



PARTNERSHIP FOR ADVANCED COMPUTING IN EUROPE

PRACE: The European HPC Research Infrastructure

Thomas Eickermann – Jülich Supercomputing Centre



Agenda

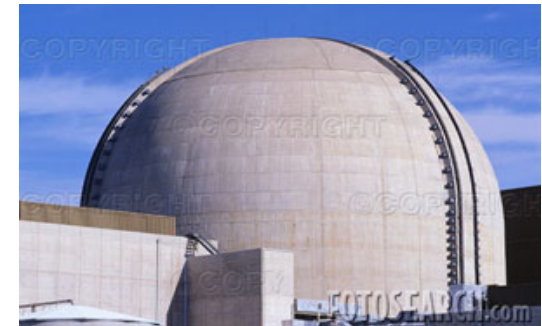
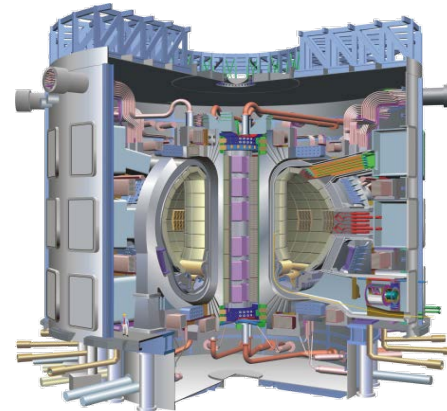
- PRACE mission and status
- Tier-0 Systems and Service
- Peer Review and Access
- User Services
- Related Work

Why does Europe need an HPC Infrastructure?

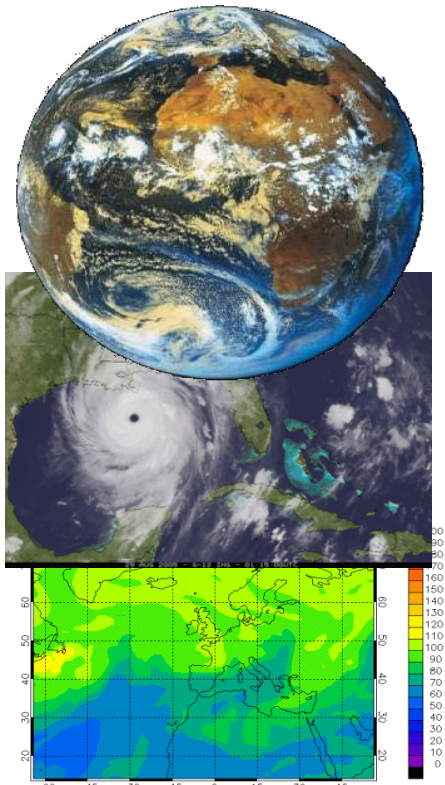
- Simulations on Supercomputers ...
 - ... are the 3rd pillar of scientific discovery
 - ... are key for industrial and scientific competitiveness
- Supercomputing is a key technology for the 21st century
- *All* European researchers and engineers need access to world-class HPC systems and services
 - There should be at least one new or renewed world-class system every year
 - A variety of architectures is needed to meet user requirements
 - No European country has the financial and intellectual resources to do this alone
 - Long-term commitments are needed to create trust in the user communities

Challenges in Engineering and Prototyping

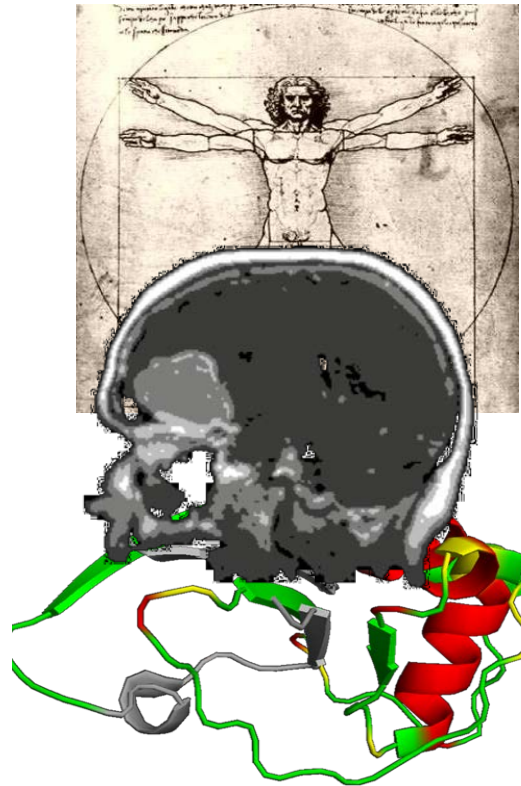
- Faster to Market by Virtual prototyping
- Avoid unethical or dangerous experiments



