



PARTNERSHIP FOR ADVANCED COMPUTING IN EUROPE

PRACE

Europe's Supercomputing Research Infrastructure

Antun Balaz – PARADOXical Training

14 October 2011, Institute of Physics Belgrade, Serbia



PARTNERSHIP
FOR ADVANCED COMPUTING
IN EUROPE





Contents

- Background and Motivation
- History
- Results of the Preparatory Phase
- Europe's Commitment
- Organization of the PRACE RI
- Resources and Access
- Peer Review
- Development Projects
- PRACE Implementation Work



PARTNERSHIP
FOR ADVANCED COMPUTING
IN EUROPE

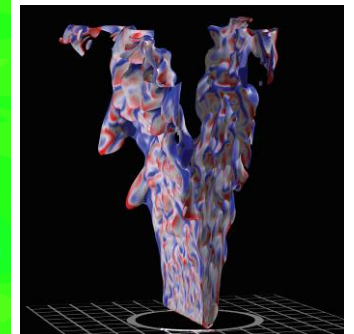
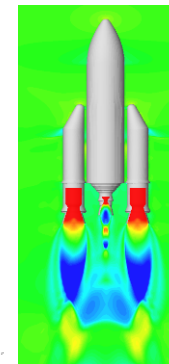
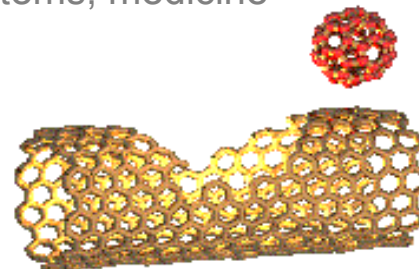
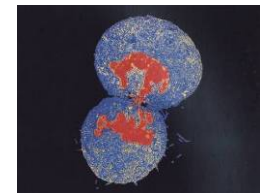
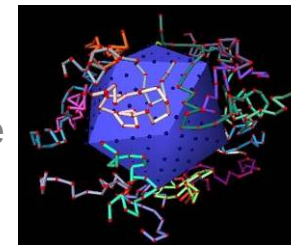
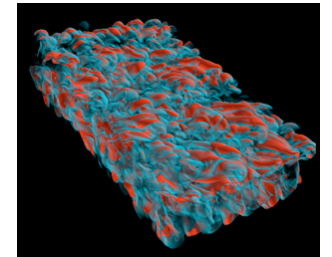
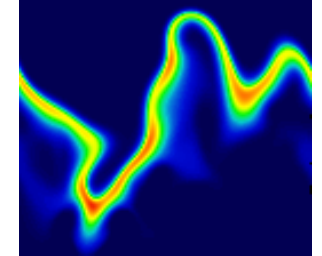
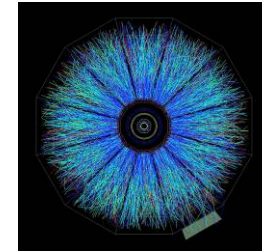
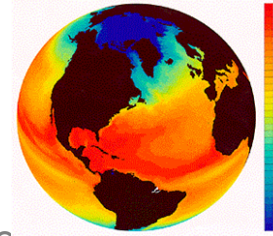


PRACE

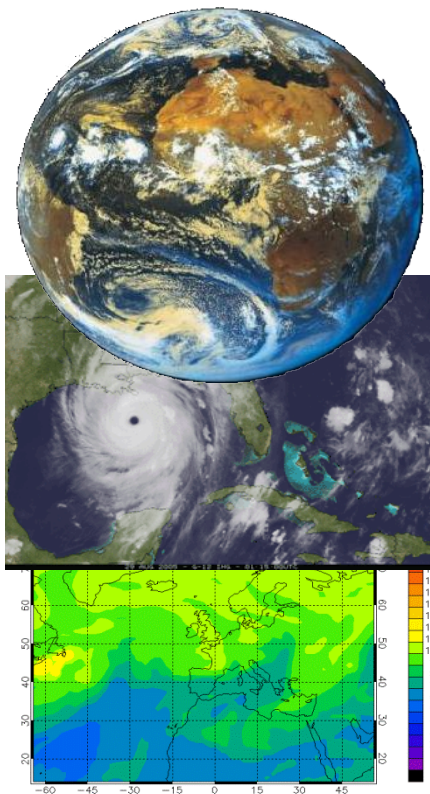
BACKGROUND AND MOTIVATION

Why?

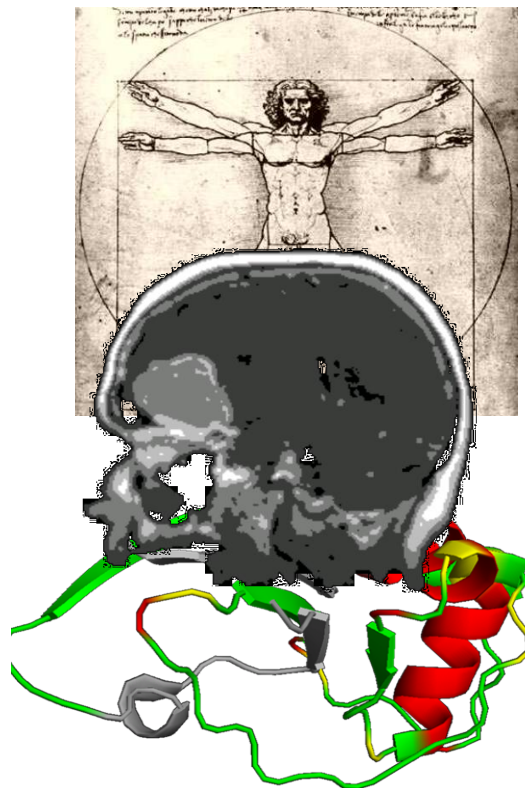
- Weather, Climatology, Earth Science
 - degree of warming, scenarios for our future climate.
 - understand and predict ocean properties and variations
 - weather and flood events
- Astrophysics, Elementary particle physics, Plasma physics
 - systems, structures which span a large range of different 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



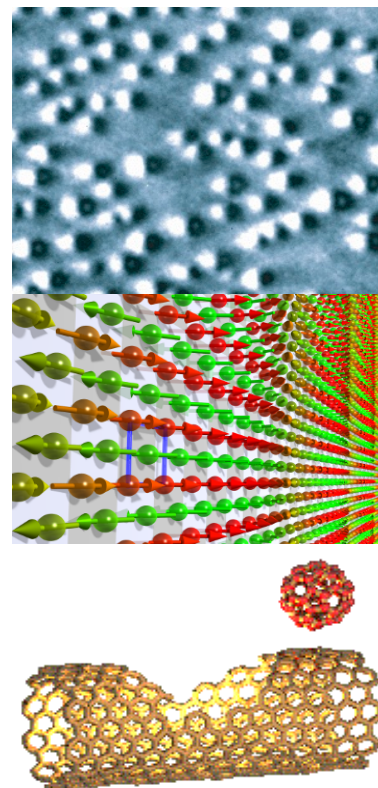
Supercomputing Drives Science through Simulation



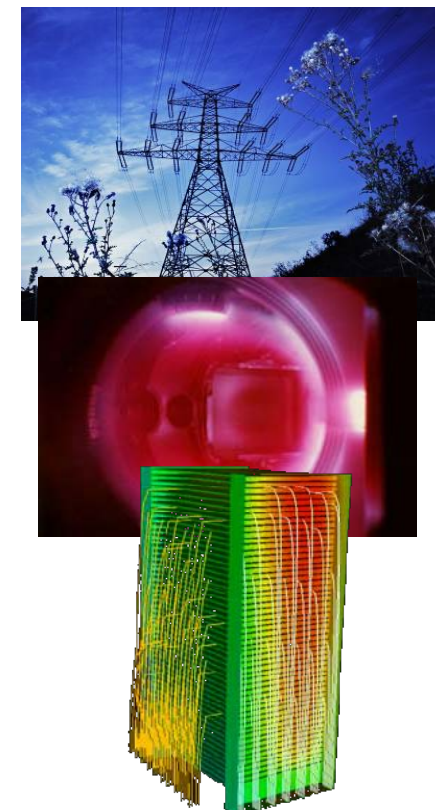
Environment
Weather/ Climatology
Pollution / Ozone Hole



