 – 4,0 billions € for a 10 year period.
- with supporting actions in the national/regional centers to maintain the transfer of knowledge and feed projects to the top capability layer

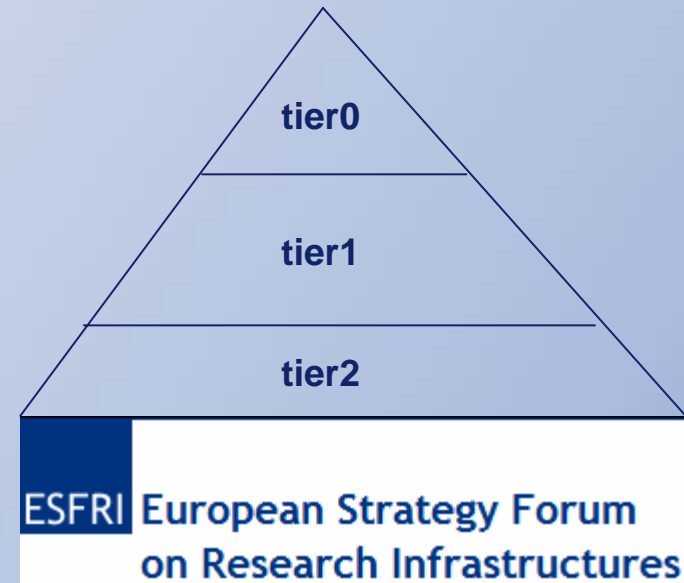
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European High Performance Computing Service includes:

- **Capability Computing**
- **Grid architectures**
- **Software**
- **Data management and curation**



There is a need for a combination of centralized, distributed, and networked aspects, based on a pyramid-like organization, starting from a few very high-end centers and going down to smaller units.

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PACE - A very significant step

The Vision:

From cooperative High Performance Computing in Europe

to

leadership class

European HPC-facilities,

**The Large Scale European Supercomputing
Infrastructure**

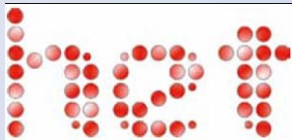
integrated in a High Performance Computing Service

– the European Ecosystem -

What has been achieved so far ?

From informal discussion between 3 countries to:

- HPCEUR (2004 – 6/2006): Bringing scientist together to discuss the scientific case and industrial applications



➔ <http://www.hpcineuropetaskforce.eu/>

6/2006 – 12/2006: chaired by Kimmo Koski

- Being listed in the ESFRI roadmap
- Proposal for funding models
- Proposal for European peer review process
- Views for HPC Ecosystem
- HET helped to build momentum and getting known to the public
- Extending the discussions to 15 European countries

Documentations ➔ <http://www.hpcineuropetaskforce.eu/>

The next step: European leadership computing facilities embedded in an European Ecosystem

- European access to a tier 0 capability HPC research infrastructure reaching and exceeding the PetaFlop/s and maintaining world-wide competitiveness
 - A sustainable infrastructure based on a sustainable and funded renewal process to follow technological progress
 - Complementing the national HPC centres and services
- ➔ EU-support is required to open access to all European countries and to industries and is a chance to promote HPC-competence on a European level for a competitive European IT-Knowledge

Why do we need a PACE-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

Which countries joined PACE so far



The PACE MoU ...

The leadership centers

- the permanent European "*Tier 0 HPC infrastructure*" will be defined during the *preparatory phase* of the "PACE-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 full additional cost for the *Tier 0 HPC infrastructure* shall be in the order of 500 M € to 600 M € over 5 years.

The PACE MoU ...

The stakeholders:

- **"Principal partner"** within PACE , is a coordinator for HPC activities, to host (and fund) one of the main *Tier 0 HPC centers* of the target *Tier 0 HPC infrastructure*.
- **"General partner"** are also involved in many aspects of definition, operation and scientific management. They participate in the definition of scientific and application domains or priorities.
- **"Associate partner"** will permit the gradual involvement of scientific communities and industrial users (e.g. climate (ENES), Fusion (EFDA), Bioinformatics (EBI), ...)