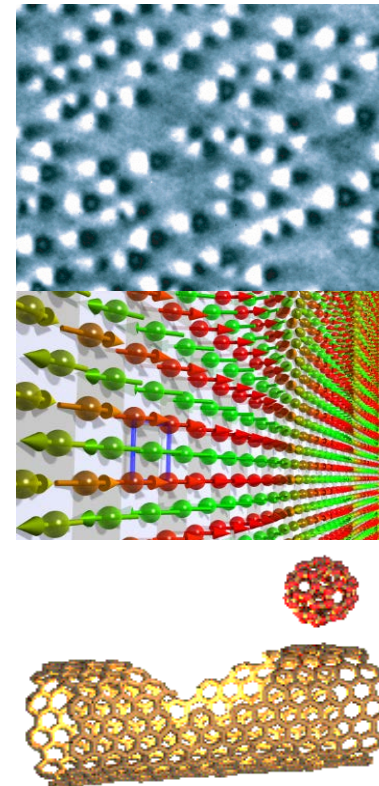
Challenges in Applied Sciences



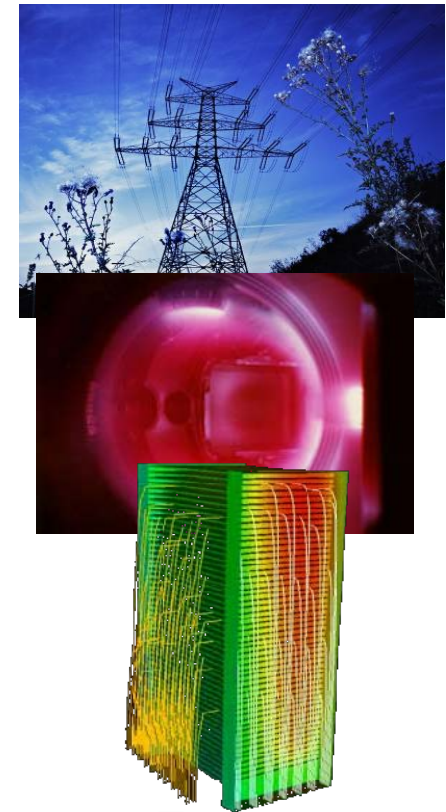
Environment
Weather/ Climatology
Pollution / Ozone Hole