Ageing Society
Medicine
Biology

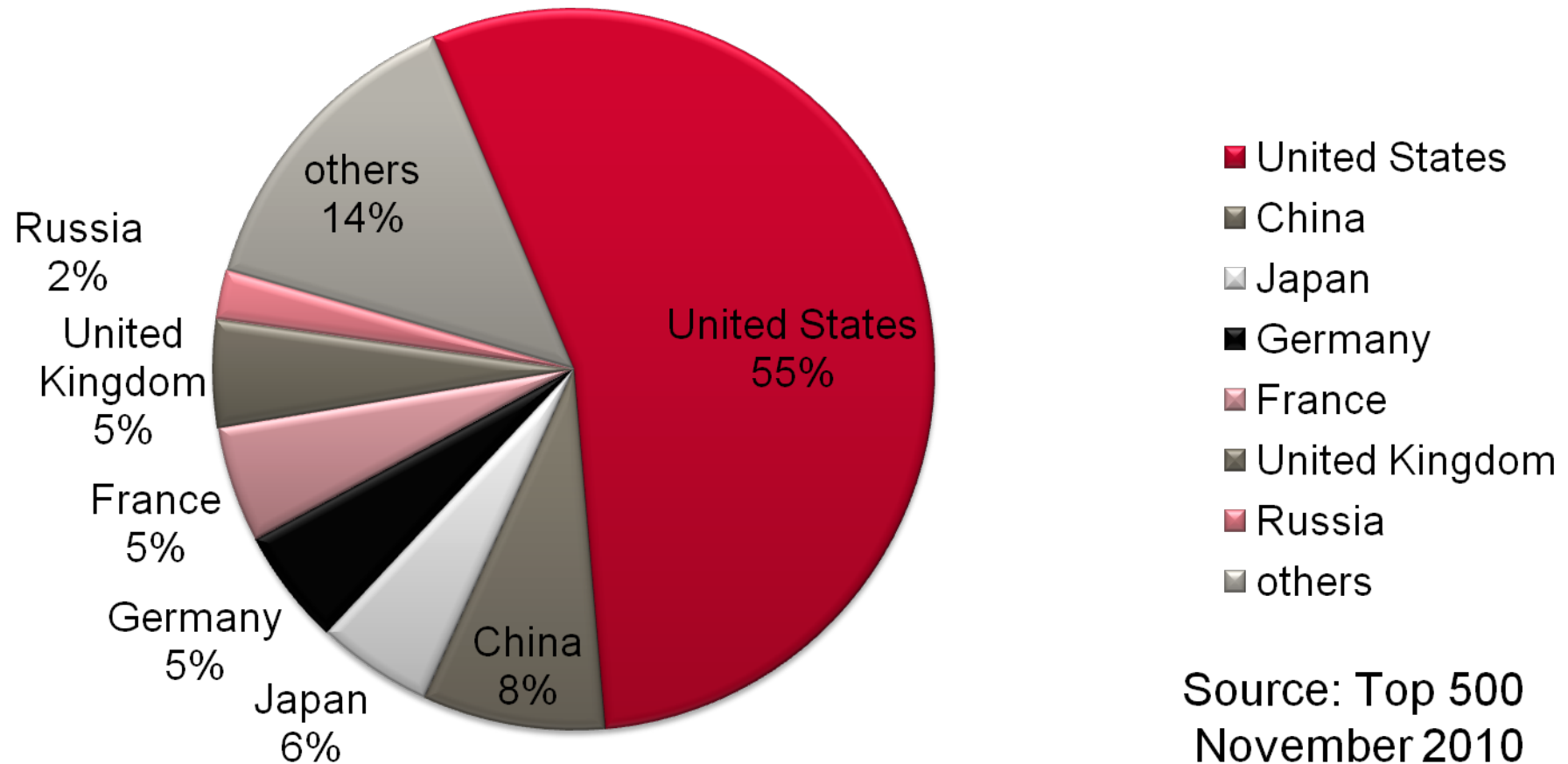


Materials/ Inf. Tech
Spintronics
Nano-science



Energy
Plasma Physics
Fuel Cells

Sum of Performance per Country



Rationale

- **Europe must maintain its high standards in computational science and engineering**
- **Europe has to guarantee independent access to HPC-systems of the highest performance class for all computational scientists in its member states**
- **Scientific Excellence requires peer review on European scale to foster best ideas and groups**
- **User requirements as to variety of architectures requires coordinated procurement**
- **EU and national governments have to establish robust and persistent funding scheme**



PARTNERSHIP
FOR ADVANCED COMPUTING
IN EUROPE



PRACE

HISTORY

HPC on ESFRI Roadmap 2006



First comprehensive definition of
RIs at European level

RIs are major pillars of the
European Research Area

- A European HPC service
- strategic competitiveness
 - attractiveness for researchers
 - access based on excellence
 - supporting industrial development

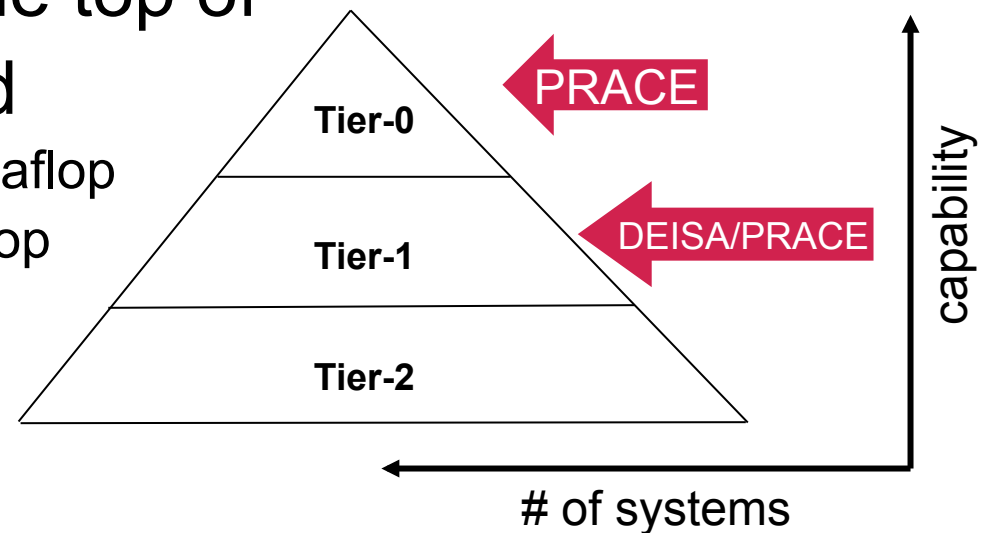
The ESFRI Vision for a European HPC service

- European HPC-facilities at the top of an HPC provisioning pyramid

- Tier-0: 3-6 European Centres for Petaflop
- Tier-0: ? European Centres for Exaflop
- Tier-1: National Centres
- Tier-2: Regional/University Centres

- Creation of a European HPC ecosystem

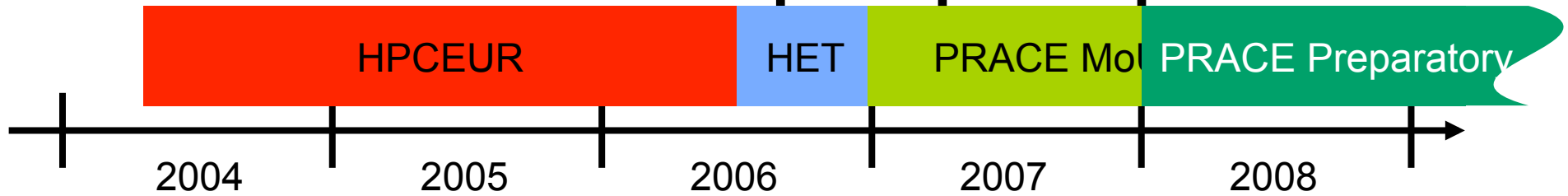
- Scientific and industrial user communities
- HPC service providers on all tiers
- Grid Infrastructures
- The European HPC hard- and software industry