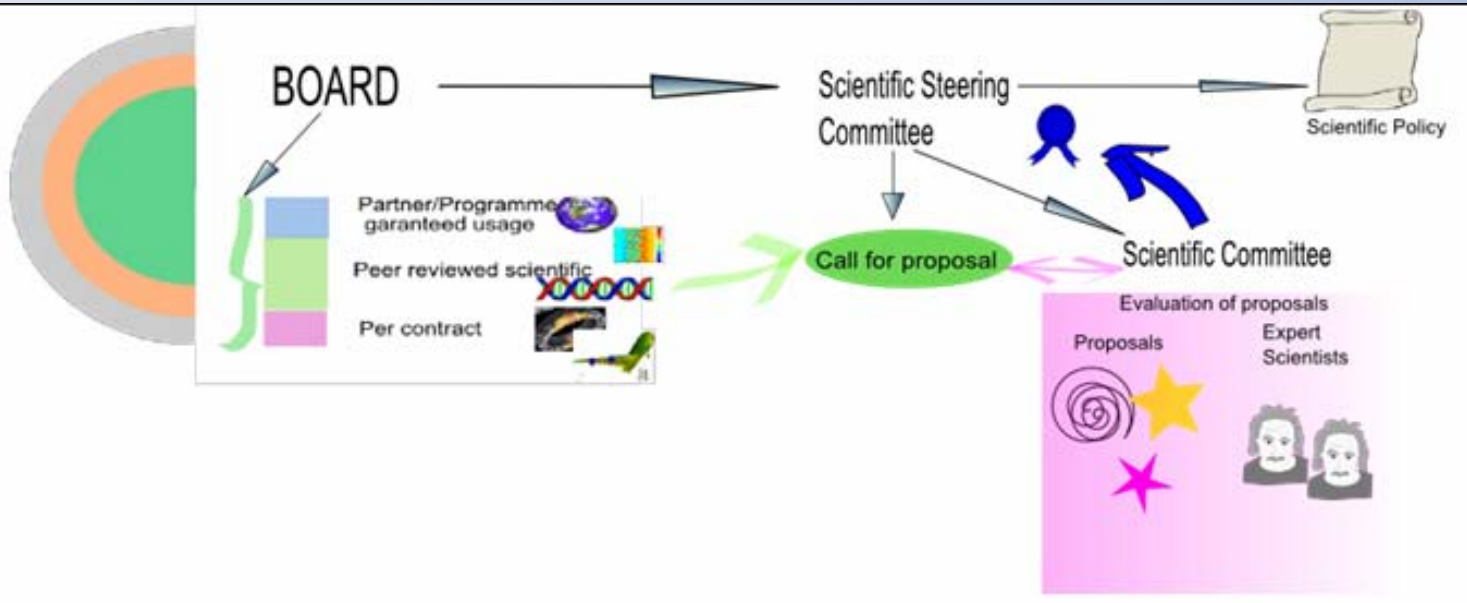
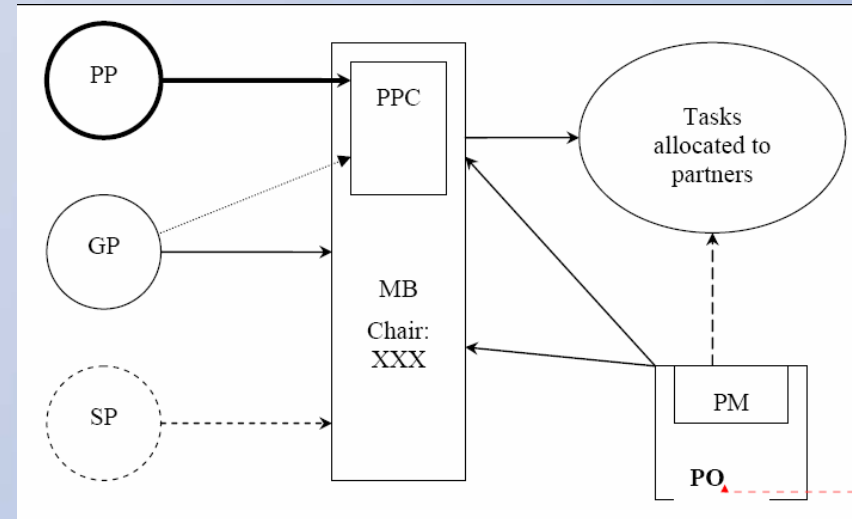
The PACE MoU ...

The 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.

