PARTNERSHIP FOR ADVANCED COMPUTING IN EUROPE

PRACE – Europe on the Road to Exascale Computing Kimmo Koski, August 31st 2010 PDC 20th Anniversary and SNIC Interaction









Topics

- Motivation for European HPC
- PRACE Short history
- Current PRACE status
- PRACE future plans
- Nordic Impact, Challenges and Opportunities
- Conclusions



Motivation for European HPC



Computational science infrastructure



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HET: The Scientific Case

- Weather, Climatology, Earth Science ٠
 - 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 ٠
 - systems, structures which span a large range of different length and time scale
 - quantum field theories like QCD, ITER
- Material Science, Chemistry, Nanoscience ٠
 - understanding complex materials, complex chemistry, nanosc
 - the determination of electronic and transport properties
- Life Science ٠
 - 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

















Europe needs independent access to Peta- and Exascale HPC-Systems for all of its member states

- We need to enable European scientists to collaborate
- Building the European Research Area:
 - We have to provide access to Tier-0-HPC power on a European level
 - Exchange of national Tier-1-HPC power should be supported on a European level
 - Make different HPC-architectures available for all users in Europe!



Europe needs Access to Peta- and Exascale HPC Systems for all Member States

- There is no sustained HPC service beyond the national scale (except topical centres like ECMWF)
- Creation of an HPC Infrastructure on a European level:
 - No single member state has the funding and overall competence to compete on an international level
 - Initially mainly national funding, complemented by an EC contribution
 - Increased European contribution e.g. through FP8
- Europe needs the skills for peta- and exascale computing of all member states and not only of those which can afford to build up its own peta- and exascale installation for national use.



The ESFRI Vision for a European HPC service



- Scientific and industrial user communities
- The European HPC hard- and software industry

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HPC-Service is an item on the ESFRI Roadmap



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

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

A European HPC service – impact foreseen:

- strategic competitiveness
- attractiveness for researchers
- supporting industrial development



PRACE unites the European HPC power to a single





A bit of history



PRACE History and first steps





| | HPCEUR | | | HET | PRACE Mol | PRACE Preparatory | |
|---|--------|------|------|-----|-----------|-------------------|---|
| | | | 2006 | | | | ╊ |
| • | 2004 | 2005 | | | 2007 | 2008 | • |

EU-Grant: INFSO-RI-211528, 10 Mio.





April, 23rd 2010 creation of the legal entity (AISBL) PRACE with seat location in Brussels, Belgium

16 founding members (today: 19 European members, +1 observer, +1 applicant)

400 Mio. € committments of 4 hosting members for the infrastructure





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Committment for hosting member provided by:

France, Germany Italy Spain





PRACE Inauguration / Barcelona June 9, 2010







PRACE Preparatory Phase Project: 01/08 – 06/10

- Perform all preparatory work for the pan-European HPC Research Infrastructure as envisioned by ESFRI
 - Legal framework
 - Governance structure
 - Sustainable funding
 - Operations
 - Ecosystem integration
 - Technical preparation
- Overall goal



Grant: INFSO-RI-211528

- Have all elements in place to begin with the implementation of the Research Infrastructure in 2010
- EC-Review in October 2009:
 - PRACE is making satisfactory progress in all areas
 - PRACE is eligible for Implementation Phase funding



Achieved so far...

In 2008/2009, PRACE has ...

- Defined the legal and organisational structure of the RI
- Secured partner funding for the next 5 years
- Performed all technical preparations for the RI implementation



PRACE is ready to start providing services to the European Scientific Communities



Status today and Next steps

Partnership For Advanced Computing IN Europe

PRACE Status and Current Activities

 The Preparatory Phase Project ended in June 2010 after 2 ¹/₂ years of successful work



- Contracts for legal entity prepared

Grant: INFSO-RI-211528

CAPACITIES

- 400 Mio € funding for the next 5 years secured from France, Germany, Italy, Spain
- Decisions about additional 100 Mio € from The Netherlands open (delay is due to national elections)
- Architectures for Tier-0 systems identified
- Created a representative benchmark suite
- Established STRATOS, a collaboration platform with industry
- Set up an extensive Training programme
- IBM Blue Gene/P in Gauss@Jülich selected as first Tier-0 system
- The first Implementation Phase Project will start in July
- The Research Infrastructure becomes operable



The Implementation Phase Project(s)

- Contract Negotiations with the EC about the first Implementation Phase Project completed
 - Budget: 28.5 Mio € (20 Mio € EC funding)
 - Duration: July 2010 June 2012
- Consortium: all 20 Partners of the Initiative
- 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
 - 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



Governance of the Association

- Council
 - General Assembly of the Association: 20 members
 - Chair: A. Bachem (Juelich), Vice-Chair: K. Koski (CSC)
- Board of Directors
 - Acting Board until Full-time Director is appointed
 - S. Girona (BSC, Chair), S. Bernardi (CINECA), Th. Eickermann (Juelich),
 - L. Johnsson (KTH), P. Michielse (NCF), Jean-Philippe Nominé (CEA)