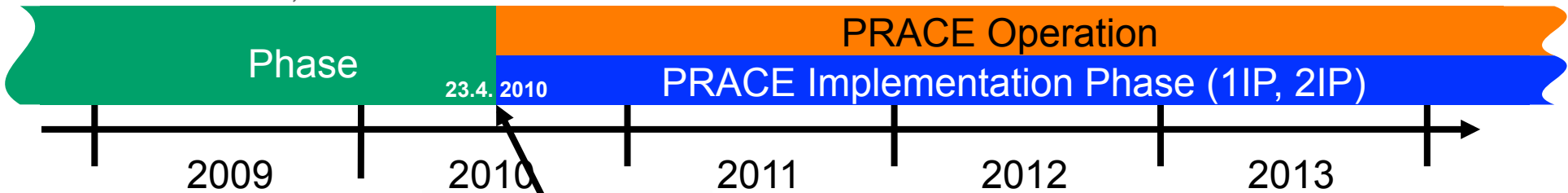
PARTNERSHIP
FOR ADVANCED COMPUTING
IN EUROPE



PRACE Timeline



EU-Grant: INFSO-RI-211528, 10 Mio. €



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



First Milestone

- Memorandum of Understanding signed by 15 States in Berlin, on April 16, 2007
- France, Germany, Spain, The Netherlands, UK and Italy committed funding for a European HPC Research Infrastructure



Second Milestone: The PRACE Project

EU approved the PRACE Preparatory Phase Project
(Grant: INFSO-RI-211528)

- 16 Partners from 14 countries
- Project duration:
January 2008 – June 2010
- Project budget: 20 M € ,
EC funding: 10 M €
- Kickoff: Jülich, January 29-30,
2008



Third Milestone: PRACE RI created

- The PRACE Research Infrastructure was created on April 23, 2010 in Brussels



Fourth Milestone: PRACE Inauguration

- Four nations (France, Germany, Italy and Spain) have agreed to provide 400 million Euro to implement supercomputers with a combined computing power in the multi Petaflop/s range over the next 5 years.
- This funding is complemented by up to 70 million Euros from the European Commission which is supporting the preparation and implementation of this infrastructure.



Fifth Milestone: PRACE project completed

- In October 2009 PRACE demonstrated to a panel of external experts and the European Commission that the project made “satisfactory progress in all areas” and “that PRACE has the potential to have real impact on the future of European HPC, and the quality and outcome of European research that depends on HPC services”. Two months before the end of the project it met the eligibility to apply for a grant of 20 million Euros for the implementation phase of the permanent PRACE Research Infrastructure.
- The First Implementation Project (PRACE 1IP) started on July 1, 2010



PARTNERSHIP
FOR ADVANCED COMPUTING
IN EUROPE

PRACE

THE PRACE PREPARATORY PHASE PROJECT

PRACE Project Achievements in a Nutshell

- Prepared the Creation of the permanent pan-European Research Infrastructure as a legal entity
- Established the PRACE brand
- Provided extensive HPC Training
- Deployed and evaluated promising Architectures
- Ported and petascaled applications

Installed prototypes



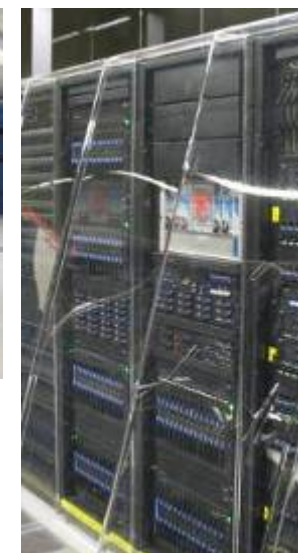
IBM BlueGene/P (FZJ)
01-2008



IBM Power6 (SARA)
07-2008



Cray XT5 (CSC/CSCS)
11-2008



IBM Cell/Power
(BSC)
12-2008



NEC SX9, vector part (HLRS)
02-2009

Intel Nehalem/Xeon (CEA/FZJ):
06-2009

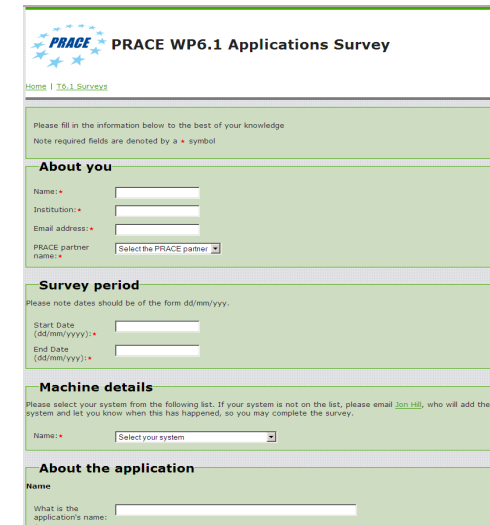


23 scientific software ported and tested to prototype-systems

- The applications studied in this work cover a broad range of scientific areas, and are representative of the European HPC usage. Most of them also originate from the European scientific community.
- The applications are: Alya, AVBP, BSIT, Code_Saturn, CP2K, CPMD, Echam5, Elmer, EUTERPE, Gadget, GPAW, Gromacs, HELIUM, NAMD, NEMO, NS3D, Octopus, PEPC, SIESTA, SPECFEM3D, QCD, Quantum_Espresso and WRF.
- These applications were ported, evaluated and scaled on the PRACE prototypes, which represent the current top of the line supercomputer architectures.
- The applications were ported, on average, to three prototype systems.

Categorisation of Applications

- Benchmark applications should be *representative* of European HPC usage
- We conducted surveys of PRACE partners' HPC systems and major applications
 - Collecting various interesting data for 24 systems and 69 applications
- Quantitative basis for selecting representative applications
- Disseminated as Technical Report



PRACE WP6.1 Applications Survey

Home | [T6.1 Surveys](#)

Please fill in the information below to the best of your knowledge
Note required fields are denoted by a * symbol

About you

Name: *

Institution: *

Email address: *

PRACE partner name: *

Survey period

Please note dates should be of the form dd/mm/yyyy.

Start Date (dd/mm/yyyy): *

End Date (dd/mm/yyyy): *

Machine details

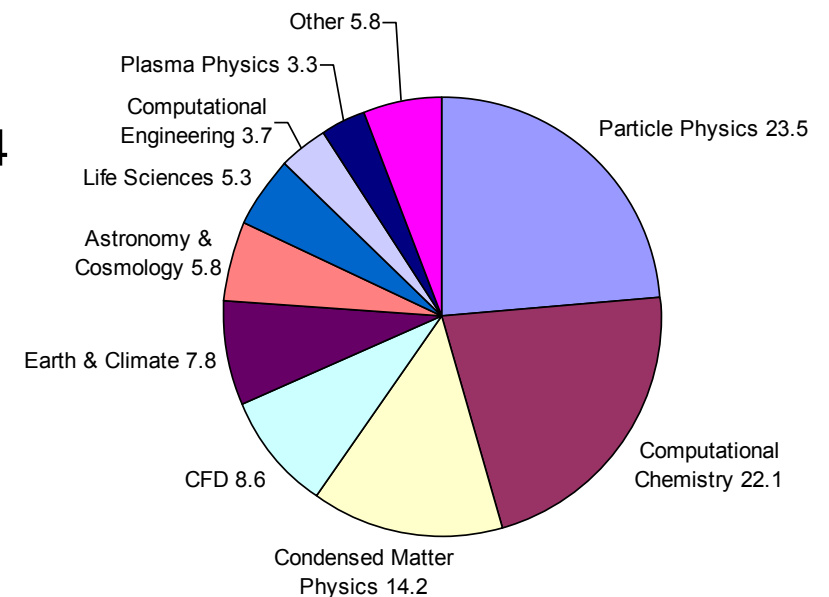
Please select your system from the following list. If your system is not on the list, please email jon.hill, who will add the system and let you know when this has happened, so you may complete the survey.