Ageing Society
Medicine
Biology

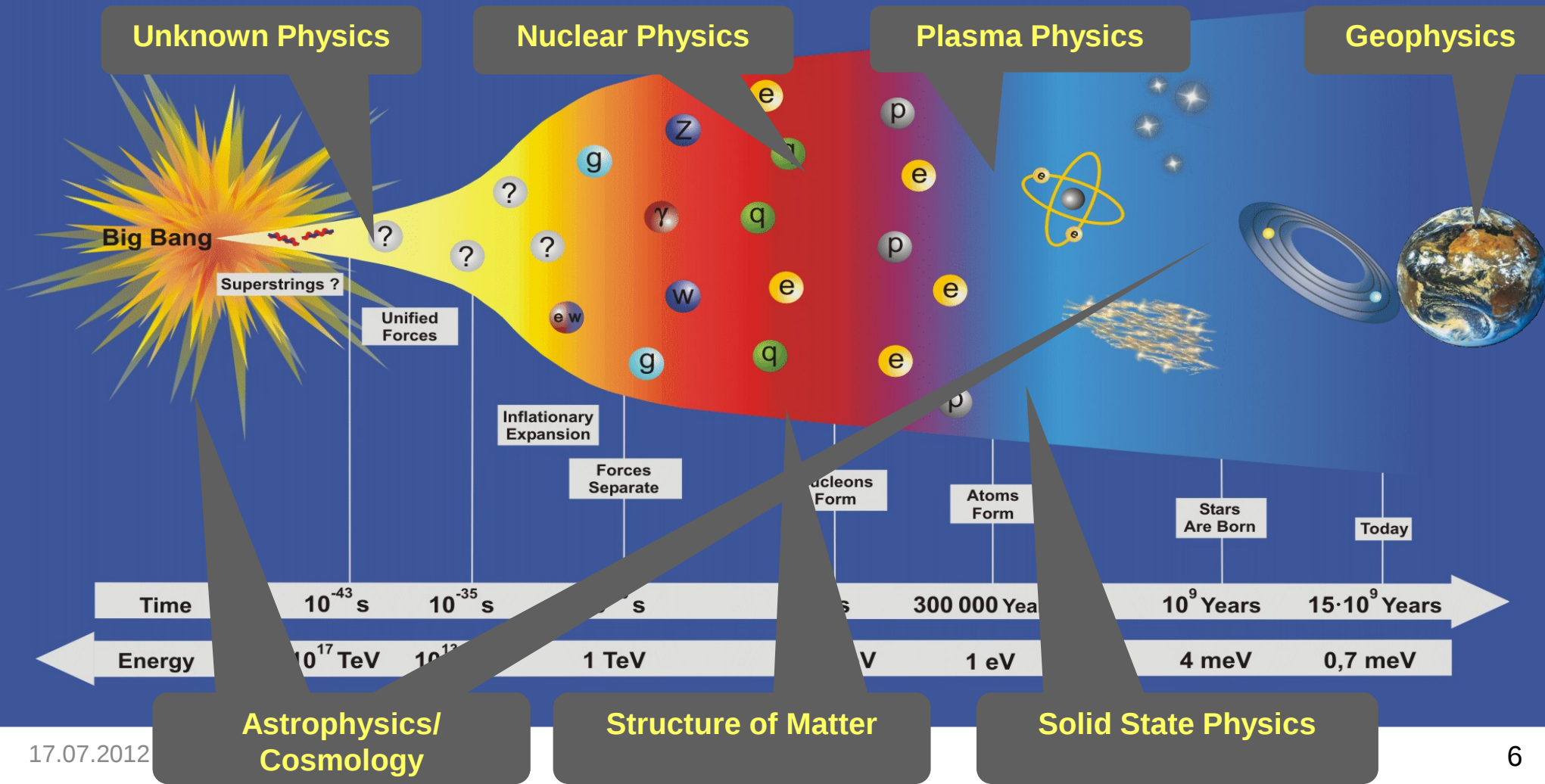


Materials/ Inf. Tech
Spintronics
Nano-science

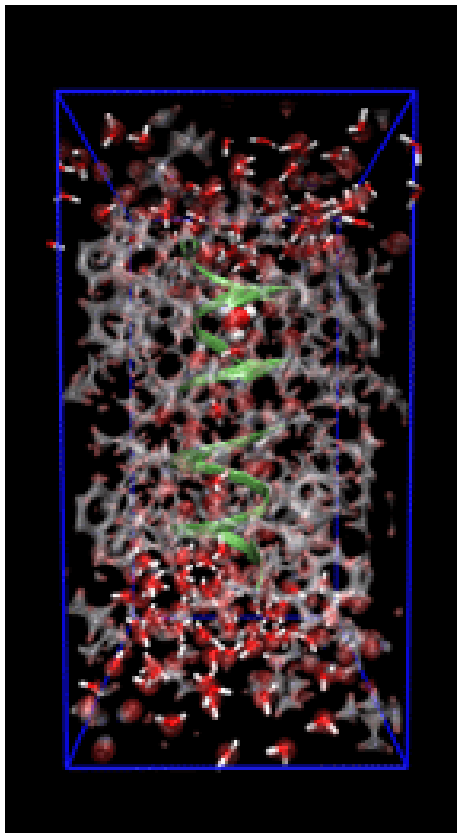


Energy
Plasma Physics
Fuel Cells

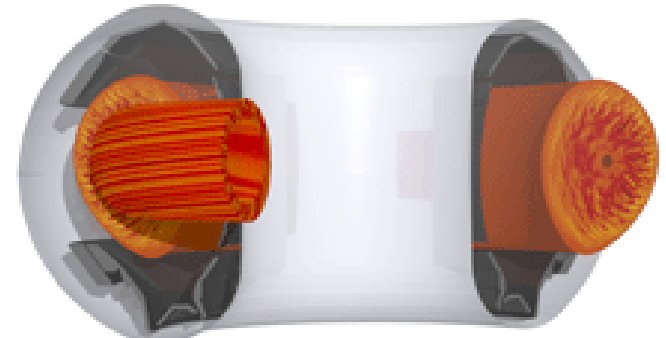
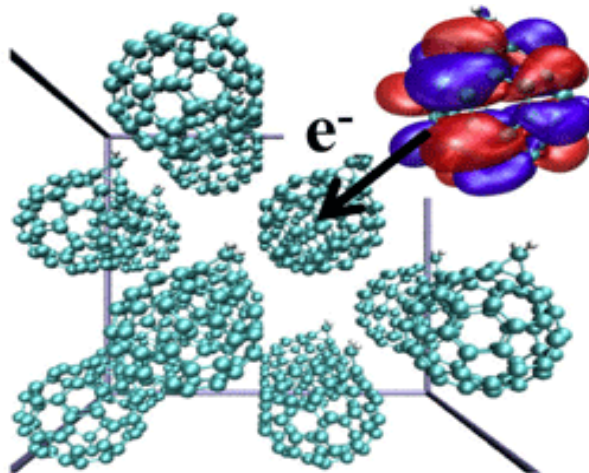
Computational Challenges in Fundamental Sciences



Examples using the PRACE Infrastructure



*Left: The simulation box
of Gramicidin A channel
48.8 M Core-hours
on Jugene awarded
November 2011*



*Above: Ab initio simulation of the ITER-
like fusion device ASDEX Upgrade with
the sophisticated plasma turbulence code
GENE.*

*50 M Core-hours on Jugene
awarded August 2010*

*Left: Charge transfer process
in an organic semi-conducting
material studied
24.6 M Core-hours on Jugene
awarded August 2010*

PRACE

CREATION OF THE PRACE PAN-EUROPEAN RESEARCH INFRASTRUCTURE

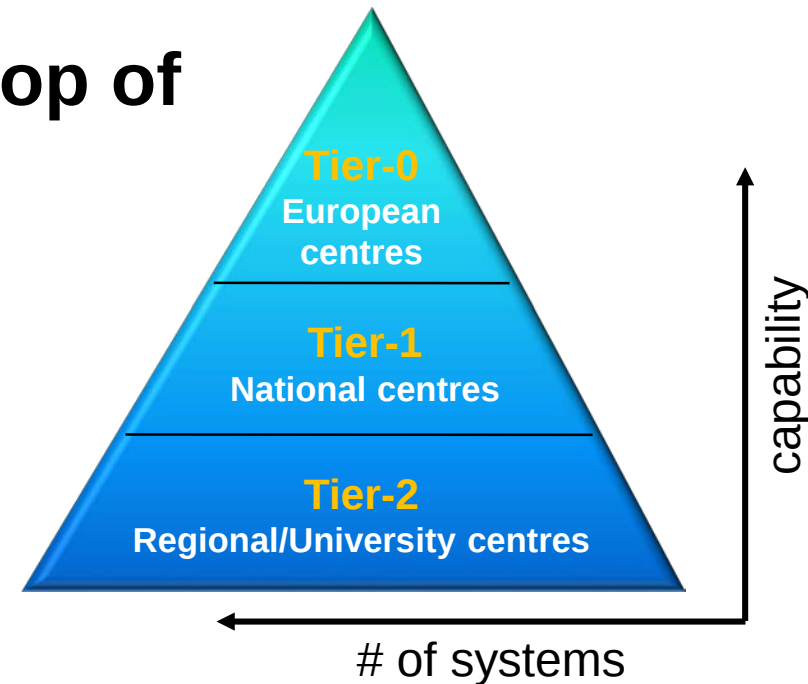
Recipe:

How to create a European Research Infrastructure

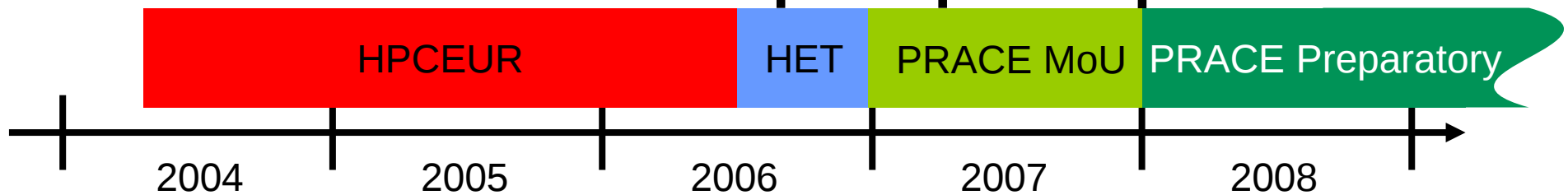
- Make a good (scientific) case
- Get the Infrastructure on Europe's agenda:
Priority list of the European Strategy Forum for Research Infrastructures (ESFRI)
- do {
 - Gather financial commitments from the national governments and the European Commission
 - Agree on the rules (governance)
 - In parallel: perform technical preparations and pilots} until (commitments are binding && contracts can be signed)
- Establish the Infrastructure and provide good service to users
- After some time: renew funding agreements or try to move forward to a fully sustainable funding model (e.g. international treaty, ERIC)

Realizing the ESFRI Vision for a HPC RI

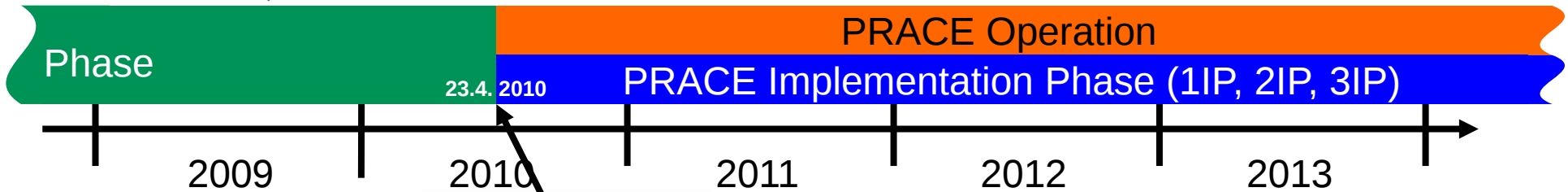
- **European HPC-facilities at the top of an HPC provisioning pyramid**
 - Tier-0: European Centres for PetaFlop/s
 - Tier-1: Coordinated National Centres
 - Tier-2: Regional/University Centres
- **Creation and interaction with the European HPC ecosystem**
 - HPC service providers on all tiers
 - Scientific and industrial user communities
 - The European HPC hard- and software industry
 - Other e-Infrastructures



PRACE History



EU-Grant: INFSo-RI-211528, 10 Mio. €



**PRACE (AISBL), a legal entity
with seat location in Brussels**





April, 23rd 2010 creation of
the legal entity (AISBL)

PRACE

with seat location in
Brussels, Belgium

24 PRACE Members

67+ Million € from EC FP7
for **preparatory and
implementation**

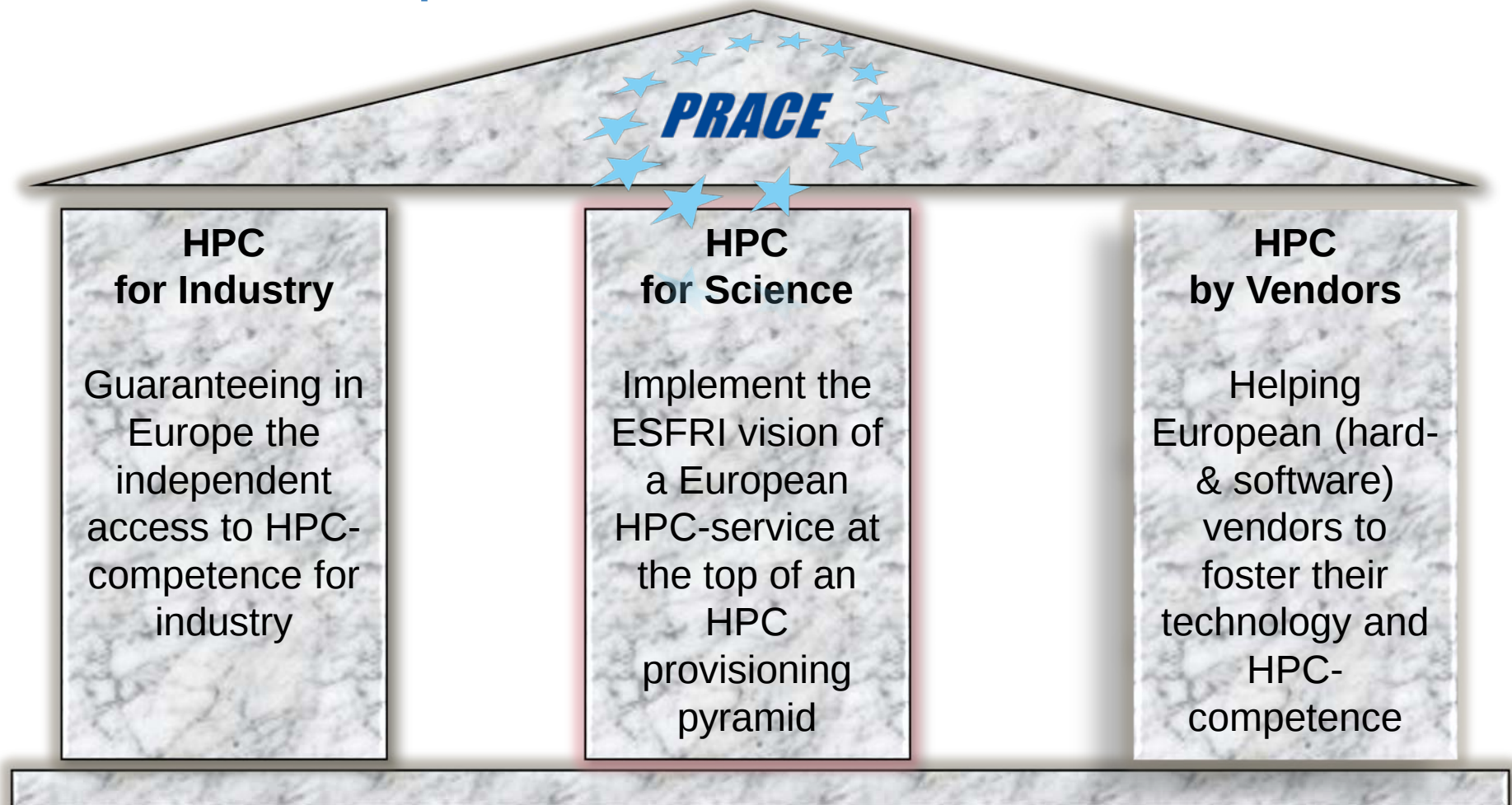
Grants INFISO-RI-211528,
261557, and 283493
Complemented by ~ 50
Million € from PRACE
members