The PACE governance structure

- Legal entity
- Peer Review
- Management Board

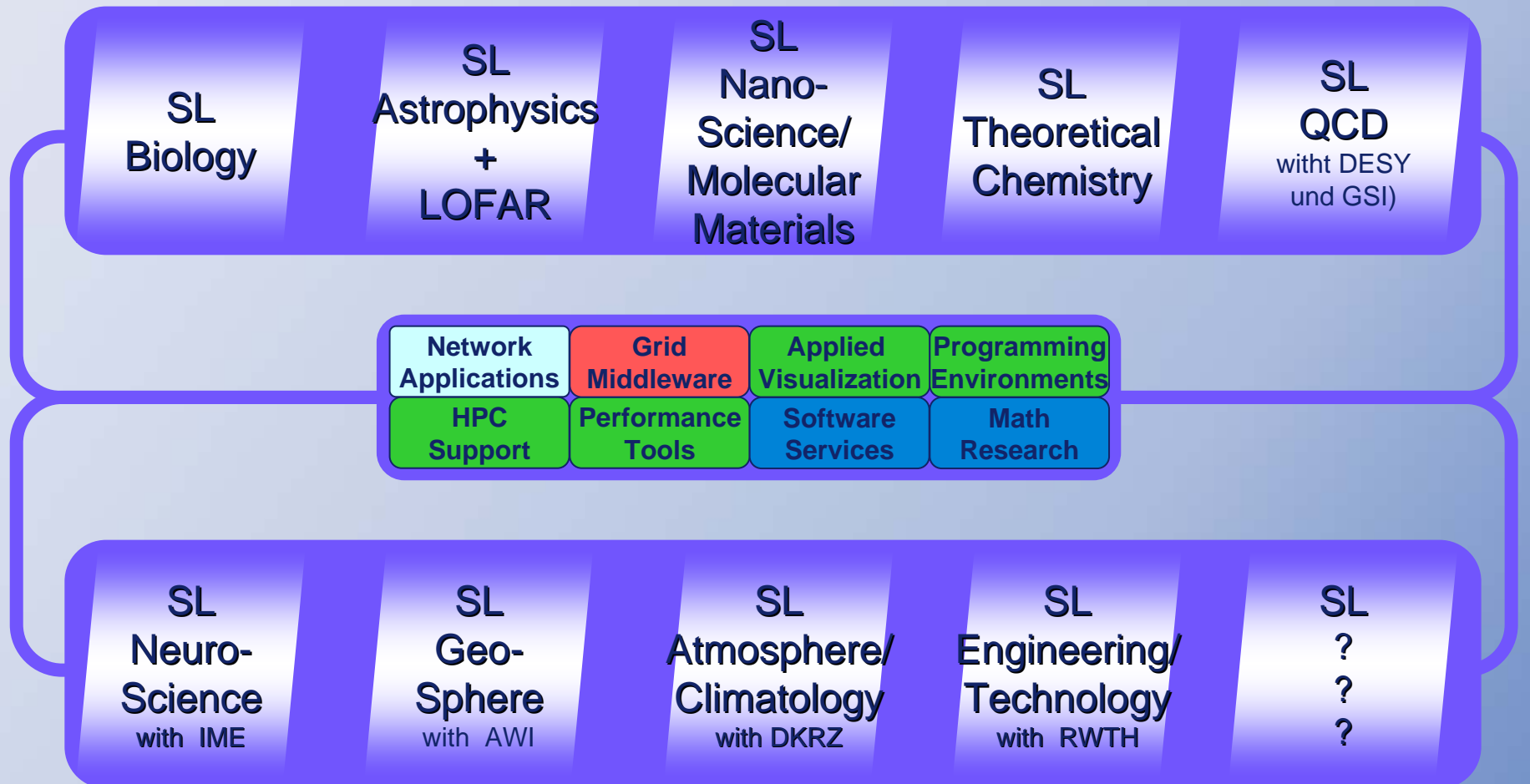


PACE: The next tasks

... growing into a mature research infrastructure

- **Recruit and consolidate partnership for financing and otherwise funding 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**

Software-Example: European Oriented Simulation Laboratories The „Experiments“



Education-Example: The German Research School for Simulation Science



PACE Roadmap

- **April, 27th 2007: Signing MoU**
- **May 2th, 2007: Delivering EU-FP7-Call supporting the preparatory phase** The logo for CAPACITIES, featuring a stylized number '7' composed of horizontal lines in red, blue, and green, with the word 'CAPACITIES' written in red below it.
- **June 2007 – May 2009: Building the European legal entity**
- **2008 – 2009: Building prototypes of Petaflop Computers**
- **2009 – 2010: Starting the production phase with Petaflop computing, servicing the scientific communities**