Name: *

About the application

Name

What is the application's name:



→ PRACE Benchmark Suite

- 12 core applications, plus 8 additional applications
 - NAMD, VASP, QCD, CPMD, GADGET, Code Saturne, TORB, ECHAM5, NEMO, CP2K, GROMACS, N3D
 - *Additional:* AVBP, HELIUM, TRIPOLI_4, PEPC, GPAW, ALYA, SIESTA, BSIT
 - Synthetic benchmarks for architecture evaluation
- Integrated into JuBE (**J**uelich **B**enchmark **E**nvironment)

Applications: Petascaling and Optimisation

Petascaling

- Mixed-mode parallelisation
- Load balancing
- Minimisation of communication overheads
- Parallel I/O
- Checkpointing

Optimisation

- Optimising serial performance
 - CPU
 - Memory
- Optimising both for general-purpose architectures and specialised architectures
- Algorithmic optimisations

*PRACE will disseminate
best practice in these areas*

Libraries and Programming Models

- Classification of Benchmark applications
- Current programming models
 - MPI, OpenMP, mixed-mode, ...
- PGAS and other future programming models
- Accelerator Languages
 - CUDA, RapidMind, openCL ...
- Petascale libraries

Survey of HPC education and training needs

- The Top 10 users at each participating PRACE member site were invited to participate in completing the survey.
- The data was obtained from the most comprehensive evaluation of user training requirements
- Over 90%) of respondents believed they would benefit from formal training in the following areas: performance optimization, debugging tools and techniques, code testing and compiler optimisations;
- Over 90% of users considered that there is an important need for improved HPC training programmes

Training: Benchmarking the survey

- After publication of the PRACE HPC Training and Education survey, a request was received from the Hong Kong Institute of High Performance Computing to use the survey as a template for a similar survey in North-East Asia (<http://survey2008.hkhpc.org/>).
- Recently a further request was received from U.S. TeraGrid trainers to use the survey as a basis for their latest TeraGrid educational and training survey."





PRACE web site

- The PRACE web presence with news, events, RSS feeds etc.
<http://www.prace-ri.eu>
- Public deliverables
- Training material
- Special presentations
- <http://www.prace-project.eu>
- <http://www.prace-project.eu/documents>
- <http://www.prace-project.eu/hpc-training>
- <http://www.prace-project.eu/hpc-training/prace-code-porting-videos>

Home Administrator log in

Welcome to PRACE

The Partnership for Advanced Computing in Europe prepares the creation of a persistent pan-European HPC service, consisting of several tier-0 centres providing European researchers with access to capability computers and forming the top level of the European HPC ecosystem. PRACE is a project funded in part by the EU's 7th Framework Programme.

Supercomputers are indispensable tools for solving the most challenging and complex scientific and technological problems through simulations. To remain internationally competitive, European scientists and engineers must be provided with leadership-class supercomputer systems. PRACE, the Partnership for Advanced Computing in Europe will create a persistent pan-European high performance computing (HPC) service and infrastructure. This infrastructure will be managed as a single European entity. European scientists and technologists will be provided world-class leadership supercomputers with capabilities equal to or better than those available in the USA and Japan. The service will comprise three to five superior HPC centers strengthened by regional and national supercomputing centers working in tight collaboration through grid technologies. In other words, the partnership will become a unique entity of the pan-European HPC ecosystem.

PRACE newsletter
Your e-mail address
HTML
Text
Subscribe

Fourth newsletter
PRACE newsletter 4/2008.

HPC training events

- > Advanced Parallel Programming (in English), Feb. 23-25, 2009, Finland
- > Iterative Linear Solvers and Parallelization (in German).

News

- > PRACE held All Hands Meeting in Jülich, Germany, February 12-13, 2009 2009-02-16
- > Serbia joins the PRACE initiative 2009-02-12
- > PRACE Part of Zero-In Magazine - Call for Papers Open 2009-02-03
- > Reminder: PRACE Award 2009 2009-01-15
- > PRACE Award 2009: Call for Papers has Started 2008-12-18

Events

- > OGF25 / EGEE User Forum, 2-6 March, Catania, Italy
- > 24th Forum ORAP, 26 March, Lille, France
- > DEISA PRACE Symposium 2009: HPC Infrastructures for Petascale Applications, May 11-13, Amsterdam, the Netherlands
- > ISC 2009, June 23-26, Hamburg, Germany

Partner vacancies

- > Research Programmer / Systems Administrator, ICHEC, Ireland

e-infrastructure European Union CAPACITIES

The PRACE website, www.prace-project.eu

Video training material already on web site

- Material from 4 workshops
- 48 hours video material



Home → HPC training → Video training material

Administrator log in

Video training material

PRACE has gathered video training material from its workshops to this site.

- Training material from PRACE workshop on application porting and performance tuning, CSC, Finland (06/2009)
- Training material from PRACE Cray XT5 Code-Porting Workshop, CSCS, Switzerland (07/2009)



PRACE workshop on application porting and performance tuning at CSC, Finland

News

- » BSC arranges a PRACE code porting and optimization workshop 2009-08-11
- » First projects granted access to the PRACE Prototype systems - 4.4 Million Core hours to 3 projects 2009-07-22
- » Presentations and pictures from ISC'09 2009-06-29
- » PRACE organises an industry seminar for potential European High Performance Computing users 2009-06-26
- » PRACE part of La Recherche magazine 2009-06-26

more...

Events

- » DFT09, August 31 - September 4, Lyon, France
- » ParCo 2009, September 1-4, Lyon, France
- » PRACE industry seminar, September 7-8, Toulouse, France
- » PPAM 2009, September 13-16, Wroclaw, Poland
- » Bio IT World Conference & Expo 09, October 6-8, Hannover, Germany

more...

Partner vacancies

PRACE at Supercomputing 2009

- PRACE gained a high visibility
- PRACE collected leads at SC09 by scanning conference passes from those people who showed interest in PRACE. A total of over 220 leads were collected and further information about PRACE sent to these people via e-mail after the event.
- Two SC presentations: "new technologies" and "future languages" published on the PRACE web site



PRACE at ISC HAMBURG

- Brochure (updated in 2009 & 2010)
- General PRACE poster (updated in 2009 & 2010)
- Prototype poster (updated in 2010)
- Production system poster (new, created in 2010)
- PRACE t-shirts (reprinted in 2010)
- 8 presentations of the network sessions available on the PRACE web site



Prace Award 2009 at ISC

- The PRACE Award 2009 winners are **J. C. Mouriño, A. Gómez, J. M. Taboada, L. Landesa, J. M. Bértolo, F. Obelleiro** and **J. L. Rodríguez** from Supercomputing Center of Galicia (CESGA), Universidad de Extremadura, Universidad de Vigo, Spain. Their work "*High Scalability Multipole Method. Solving Half Billion of Unknowns*" was declared as the winning paper among the excellent submissions.



PRACE Award 2010 at ISC

- The PRACE Award 2010 winners were **Klaus Iglberger**, M. Sc. and Prof. **Ulrich Rüde** from the University of Erlangen-Nuremberg, Germany. Their paper “Massively Parallel Granular Flow Simulations with Non-Spherical Particles”



The Second Industry Seminar 2009

- The second PRACE industry seminar “Europe goes HPC” was held in Toulouse on 7–8 September.
- It attracted more than 100 participants from 21 countries with executive attendees representing 57 companies from a wide variety of industry fields
- 14 presentations are available on the PRACE web site



First DEISA-PRACE symposium

- The DEISA PRACE Symposium 2009 took place at the Royal Tropical Institute in Amsterdam on May 11 - 13, 2009.
- 97 per cent of the respondents thought that the symposium was very productive (62%) or productive (35%).
- It attracted almost 200 participants from more than 20 countries and four continents
- 28 presentations were published on the Prace web site



Second DEISA- PRACE symposium 2010

- The symposium was held from May 10 to May 12 at Casa Milà, in Barcelona,
- It received more than 130 participants from 23 countries and three continents.
- 14 computational science grand-challenge projects from all over Europe and various disciplines were presented.
- 25 presentations published on the Prace web site
- The Third Scientific Conference had over 130 participants



STRATOS

- Strategic Advisory Group for Advanced Technologies
 - A cooperation platform between PRACE and industrial consortia
 - Members: 15 PRACE partners, PROSPECT, Teratec
 - 3 Working Groups: Exascale Software, Technology Watch, Green-IT and HPC Leadership resources

Vision:

Reinforce Europe's excellence in HPC Architectures, software and tools.