PRACE

PROVIDING SERVICES TO THE EUROPEAN SCIENCE COMMUNITIES

Three pillars of the PRACE Mission



Tier-0 PetaFlop Capability in PRACE



IBM BlueGene/P JUGENE
PRACE@GCS@Jülich



Bull Cluster CURIE
PRACE@GENCI@CEA



2012: IBM BlueGene/Q
PRACE@CINECA FERMI +
PRACE@GCS@Jülich



CRAY XE6 HERMIT
PRACE@GCS@HLRS

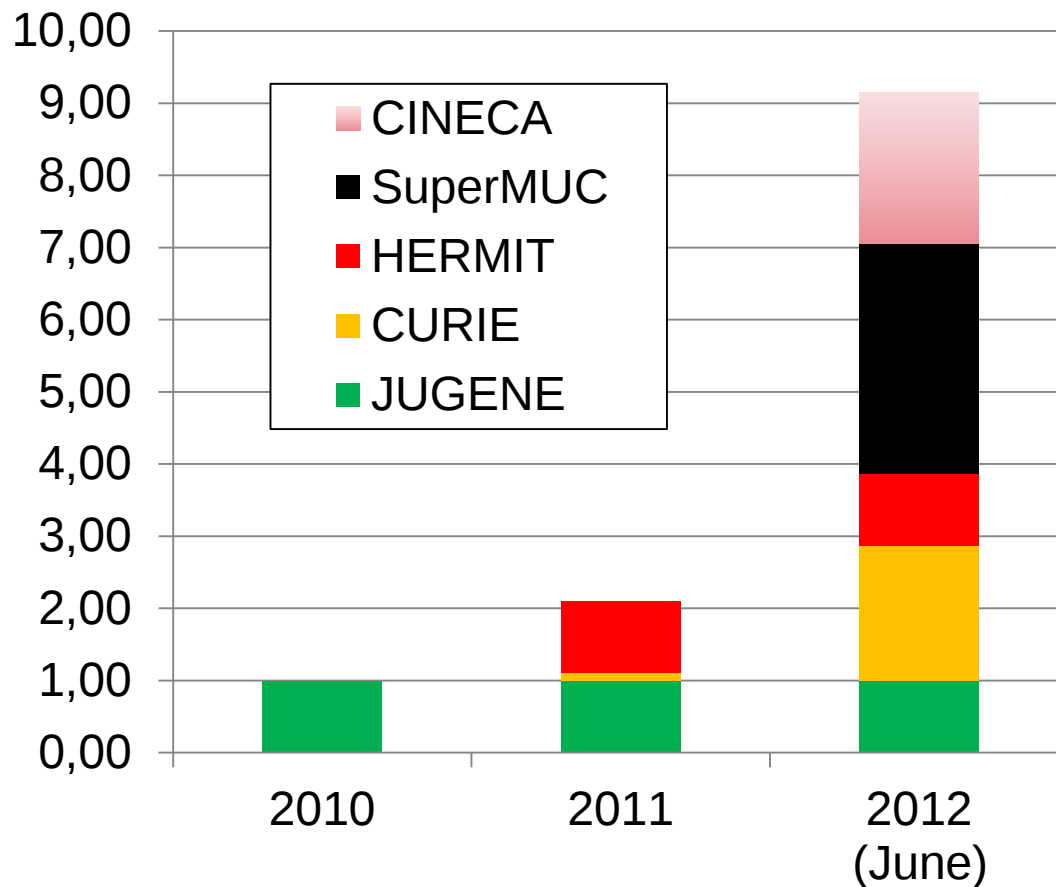


2012: IBM x IDataPlex SuperMUC
PRACE@GCS@LRZ



2012 : Mare Nostrum
PRACE@BSC

PRACE Tier-0 Capability and Support



- Accumulated Tier-0 capability > 13 PFlop/s by end of 2012
- PRACE includes **18 Tier-1 systems** with accumulated capability of > **2 PF** (building on DEISA / DECI)
- PRACE provides capability support competence centres over **several** sites

Provision of Capacity and Access

- **Binding commitments: France, Germany, Italy, Spain**
 - GENCI – GCS – CINECA – BSC
 - Each: 100 Mio € over 5 years in terms of cycles
 - Contribution accounted as TCO
- **Access strictly by peer review at a European level**
 - 6-monthly calls: 5/2010, 9/2010, 2/2011 ... incl. DECI calls
 - Start of provision: 8/2010

PRACE

PEER REVIEW AND ACCESS

Getting Access to PRACE Resources

- **Access is ...**
 - ... granted based on scientific merit only – through peer review
 - ... open to all Researchers in public and private organisations
 - ... free of charge for all users
- **Different types of access are offered**
 - Preparatory access
 - only technical peer review
 - prepare for project access, optionally with PRACE support
 - Project access
 - both technical and scientific peer review by 3 independent reviewers
 - 12 month allocations, 2 calls per year: watch www.prace-ri.eu
 - Multi-Year access (pilot in current call: allocations from Nov. 2012)
 - both technical and scientific peer review
 - demand has been assessed through a call for Eols

Getting Access to PRACE Resources cont.