Governance of the Association

- Scientific Steering Committee
 - "SSC Establishment Workshop" in Jülich on June 14
 - planned by 6 independent scientists chaired by Richard Kenway (UoEdinburgh)
 - Participation of 33 scientists from all over Europe
 - Workshop proposed 21 SSC members for approval by Council on October 5





PRACE Tier-0 Access

- Europe-wide calls for proposals for access to the first Tier-0 System (IBM BlueGene/P in GCS@Juelich)
- Early Access Call in May 2010
 - 68 proposals asked for 1870 Million Core hours
 - 10 projects granted with 328 Million Core hours
 - 2 Allocation periods: August November, December March
- 1st Regular Call closed on August 15
 - 58 proposals received
 - 360 Million Core hours available for a 12 months allocation period starting November 2010
- 6 monthly regular calls scheduled



Funding Principles for the Association

- Funding of Tier-0 resources
 - Each hosting member commits to provide Tier-0 resources worth 100 Mio. € based on TCO in the next 5 years
 - National procurements of Tier-0 systems follow an agreed procurement plan
 - Meeting requirements of the user communities with previously identified technology options
- Funding of the HQ operation
 - All partners provide equal cash contributions
- User support, training and other tasks
 - Provided in kind by members on as-needed basis
 - Supported by the planned Implementation Phase project where eligible



Governance Considerations (1/2)

- PRACE is not very different from "non-e" distributed Infrastructures
 - A limited number of Tier-0 centres providing the core services
 - There are many successful examples in Europe for such RIs; their experience is leveraged (e.g. EMBL)
- Governance shall support the mission to enable the best science on the best HPC systems
 - Science Communities must drive the Peer Review process and should provide advice to the RI in terms of scientific policy including procurements of HPC systems
 - ➔ Scientific Steering Committee
 - A coherent and coordinated procurement plan will ensure complementarity of architectures and systems that match the needs of the science communities



Governance Considerations (2/2)

Balance interests of stakeholders

- 4 Hosting Members (hosting one of the Tier-0 systems) commit to 100 Mio € over the next 5 years each
- All members contribute cash and in kind services, e.g. training and software support
- Voting rights in the Council have to reflect this
 - In matters concerned with providing and using of funds: voting ~ contributions
 - In scientific matters: double majority of contributions and countries
- EC contributes up to 10% of the budget for the implementation phase (FP7)

Sustainability of funding

- Member states need to see ROI and have appropriate influence on RI
- Long-term national support will mainly depend on user satisfaction
- Member states have to give long-term commitments (above the initial 5 years)



PRACE Next steps

- The PRACE Research Infrastructure
 - is established as a legal entity on April, 23rd 2010 in Brussels as an international not-for-profit association under Belgian law: Association Internationale sans but Lucratif (AISBL)
 - will start providing Tier-0 Services in August 2010
- Focus of the Implementation Phase Project
 - User & Community support through application enabling
 - Deployment and operation of the Technical Infrastructure
 - Collaboration with Communities and other Research Infrastructures
 - Cooperation with vendors for future HPC technologies
 - Further development of the legal, organisational and financial framework



Nordic impact



Topics to consider

- Installing of Tier-0 or accessing it?
 - Number of scientists with ability to use +100000 cores in parallel?
 - Investment vs. benefits?
 - Possibilities to get access, if not in own control?
 - Competitive position if resources not available (with short notice)?
- Position of Nordic countries
 - Potential for 'virtual Tier-0', but where to place it and is it really needed?
 - Joining forces for applications, training, competence building etc.
 - Raise of the eco-efficient ICT: all the datacenters to the cool climate?



Some challenges with PRACE

- What is the cost to use Tier-0?
 - 'Donation only' is not sustainable
 - Paying is more difficult than in-kind
 - What kind of in-kind is accepted?
 - Will the 'market' work?
- Integration of different Tiers
 - How to link Tier0 Tier1?
 - What are the links to Tier2?
 - Users could not care less in what Tier they are working in case they get their work done
- Relations between scientists (users) and PRACE centers
 - Need to speak the same language



More issues



- 1. How to guarantee access to the top for selected groups?
- 2. How to ensure there are competent users which can use the high end resources?
- 3. How to involve all countries who can contribute?
- 4. How to develop competence in home ground?
- 5. How to boost collaboration between research and e-infrastructure providers?
- 6. What are the principles of resource exchange (in-kind)?



How to benefit from the opportunity in Nordics



- National infrastructure close enough to the top
 - Stepping stone for code development
 - Ability to use high end (hard to jump from laptop to 100000 cores)
 - Potential for resource exchange Tier1-Tier2
- Focus on application development, balanced einfrastructure and competence development
- Nordic collaboration



Some conclusions

- PRACE is a unique opportunity, but it needs still a lot of work
- Considerable development has been achieved since the first HPCEUR project back in 2004
 - Working with the full HPC Ecosystem instead of just peak performance hardware
- Nordic countries should be active, this way we can impact
- There was not much Exascale in this presentation, but we have not either seen much of petascale yet ...