Mission:

Guarantee a continuous HPC technology evaluation and system evolution within the future European HPC Research Infrastructure.

Become a permanent European Coordination, Research and Development Platform for HPC.

- Expected impact
 - STRATOS allows PRACE to enter industry cooperations through its members and yet maintain vendor independence, e.g. during procurements
 - Technology assessment guides the technological/scientific plans of PRACE in collaboration with HPC technology providers



PARTNERSHIP
FOR ADVANCED COMPUTING
IN EUROPE



Member States

**PRACE RESEARCH
INFRASTRUCTURE CREATED**

PRACE Research Infrastructure Created

- Establishment of the legal framework
 - PRACE AISBL created with seat in Brussels in April (Association Internationale Sans But Lucratif)
 - 20 members representing 20 European countries
 - Inauguration in Barcelona on June 9



- Funding secured for 2010 - 2015
 - 400 Million € from France, Germany, Italy, Spain
Provided as Tier-0 services on TCO basis
 - Funding decision for 100 Million € in The Netherlands
expected soon
 - 70+ Million € from EC FP7 for preparatory and implementation
Grants INFSO-RI-211528 and 261557
Complemented by ~ 60 Million € from PRACE members





PARTNERSHIP
FOR ADVANCED COMPUTING
IN EUROPE



PRACE

COMMITMENT

Provision of Capacity and Access

- **Binding commitments** by Germany, France, Italy, Spain
 - 100 Mio € over 5 years in terms of cycles
 - Contribution accounted as TCO
- Access strictly by **peer review** at a European level
 - Early access call: May 2010
 - Start of provision: 1.8.2010
 1. Test / evaluation access
 2. Project access – for a specific project, grant period ~ 1 year
 3. Programme access – resources managed by a community
 - **Free-of-charge** for European scientific communities

Provision of Capability and Support

- PRACE goes for a set of machines with successively increasing **capability**
 - 1 PF (2010) + 1.5 PF (2011) + 2 PF (2012) + 3 PF (2012) + 5 PF (2013) and will add **upgrade steps**
 - Accumulated capability of more than **10 PF** in 2013
 - PRACE will include **Tier-1** sites (continuing DEISA)
- PRACE will provide support competence centres over **several** sites

PRACE Tier-0 Systems

- 1st Tier-0 System provides cycles since August 1
 - Jugene: BlueGene/P in GCS@Juelich
 - 72 Racks, 1 PFlop/s Peak
 - 35% of capacity provided to PRACE
- 2nd Tier-0 System announced by GENCI on October 5
 - Curie: Bull Cluster with Intel CPUs operated by CEA
 - 1.6 PFlop/s peak in Oct. 2011 (1st step in 2010)
 - Largest fraction of capacity provided to PRACE
- Next Procurements (in alphabetical order)
 - BSC, CINECA, GCS@HLRS, GCS@LRZ
 - Procurement plan based on analysis of user requirements and market



Ramp Up Until 2012

Country	2010	2011
Germany / GCS	FZJ 1 PF peak	
France / GENCI		CEA 1.6 PF peak
Italy / CINECA		
Spain / BSC		

Further installations planned in 2011-2013 by Italy, Spain, Germany

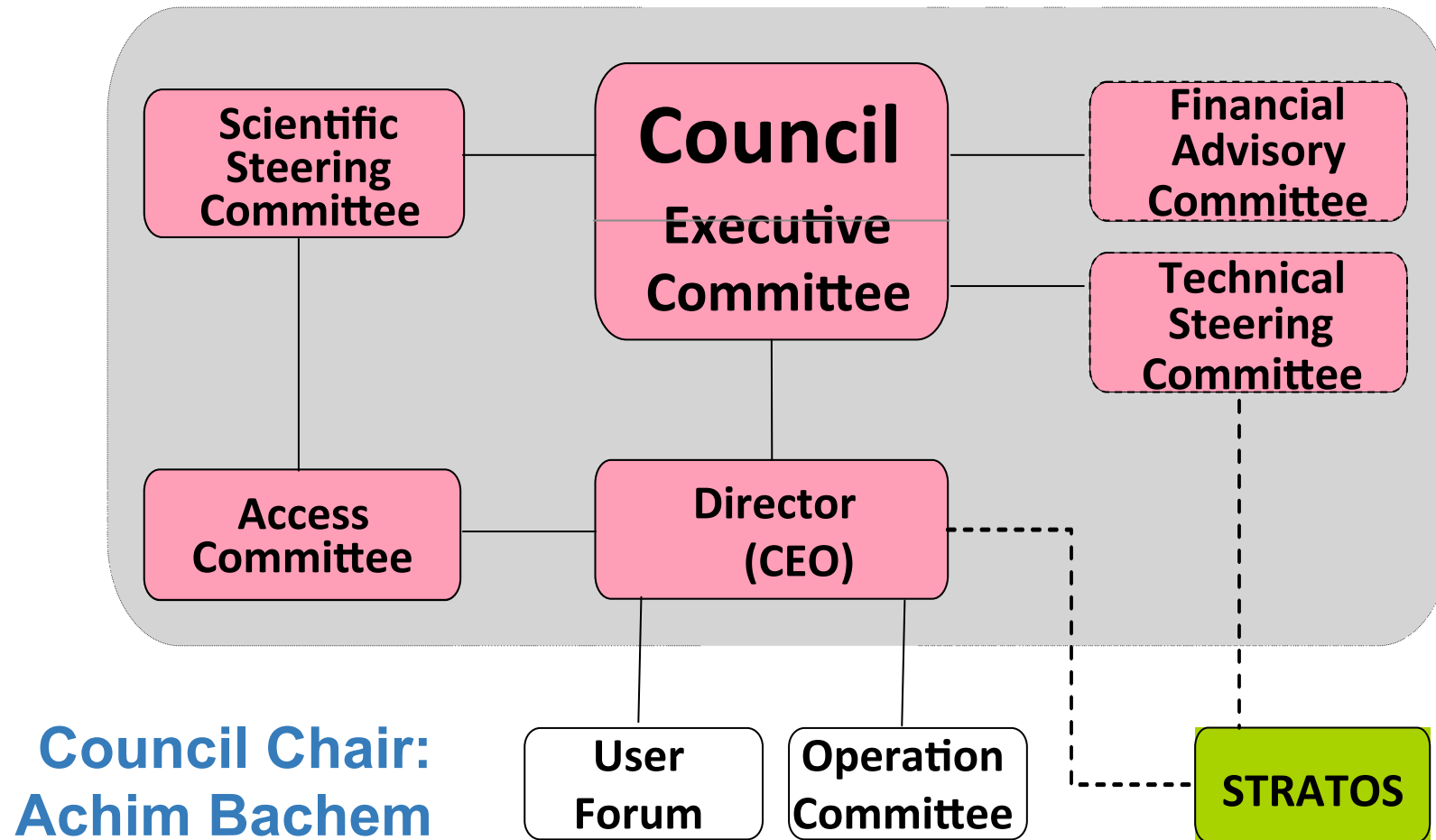


PARTNERSHIP
FOR ADVANCED COMPUTING
IN EUROPE

PRACE

ORGANIZATION

Organization



SSC “bootstrap” Group

- Richard Kenway (UK, Part. Phys., Chair)
- E.J.Baerends (Netherlands, Chemistry)
- Kurt Binder (Germany, Cond. Matter)
- Miquel Coll (Spain, Biology)
- Filippo Giorgi (Italy, Climate)
- Olivier Pironneau (France, Math)