- Eligibility
 - Main target group: Researchers employed in Universities or public research labs in EU or PRACE member countries and their collaborators world-wide
 - The call closing May 30, 2012 pilots:
 - Access for Industrial users as PI for Open R&D projects (similar to INCITE)
 - Access for non-European PIs
- Is this enough to support existing and encourage new international collaborations?



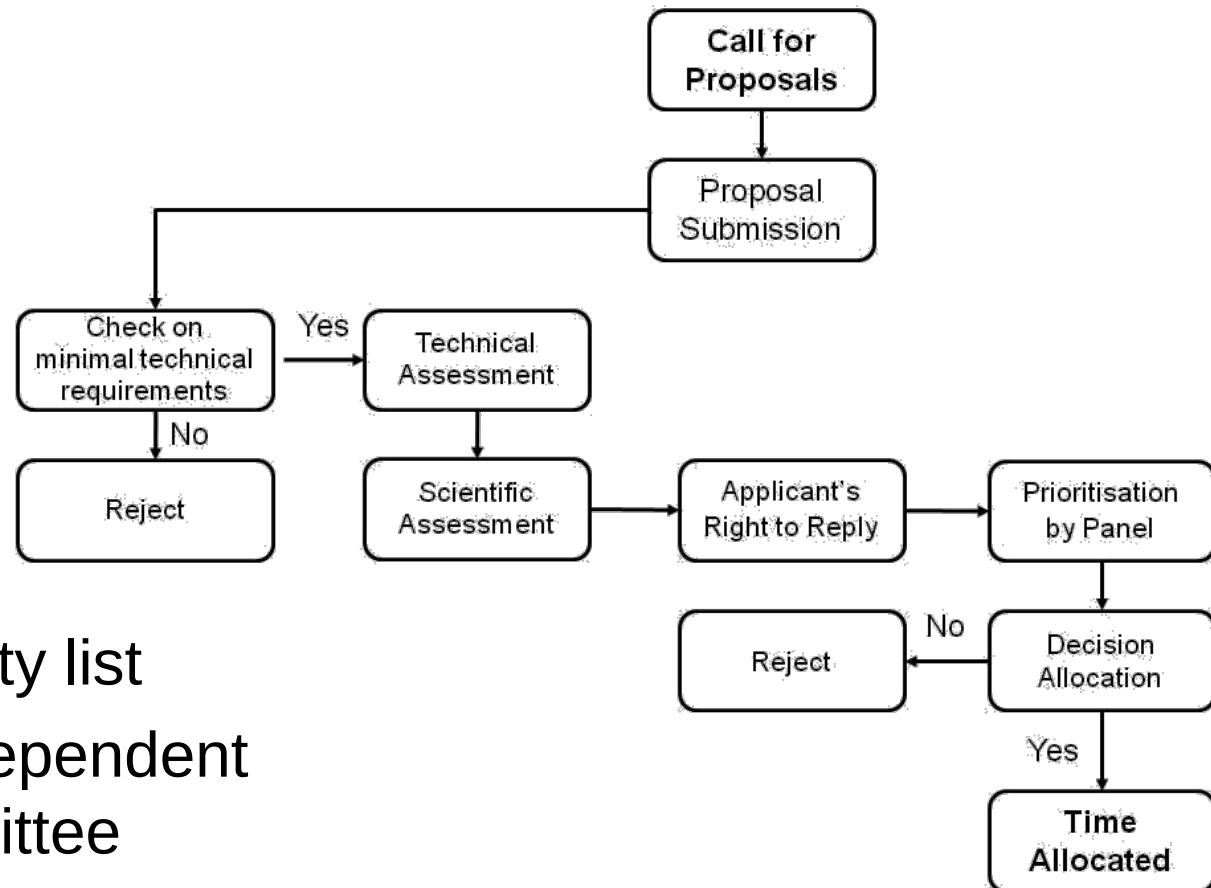
PRACE – XSEDE Call for Eols



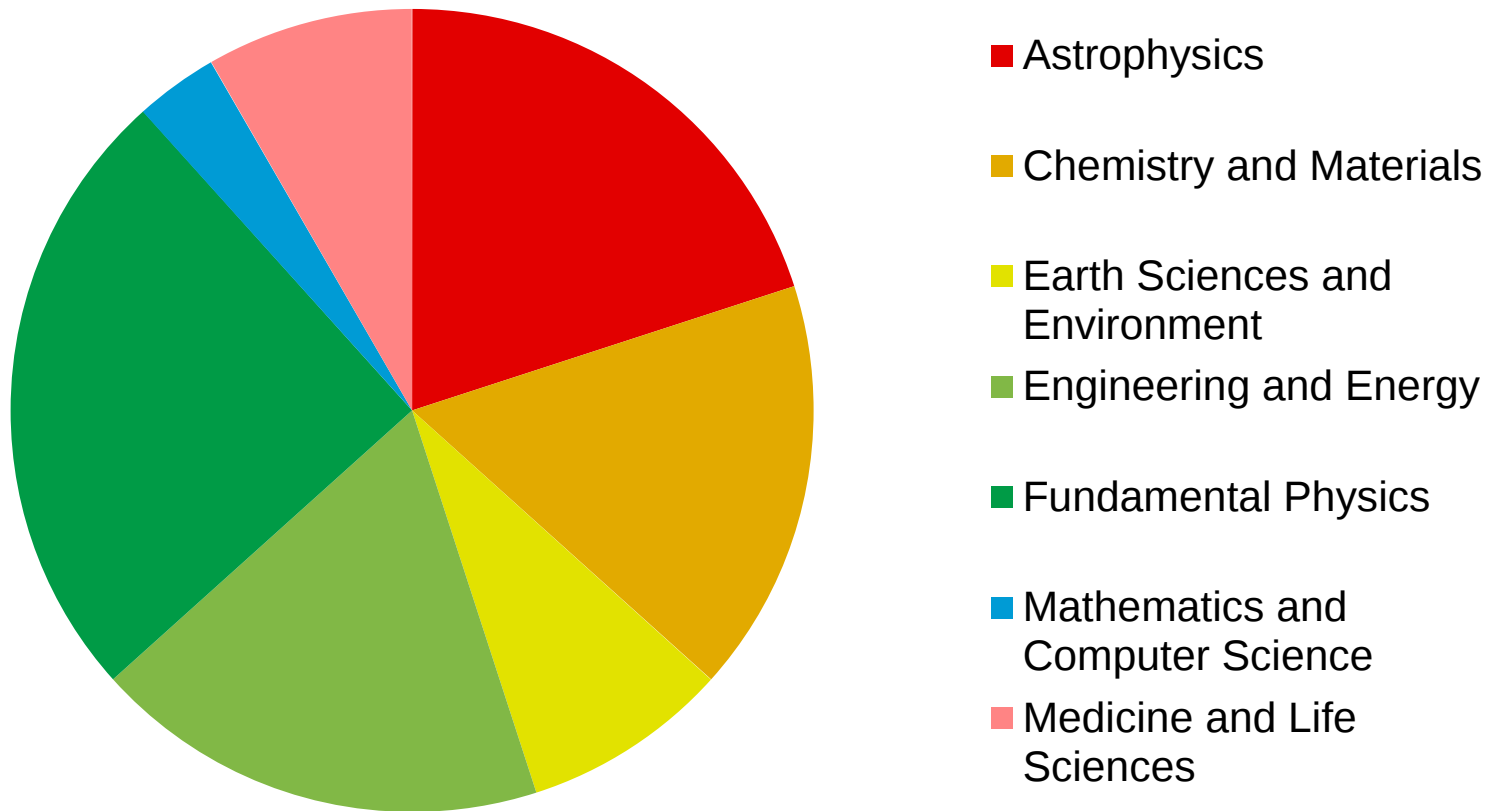
- PRACE and XSEDE explore options for activities to effectively support collaborating research teams spanning the US and EU
- Call for Expressions of interest has been issued
 - <https://www.xsede.org/xsede-and-prace-eoi> and
 - <http://www.prace-ri.eu/Expressions-of-Interest>
- Next steps will be based on the feedback until Sept. 15
- Envisaged actions
 - Joint call for resource allocations
 - Interoperable services

Peer Review Principles and Process

- Technical assessment by Centre staff
- Scientific assessment by independent peers
- Prioritization by independent panel
- Allocation by Director, strictly following the priority list
- Process overseen by independent Scientific Steering Committee



103 Awarded Proposals in 5 Calls



2.7 billion Core-hours granted