Partnership for **A**dvanced **C**omputing in **E**urope MoU signed April, 17th 2007



Conclusion

- **PACE gives Europe the unique opportunity to set ambitious goals**
 - to boost European competitiveness
 - to position itself strategically at a leading rather than follower role in HPC and it's applications
- **PACE is open for new European members**

COMBINATION OF COLLABORATIVE PROJECT AND COORDINATION AND SUPPORT ACTION

Construction of new infrastructures - preparatory phase

FP7-INFRASTRUCTURES-2007-1

INFSO: Supercomputing in Call 2007.2.2.1

Partnership for Advanced Computing in Europe

PACE

partners are 16 “Legal Entities” from 14 European countries

Budget: 19 Mill. €

application was delivered on Mai 2, 2007

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

National governmental support

Bundesministerium für Bildung und Forschung	Germany	The Federal Ministry of Education and Research supports PACE and endorses the participation of GAUSS in PACE, 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 PACE and authorizes GENCI to represent France
Ministerio de Education y Ciencia	Spain	The Director-General for Technology Policy, within the Spanish ministry for Education and Science, supports the participation of BSC in PACE
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
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 PACE
Ministero dell' Università e della Ricerca	Italy	The Ministry of University and Research recognizes the importance of PACE 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 PACE and facilitates the participation of PSNC in PACE
Research Council of Norway	Norway	The Division of Science within the Research Council of Norway expresses its support for PACE and endorses UNINETT Sigma to represent Norway in PACE
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 PACE
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

<p>DEISA</p>	<p>EU- Project</p>	<p>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 PACE as an absolutely necessary and complementary initiative. DEISA offers its services and support for deployment in PACE.</p>
<p>HPC-Europa</p>	<p>EU- Project</p>	<p>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.</p>
<p>OMII-Europe</p>	<p>EU- Project</p>	<p>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 PACE towards provisioning of High end computing resources within Grid computing frameworks.</p>
<p>EGI</p>	<p>EU- Project Proposal</p>	<p>The consortium of EGI aims at establishing a sustainable Grid infrastructure in Europe, coordinating national Grid initiatives. EGI is interested to collaborate with PACE by receiving requirements from the HPC community towards EGI, concerning governance, legal, and political issues.</p>

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 PACE 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 PACE. ENES involvement includes porting of applications on prototype systems of PACE 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 PACE on specific applications.
ESF	Europe	The European Science Foundation is interested to contribute to PACE, 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 PACE by porting their major applications to the prototype systems installed by PACE.
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 PACE.

work packages (I)

Work Package	Descriptive Title	Short description and specific objectives of the task	Leading Participant
WP1	Management of the contract	Result oriented management of all aspects of the project.	FZJ
WP2	Organisational concept of Research Infrastructure (SUPP)	Preparation of the organisational framework to enable the Research Infrastructure (RI) can start operation at the end of the PACE project as a legal entity. Signature ready contracts.	BSC
WP3	Dissemination, Outreach and Training (COORD)	Disseminate project results and educate users.	CSC
WP4	Distributed system management (RTD)	Ensure that the tier-0 systems of the RI can be managed consistently and interoperate with the European HPC ecosystem.	ETHZ
WP5	Deployment of prototype systems (RTD)	Deploy prototypes of potential future Petaflop/s systems at selected PACE sites and assess their viability. The selections will be decided by the Management Board upon recommendation by WP7.	NCF

work packages (II)

WP6	Software enabling for Petaflop/s systems (RTD)	Prepare key applications to use the future Petaflop/s systems efficiently; capture requirements for WP7 and WP8 and create a benchmark suite.	EPSRC
WP7	Petaflop/s Systems for 2009/2010 (RTD)	Identify potential Petaflop/s systems for PACE that can be installed in 2009/10 with prototypes deployed by WP5. Prepare the procurement process including acceptance criteria.	GENCI
WP8	Future Petaflop/s computer technologies beyond 2010 (RTD)	Start a permanent process to identify technologies for future multi-Petaflop/s systems of the RI and work with hardware and software vendors to influence the direction they are taking. Establish PACE as a leader in HPC technology.	FZJ