Scientific Steering Committee

Scope defined in the Statutes of the AISBL

- The SSC is responsible for giving opinions on all matters of scientific and technical nature
- 21 members
- Members appointed by Council based on a list of candidates prepared by the SSC
- Two year term (renewable twice)
- Propose the members of the Access Committee

Access Committee (Article 25-26)

- Advice on scientific use of Tier-0 Infrastructure
- Recommendations on the allocation of computational resources based on the Peer Review process
- Proposed by the SSC based on competence in the areas of science
- Appointed by the Council, minimum of 5 members
- Two years term (renewable once)
- The Access Committee will define its iworking rules



PARTNERSHIP
FOR ADVANCED COMPUTING
IN EUROPE



PRACE

CALLS FOR PROPOSALS

PARTNERSHIP
FOR ADVANCED COMPUTING
IN EUROPE



JUGENE@Jülich: #5 worldwide, #1 in Europe



IBM Blue Gene/P

1st

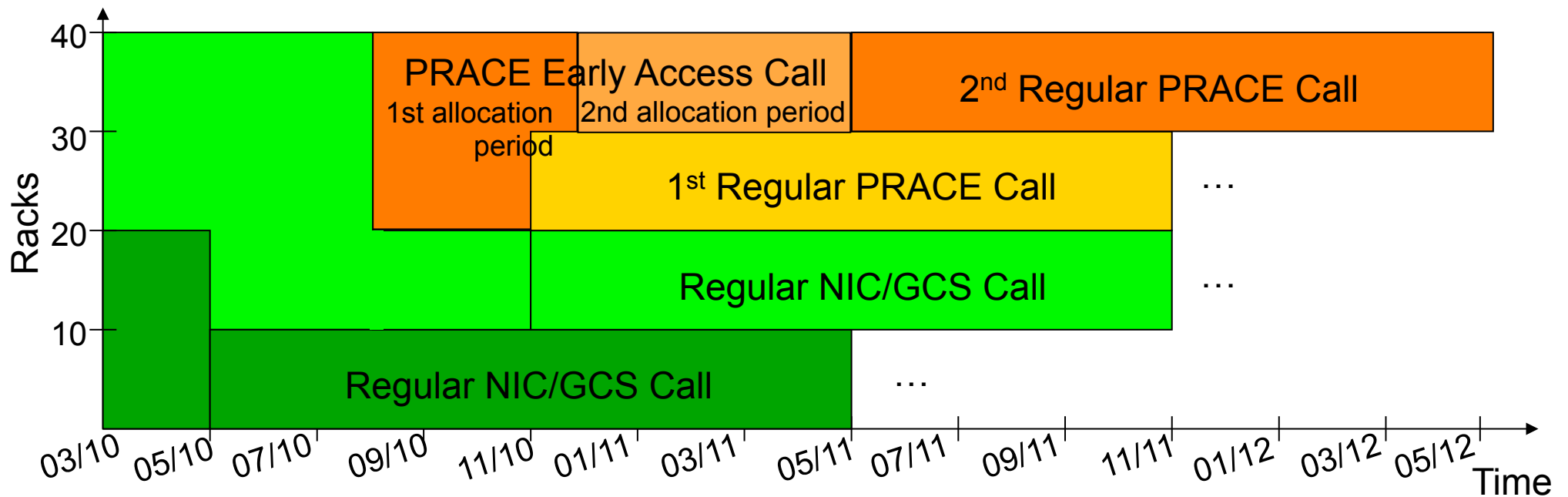
**PRACE
system**

Jülich Blue Gene/P Configuration

72 Racks Blue Gene/P

- 73728 Compute Nodes
(4 processor cores, 2 GB memory)
- **294912 CPU cores**, 144 TB memory
- 1 PFlop/s peak performance
- 825.5 TFlop/s Linpack
- 600 I/O nodes (10GigE) → **>60 GB/s I/O**
- 2.2 MW power consumption

Scheme of Calls for JUGENE



35% of Capacity provided by PRACE corresponding to 40 Racks
Early Access Call assisted by the SSC Establishment Group

Proposal Statistics

- **65 proposals**

- 47 for project access
- 11 for the 1st of December
- 36 for the 1st of August
- 18 for combined access

- **Project leaders from 16 countries**

- Belgium – 1
- Denmark – 1
- France – 5
- Greece – 2
- Italy – 4
- Poland – 2
- Spain – 11
- Switzerland – 3
- Bulgaria - 2
- Finland - 2
- Germany - 11
- Ireland - 2
- Netherlands – 2
- Portugal – 4
- Sweden – 1
- UK - 12

Proposal Statistics II

- 1,471,509,270 core hours
- Oversubscription: factor 5
 - Astrophysics - 7
 - Chemistry and Materials - 11
 - Earth Sciences and Environment - 4
 - Engineering and Energy - 15
 - Fundamental Physics - 17
 - Mathematics and Computing - 3
 - Medicine and Life Sciences - 8

Tier-0 Early Access Projects (1/2)

1. Simulation of electron transport in organic solar cell materials
(J.Blumberger UCL, UK, 24,7 Mio core hours)
2. Excess proton at water/hydrophobic interfaces: A Car-Parrinello MD study
(P. Carloni, GRS, Germany, 40,7 Mio core hours)
3. Parallel space-time approach to turbulence: computation of unstable periodic orbits and the dynamical zeta function
(P. Coveney, UCL, UK, 17 Mio core hours)
4. QCD Thermodynamics with 2+1+1 improved dynamical flavors
(Z. Fordor, Uni Wuppertal, Germany, 63 Mio core hours)
5. Ab initio Simulations of Turbulence in Fusion Plasmas
(F. Jenko, MPI-IPP, Germany, 50 Mio core hours)

Tier-0 Early Access Projects (2/2)

6. Providing fundamental laws for weather and climate models
(H. Jonker, Uni Delft, NL, 35 Mio core hours)
7. Plasmoid Dynamics in Magnetic Reconnection
(N. Loureiro, Inst. Superior Técnico, Port., 20 Mio core hours)
8. A dislocation dynamics study of dislocation cell formation and interaction between a low angle grain boundary and an in-coming dislocation
(D. Raabe, MPI Eisenforschung D'dorf, Germany, 15.6 Mio core hours)
9. Type Ia supernovae from Chandrasekhar-mass white dwarf explosions
(F. Röpke, MPI Garching, Germany, 23.6 Mio core hours)
10. QCD Simulations for Flavor Physics in the Standard Model and Beyond
(S. Simula, INFN, Italy, 35 Mio core hours)

<http://www.prace-project.eu/hpc-access/page-11/>

PRACE Regular Calls: Reviews

- **1st Regular Call**
 - Analogous to Early Acces Call
 - New extended Priorization Panel (composed by bootstrap group, BoD approval)
 - Start of provision 1.12.2010
- **2nd Regular Call**
 - Council approves SSC on October 5
 - SSC proposes Access Committee
 - Council aprooves AC
 - AC establishes Priorization Panel
 - Provision starts on 1.5.2011

Accessing the PRACE RI

Access Model

- Based on peer-review: “the best systems for the best science”
- Three types of resource allocations
 - Test / evaluation access
 - Project access – for a specific project, grant period ~ 1 year
 - Programme access – resources managed by a community
- Free-of-charge

Funding

- Mainly national funding through partner countries
- European contribution
- Access model has to respect national interests (ROI)



PARTNERSHIP
FOR ADVANCED COMPUTING
IN EUROPE



Access for the systems

<http://www.prace-project.eu/hpc-access>



PARTNERSHIP
FOR ADVANCED COMPUTING
IN EUROPE



PRACE

FIRST PROJECT RESULTS

Providing fundamental laws for weather and climate models

Objective: Determine the growth-rate law of turbulent atmospheric boundary layers under the influence of wind shear. Such a law plays a vital role in weather and climate models.