PRACE USER SERVICES

User Services

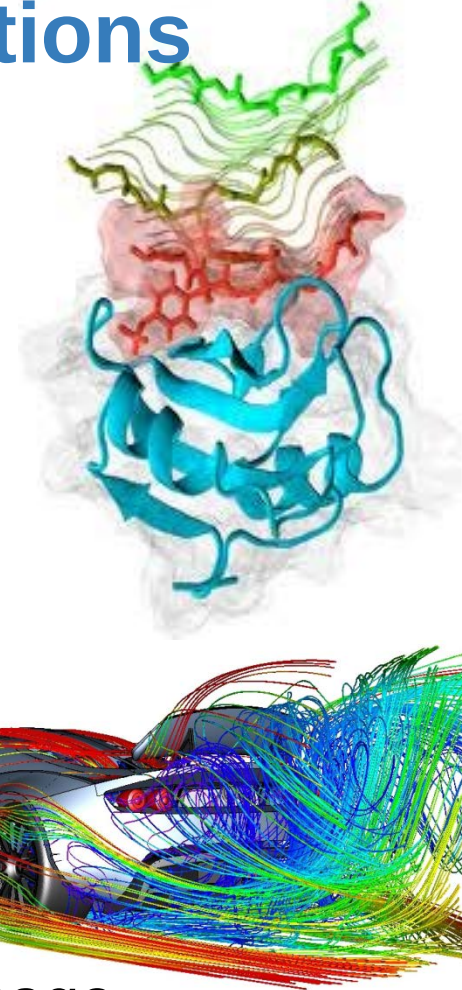
- The PRACE RI is funding Tier-0 access through
 - Tier-0 resources provided by the hosting member countries (400 Mio €)
 - Peer Review management by the membership fees from all member countries
- Additional key services are provided through the EU co-funded PRACE Implementation projects (67 + 50 Mio €)
 - **Application Support and Petascaling of applications**
 - **HPC Training** and Dissemination
 - **Cross-national Tier-1 Access**
 - Services for the Research Infrastructure
 - Advice for the further legal, organisational, and financial development
 - **Operation of the distributed Infrastructure**
 - Market and technology watch, preparation of Tier-0 procurements
 - Prototyping and assessment of future HPC technologies

Application Support

- PRACE offers Application support to
 - Tier-0 Preparatory Access projects
 - Tier-1 DECI projects
 - ~ 3 PM effort from a PRACE expert to help porting, optimising, and scaling an application
- Community applications require a different approach
 - Codes are often well tuned
 - Substantial scalability improvements require code refactoring
 - Close collaboration between code developer and HPC expert
 - Substantial effort: ~ 2 PY per code