WP1: Management

- Target- and result-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

WP2: Organizational Concept of RI

- 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

WP3: Dissemination Outreach and Training

- 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

WP4: Distributed System Management

- 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

WP5: Deployment of Prototype Systems

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

WP6: Software Enabling for Petaflop/s Systems

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

❑ **Petaflop/s-Systems for 2009/2010**

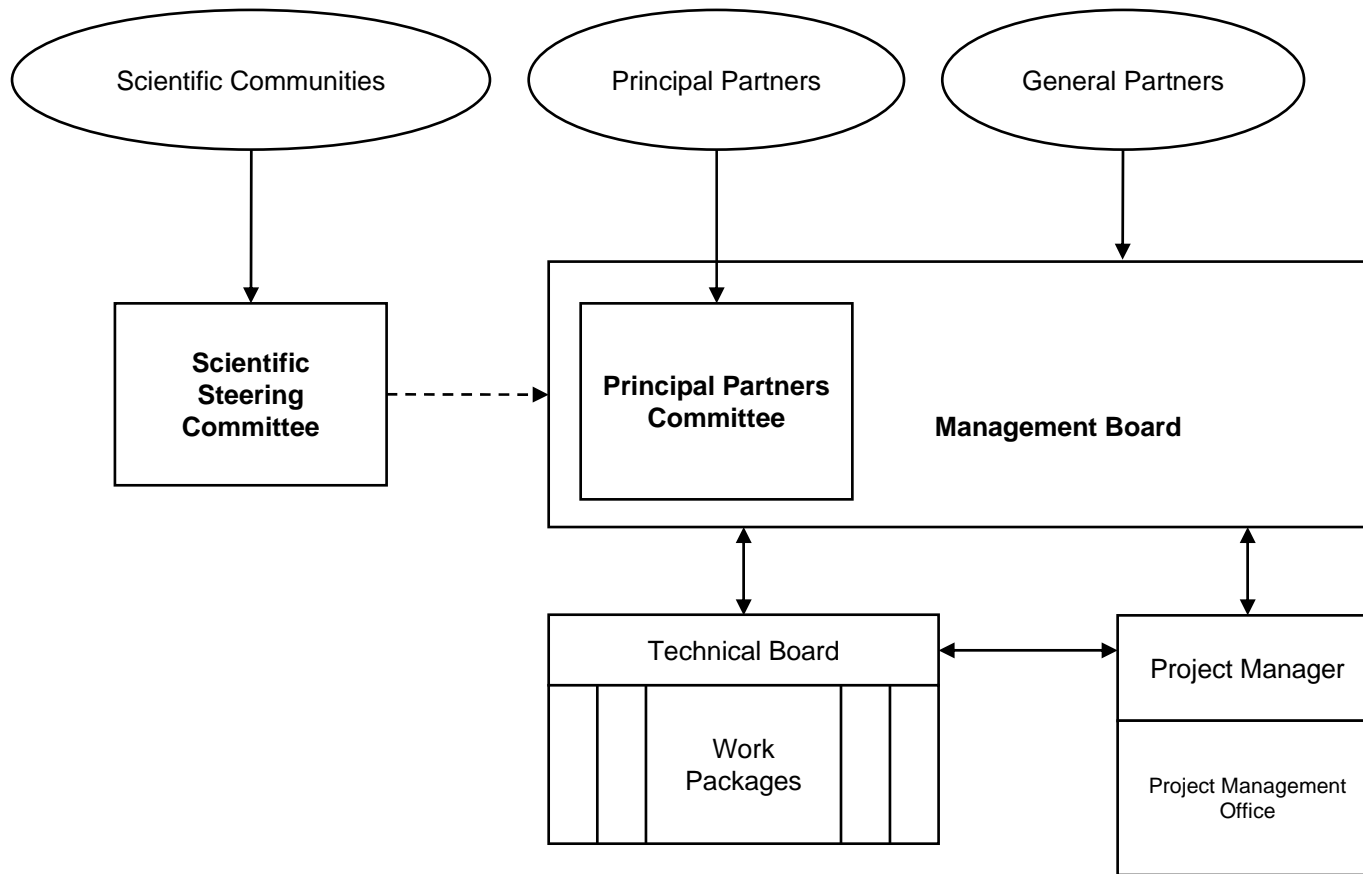
- ❑ Identify architectures and vendors capable of delivering Petaflop/s systems by 2009/2010
- ❑ Translate user requirements into architecture and configuration outline
- ❑ Define installation requirements for Petaflop/s systems and evaluate consistency with possible installation sites
- ❑ Perform a 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

❑ **Future Petaflop/s Computer Technologies beyond 2010**

- ❑ 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

Management structure

- ❑ PACE-Project follows the rules of the PACE-MoU



Project Management Structure