Expected results: From simulations of developing boundary layers for different wind speeds and atmospheric stability conditions, a generic growth-rate law will be determined.

Resources granted: 35 million core hours on BG/P

Project duration: August 2010 – December 2010

Principal Investigator: prof dr Harmen Jonker, H.J.J.Jonker@tudelft.nl, TU Delft, Netherlands

Met Office Unified Model Scalability

Objective: To compare performance of the Met Office Unified Model on IBM Power 6 and an Intel cluster

Achieved results: IBM Power 6 was up to 15% quicker up to 512 cores but the Intel cluster was up to 18% quicker on higher core counts due almost entirely to better OpenMP performance on this architecture.

Resources granted: 20,000 core hours on Juropa cluster

Project duration: June – August 2010

Principal Investigator: Paul Selwood, UK Met Office,

<http://www.metoffice.gov.uk>

CEDRE: MULTI-PHYSICS PLATE-FORM FOR ENERGETICS AND PROPULSION ON GENERAL UNSTRUCTURED GRIDS

Scope of application :

Aerodynamics, aerothermal coupling, combustion, propulsion, aeroacoustics for aero-engines, missiles, launchers, ramjet engines, etc. A software for industrial applications and research.

Objective: [Code porting for identify bottleneck's points](#)

Results: Test of compiler options (35 executables generated), test of tools (HPM, mpi trace, scalasca, ...), routines optimization (6 routines for CPU, 3 for memory), test of environment 's variables (DCMF_EAGER, BGLMPIO_COMM,), great stability of the machine, good reproducibility of results of measure, good scalability of the code, but in the future :

- Above 8192 cores necessary to adapt the code (memory size : array function of number of core **2, Replace MPI_Allgather by MPI_AlltoAll).
- Adapt the pre processor for treat 1 Billion's cells : in multi-domains approach problem of memory and time for split one mesh in a great number of sub-meshs with a sequential pre-processor.

Resources granted: 1000000 core hours on BG/P

Project duration: 3 months

Principal Investigator: Refloch Alain, ONERA (the *French Aerospace Lab*)

(refloch@onera.fr, www.onera.fr, www.cedre.onera.fr)

Quantum Chromo Dynamics

Objective: Determination of the equation of state of QCD
- including the dynamics of the charm quark

Expected results: Continuum extrapolated equation of state (EOS) of QCD; charm effects contributing to EOS; cross-check of available EOS results

Resources granted: 63 000 000 core-hours

Project duration: 08.2010 – 11.2010

Principal Investigator: Zoltán Fodor, Bergische Universität Wuppertal, Wuppertal, Germany

fodor@physik.uni-wuppertal.de

Simulations of Turbulence in Fusion Plasmas

Objective: A better understanding and control of plasma turbulence – a key physics problem on the way to efficient fusion power plants

Expected results:

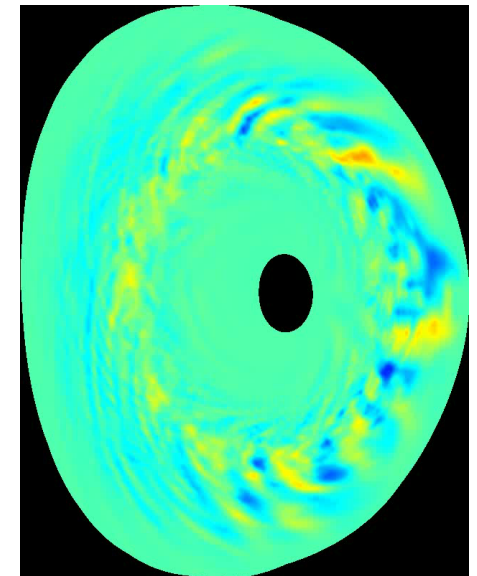
- Temperature and density profile predictions by coupling the premier gyrokinetic plasma turbulence code GENE with a transport solver
- Full-torus GENE simulations of “Internal Transport Barriers”

Resources granted: 50,000,000 core hours

Project duration: 1st August – 30th November

Principal Investigator: Prof. Frank Jenko, Max-Planck-Institute for Plasma Physics at Garching, Germany

More info: <http://gene.rzg.mpg.de>



Full-torus gyrokinetic plasma turbulence simulation with GENE (TCV tokamak, Lausanne)

Excess proton at water/hydrophobic interfaces: An ab initio Molecular Dynamics study

Objective: Recently, experimental studies have led to the suggestion that protons may be located in the close proximity of water/hydrophobic liquid surfaces [1]. Providing the physical basis of this phenomenon may enhance our understanding of a variety of key biological processes, including protein folding, protein/protein interactions and drug/target binding.

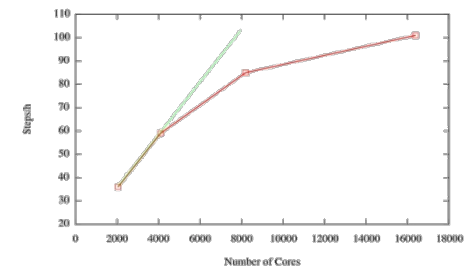
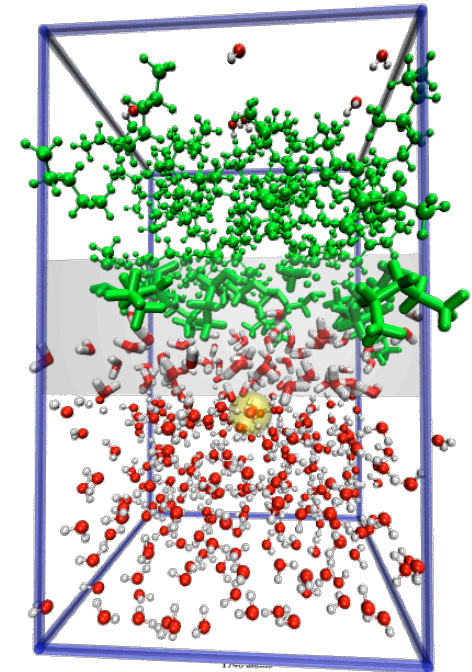
Expected results: We will predict the structure and the energetics of an excess proton at the interface between water and an hydrophobic liquid (n-decane) using ab initio molecular dynamics (system size ~1800 atoms). The free energy profile of the proton from bulk water to the surface will be calculated using the metadynamics method.

Resources granted: 40.5 million core hours on BG/P

Project duration: 1-10-2010 – 31-3-2011

Principal Investigator: Prof. Paolo Carloni,

German Research School for Simulation Sciences GmbH, Forschungszentrum Juelich and RWTH Aachen University



Scaling performance of CPMD for the investigated system on BG/P (red). Ideal scaling (green).

[1] Peter Pohl, personal communication.