Petascaling Key Community Applications

- Material Sciences and Life Sciences
 - GPAW, GROMACS, Quantum_Espresso, CP2K
- Computational Chemistry
 - DL_POLY, DALTON
- Astrophysics, Cosmology and Plasma Physics
 - EUTERPE
- Engineering and CFD
 - OpenFOAM, Code_Saturne, ELMER
- Meteo-Climatology and Earth Sciences
 - EC Earth 3 (NEMO/IFS/Oasis), SPECFEM3D
- Selected based on a survey of European HPC usage



HPC Training

- PRACE offers an extensive HPC training programme
 - 4 seasonal schools per year
 - Workshops for specific topics (e.g. GPGPU programming)
- Online Training
 - Training material (slides and videos) available on the PRACE web
 - A training portal is in preparation
- Annual EU US Summer School jointly organised with XSEDE
 - continuing the series started in 2010 by TeraGrid and DEISA
 - 2012 School in Dublin from June 24-28
 - 230 applicants, 60 participants
 - 2013 School will take place in the US
 - Involvement of Asia considered



PRACE Advanced Training Centres (PATC)

- HPC training is key for advancing and extending the user base
- Training must become sustainable
 - Migration from a EU funded project activity to an Infrastructure Service
- HPC training is almost non-existing in University curricula
- Creation of 6 PATCs
 - Spain (BSC), Italy (CINECA), Finland (CSC), UK (EPCC), Germany (GCS), France (Maison de la Simulation)
 - Coordinated annual curricula from basic MPI courses to specialized topics, community-oriented events, training for trainers

Distributed Infrastructure Operation and Evolution

- Provision of a comprehensive set of common services across Tier-0 and Tier-1 systems
- Services are documented in a Service Catalogue
- Classification
 - Core services – mandatory for all Tier-0 and Tier-1 sites
 - Additional services - mandatory, where possible
 - Optional services – availability and long-term support not guaranteed
- In Preparation: Key Performance Indicators for the services
 - Ensure quality standards in an increasingly distributed environment
- Monitoring, assessment and preparation of technologies and software for new services

PRACE Service Catalogue: Core Services

- Network Services
 - Operation of a dedicated secure 10 Gbit/s network based on GEANT and NRENs (former DEISA network)
- AAA: User administration and accounting
- Compute and Data Services
 - ssh and UNICORE access, GridFTP
- Monitoring and Reporting
 - Inca, DART
- User Services
 - Common Production Environment
 - 1st and 2nd level support, helpdesk, extensive documentation, training

Cross-National Tier-1 Access

- Rationale
 - Not all applications / projects have Tier-0 requirements
 - Most users will use both Tier-1 and Tier-0 class systems and benefit from a close coordination between the tiers
 - Users may require access to a Tier-1 architecture not available in their country
 - Petascaling and user support applies to both tiers
 - Tier-0 is funded by PRACE hosting members and resources are provided under a joint European governance / peer review
 - Tier-1's are funded nationally and are under national governance
- PRACE is
 - committed to manage the coordination of Tier-0 with Tier-1
 - developing a cross-national Tier-1 Access Programme, building on the DEISA DECI initiative and synchronized with Tier-0 Access
 - executing pilot calls, offering access to 18 Tier-1 systems

PRACE

RELATED WORK IN EUROPE

Data Handling

- Storing simulation data is not an issue as such – its part of the HPC centres job
- PRACE Tier-0 operation
 - PRACE users to not have a permanent home at a Tier-0 site, data needs to be moved and preserved after a 12 month project
 - Example: a UK group received a 144 Mio Core-hour Grant on HERMIT for high resolution weather simulation; 2 TB of data transferred daily
- Users change the way they use data
 - Share it in community
 - Keep it accessible for a longer period for analysis
- The European approach: EUDAT
 - “provide a pan-European solution to the challenge of data proliferation in Europe's scientific and research communities”



Towards Exascale Computing

- PRACE Prototypes
 - Assessment of new technologies and cooperation with technology providers
 - Main objective is guide future procurements of energy-efficient systems
- Pre-Commercial Procurement – stimulate R&D of European vendors
- PRACE participates in EESI2 – European Exascale Software Initiative
 - Expert consultation to specify requirements and potential solutions
- EU funds 3 Exascale Projects
 - MontBlanc: Supercomputers based on low-power components (ARM) [BSC]
 - DEEP: Cluster + Intel MIC-based Booster [JSC]
 - CRESTA: Collaborative Research into Exascale Systemware, Tools, and Applications [EPCC]
- ETP4HPC: vendor-driven “European Technology Platform”
 - Will develop a strategic research agenda for HPC hardware technology

Ecosystem Relations

- EEF - European e-Infrastructure Forum
 - Open Forum for exchange among European e-Infrastructures
 - Current members: PRACE, EGI, EGEE, Terena, GEANT, EUDAT
 - Strives for seamless interoperation to provide added value for users
 - Share information, peer with similar activities outside Europe
 - <http://www.einfrastructure-forum.eu/>
- EGI – European Grid Initiative
 - Work on AAA, investigate options for joint dissemination & training
- EMI – European Middleware Initiative
- IGE – Initiative for Globus in Europe
 - EMI and IGE pick up PRACE requirements, provide middleware
 - PRACE evaluates EMI and IGE work

UNICORE

 (GridFTP)

Recipe revisited: State of PRACE

- PRACE is the European HPC Research Infrastructure
 - It provides access to European Tier-0 systems
 - It coordinates access to national Tier-1 systems through DECI
 - It provides extensive training and support
- Infrastructure is established and funding is secured until 2015
 - 400 Mio € by member states + 67 Mio € by European Commission
 - More than 13 Pflop/s aggregated Peak-Performance by the end of 2012
 - 2.7 billion core hours granted to 103 projects since August 2010

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FOR ADVANCED COMPUTING
IN EUROPE



These people build PRACE