PARTNERSHIP
FOR ADVANCED COMPUTING
IN EUROPE



PRACE

PEER REVIEW

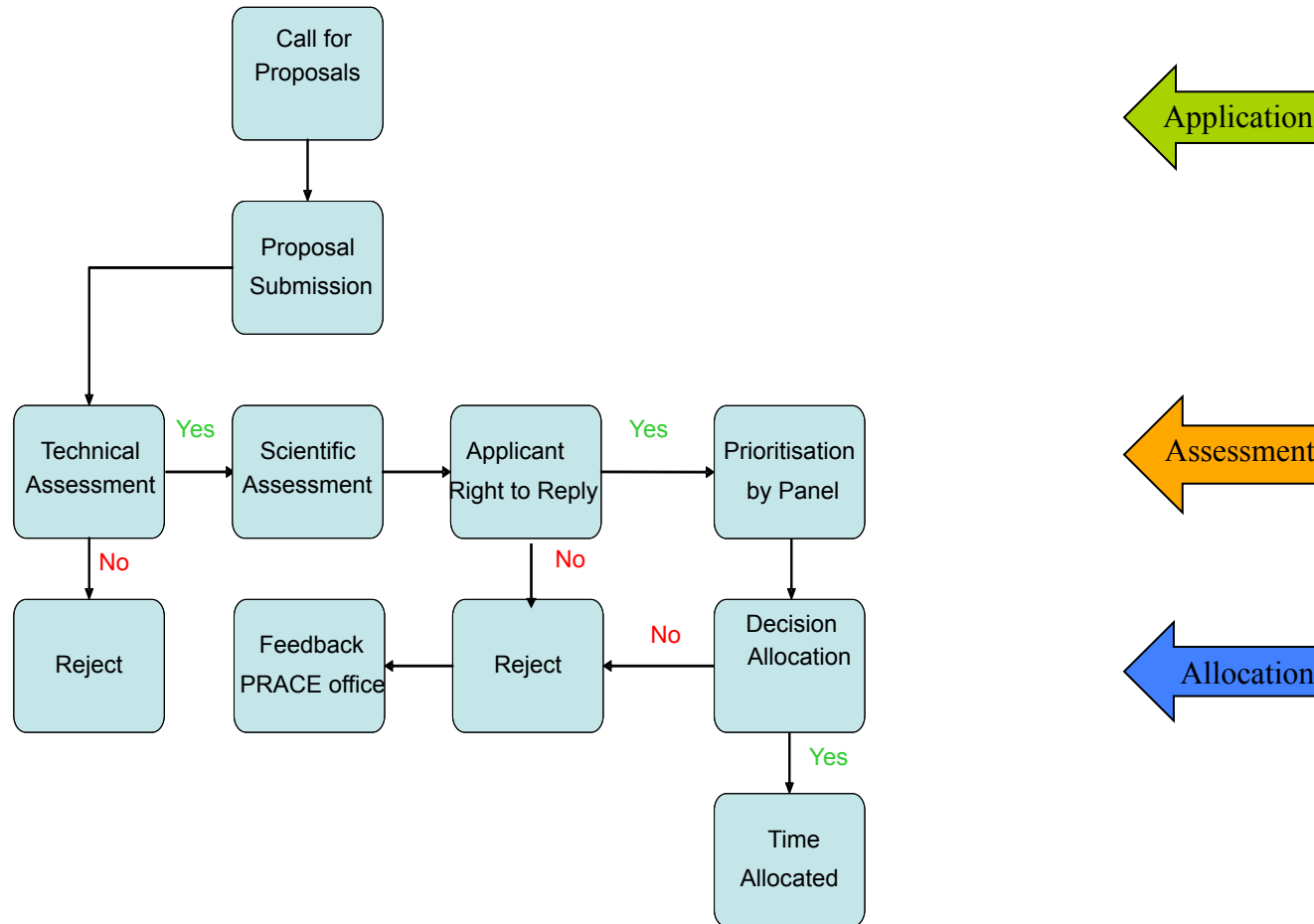
PRINCIPLES

- Transparency
- Expert assessment
- Confidentiality
- Right to reply
- Prioritisation
- Managing interests
- No parallel assessment
- Ensure fairness to the science proposed

Types of Access

- Preparatory access
 - only technical peer review
- Project access
 - both technical and scientific peer review
- Programme access
 - both technical and scientific peer review

Peer review process



Council's Role

- Council will be informed on resource distribution
- In case of significant imbalance between total allocation of resources made to particular member in comparison with the contributions of such members
- → Council will ensure a fair distribution of the Infrastructure's resources

Procedure

- Technical peer review (system and code suitability) by hosting centre representatives
- Scientific peer review by 3 external reviewers
- Applicants have the right to comment on the reviewers remarks; these remarks are sent together with the reviewers comments to the (priorization) panel
- Applicants have the right to appeal to a decision of the Council



PARTNERSHIP
FOR ADVANCED COMPUTING
IN EUROPE



PRACE

DEVELOPMENT PROJECTS

Preparatory Project

- 16 Partners (14 countries), funding 10 Million €
- Coordination: FZJ/JSC
- 1.1.2008 – 30.6.2010, successfully finished
- Review October 1st in Brussels

PRACE All-Hands meeting February 2009

PARTNERSHIP
FOR ADVANCED COMPUTING
IN EUROPE



Preparatory Phase Project Achievements

- The project was indispensable for creating the RI !
- Legal, administrative, finance → see previous slides
- Technical / Scientific
 - Definition of operation processes and user environment
 - Creation of a representative benchmark suite
 - Tier-0 enabling of 20+ important applications
 - Definition of a procurement strategy and process toolbox, synthesising surveys, analysis and technical results
 - Prototype assessment, benchmarking
 - User and technology surveys
 - Site requirements
 - Market surveys, foreseen procurements elsewhere
 - Creation of STRATOS

The First Implementation Phase Project

- First Implementation Phase Project started
 - Budget: 28.5 Mio € (20 Mio € EC funding)
 - Duration: July 2010 – June 2012
- Consortium: all 20 Partners of the AISBL
- 2 more Implementation Phase Projects envisaged
 - 20 Mio € EC funding each
 - Major Challenges:
Tier-1, Industry involvement, Application scaling with communities
- Total EC funding for PRACE
 - up to 70 Mio € in FP7 for preparation and implementation
 - 25 Mio € in open calls for Exascale projects
 - Co-funding of the Infrastructure in FP8 would further strengthen the European integration

First Implementation Phase Project

- User & Community support through application enabling
 - > 40% of the total workforce in the project is here!
 - Support can be requested along with proposals for Preparatory Access to the Tier-0 systems
- Deployment and operation of the Technical Infrastructure
- Collaboration with Communities and other Research Infrastructures
- Development of a model for cross-national Tier-1 access
 - This activity will be extended in the future implementation phase projects
- Cooperation with vendors for future HPC technologies
 - ~20% of the total workforce + 5 Million € for prototypes (50% EC-funded)
- Further development of the legal, organisational and financial framework
- Continuation and further extension of the very successful training programme started in the Preparatory Phase project

PRACE Implementation Phase Work Packages

- WP1 Management
- WP2 Evolution of the Research Infrastructure
- WP3 Dissemination and training
- WP4 HPC Ecosystem Relations
- WP5 Industrial User Relations
- WP6 Technical Operation and Evolution of the Distributed Infrastructure
- WP7 Enabling Petascale Applications: Efficient Use of Tier-0 Systems
- WP8 Support for the procurement and commissioning of HPC services
- WP9 Future Technologies

The growing PRACE family

PARTNERSHIP
FOR ADVANCED COMPUTING
IN EUROPE



PRACE-1IP Kick-off meeting in Garching

Second Implementation Phase Project

- Schedule: mid 2011 – mid 2013
- Foreseen budget: 38 Million € / 20 Millio € EC contribution
- Main objectives
 - Integration of Tier-1 services (DEISA-type)
 - Enter close collaborations with scientific and industrial communities to scale important codes for Tier-0 and Tier-1
 - Continue and extend the started programmes for
 - Technology assessment
 - Procurement guidance
 - Education and Training

Towards Exascale

- Europe needs to ...
 - invest more and with a long-term vision and commitment
 - build on its proven strengths in software and hardware, e.g. energy-efficient components and devices
 - set ambitious goals:
strive for global leadership or end in the second league
- PRACE is actively participating
 - Through STRATOS, a member of the EESI
 - Through PRACE partners in the IESI
 - Consortia involving PRACE partners and technology providers expected for the current FP7 Exascale call (24+1 Million €)
 - PRACE is ready to provide its competence and guidance
 - Development of future technologies needs an element of competition



PRACE

The Partnership for Advance Computing in Europe
is *the* European HPC Research Infrastructure

- PRACE enables world-class science through large scale simulations
- PRACE provides HPC services on leading edge capability systems on a diverse set of architectures
- PRACE operates up to six Tier-0 systems as a single entity including user and application support
- PRACE offers its resources through a single pan-European peer review process
- PRACE is providing services since August 2010
- The first Tier-0 system is the fastest Supercomputer in Europe

PARTNERSHIP
FOR ADVANCED COMPUTING
IN EUROPE



Thank you on behalf of the European Heavy Computing
Community!

