International HPC – Building a Bigger Pyramid

Richard Kenway

Chairman of the PRACE Scientific Steering Committee

CAPACITIES

e-infrastructure

the case for HPC … is made

PRACE – The Scientific Case for HPC in Europe 2012 - 2020

*"Molecular simulation is a key tool for computer-aided drug design … **Biomedical Simulation** will reduce costs, time to market and animal experimentation. In the medium to long term, simulation will have a major impact on public health, providing insights into the cause of diseases and allowing the development of new diagnostic tools and treatments. It is expected that understanding the basic mechanisms of cognition, memory, perception etc. will allow the development of completely new forms of energy efficient computation and robotics. The potential long-term social and economic impact is immense."*

*"**Computational materials science, chemistry and nanoscience** is concerned with the complex interplay of the myriads of atoms in a solid or a liquid, thereby producing a continuous stream of new and unexpected phenomena and forms of matter, characterised by an extreme range of length, time, energy, entropy and entanglement scales. The target of this science is to design materials ranging from level of a single atom up to the macroscopic scale, and unravel phenomena and design processes from electronic reaction times in the femtosecond range up to geological periods."*

*"… whilst there is great confidence in the fact that **climate change** is happening, there remain uncertainties … Increasing the capability and comprehensiveness of 'whole Earth system' models that represent in ever-increasing realism and detail, scenarios for our future climate is the only way to reduce these latter uncertainties."*

Communication from the Commission to the European Parliament

"High-Performance Computing: Europe's place in a Global Race", Brussels, 15.2.2012

"The race for leadership in HPC systems is driven both by the need to address societal and scientific grand challenges more effectively … and by the needs of industry to innovate in products and services."

"Access to rapid simulations carried out by ever-improving super computers can be the difference between life and death; between new jobs and profits or bankruptcy."

*"The **automotive industry** is actively pursuing important goals that need exaflop computing capability or greater. Examples include (i) vehicles that will operate for 250,000 kilometres on average without the need for repair; … and (ii) Insurance companies require full-body crash analysis that includes simulation of soft tissue damage"*

*"The impact of **computer simulation in aircraft design** has been significant … Boeing, for example, exploited HPC in order to reduce drastically the number of real prototypes from 77 physical prototype wings for the 757 aircraft, to only 11 prototype wings for the 787 "Dreamliner" plane. HPC usage saved the company billions of dollars"*

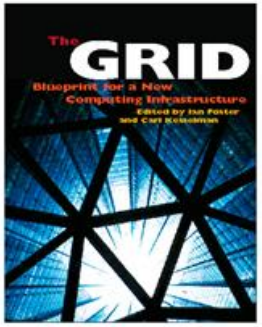
*In **Astrophysics** determination of the nature of dark energy and dark matter requires a detailed comparison of predictions from large classes of cosmological models with data from the new satellites and ground based detectors which will be deployed until 2020.*
*In **high-energy physics**, one of the tasks is to explore many possible extensions of the Standard Model to such a degree, that even minute deviations between experimental data and Standard Model predictions can serve as smoking guns for a specific realization of New Physics.*
*In **plasma physics**, one of the tasks is to understand the physics observed at ITER at such a high level that substantially more efficient fusion reactors could be reliably designed based on theoretical simulations which explore a large range of options."*

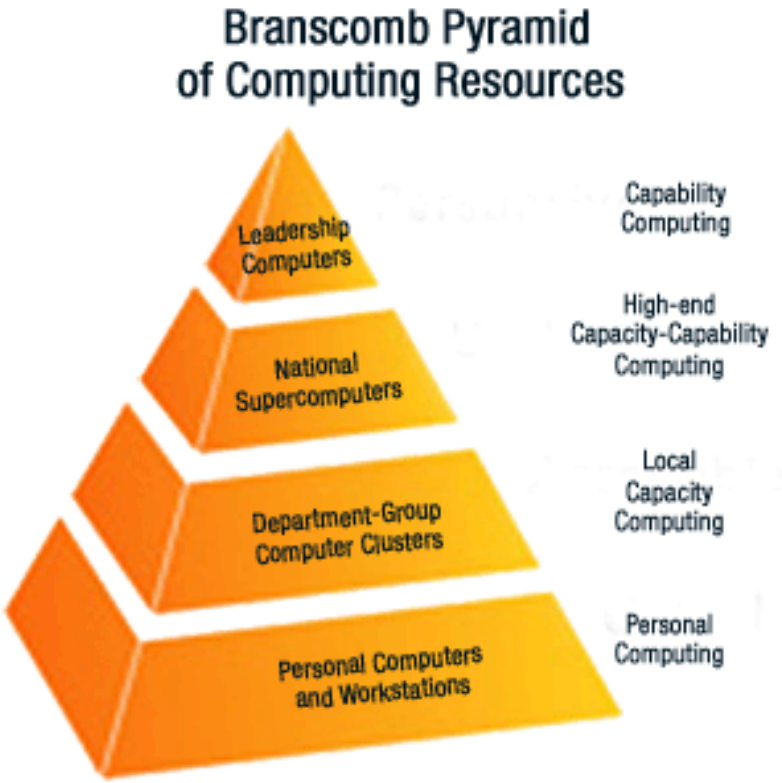
… but there are many challenges

- new software and algorithms
  - scaling to >100 million cores
  - 1/100 memory bandwidth
  - fault tolerance
  - validation and verification
- data deluge
  - sensors everywhere
  - new applications eg without theory
- 100x more power efficient technology
  - or a better value proposition

co-design
+
new skills

the research computing ecosystem





organisation at an international level

PRACE past

- Mar 2004: Hugh Pilcher-Clayton and Richard Kenway attend German Science Council

ERA – NET
High Performance Computing Proposal

Aim: without prejudicing the national programmes for high performance computing, to create a European high performance computing service by 2009 with a capability that matches that of the current world leaders, the USA and Japan.

Partners: UK, Germany, France, and others

RESEARCH COUNCILS UK

- Apr 2006: Scientific Case for a European Supercomputing Infrastructure

German HSC 18.3.04

WR WISSENSCHAFTSRAT

The conviction that isolated European countries would not be able to provide their researchers and engineers with resources competitive on the world stage lies at the heart of the HPCEUR initiative.

- Jan 2007: HPC in Europe Task Force (HET)

HET recommends establishment of a small number of European HPC facilities to provide extreme computing power – exceeding petaflop capability – for the most demanding computational tasks. In addition, a funding model based on national investments with an additional European share and a possible new collaborative entity governing it is recommended.

PRACE Timeline

HPCEUR | HET | PRACE MoU | PRACE Preparatory

2004 2005 2006 2007 2008

EU-Grant: INFSO-RI-211528, 10 Mio. €

EC: 60 Mio. € + Member States: 60 Mio. € + 400 Mio. € cycles

Phase | PRACE Operation

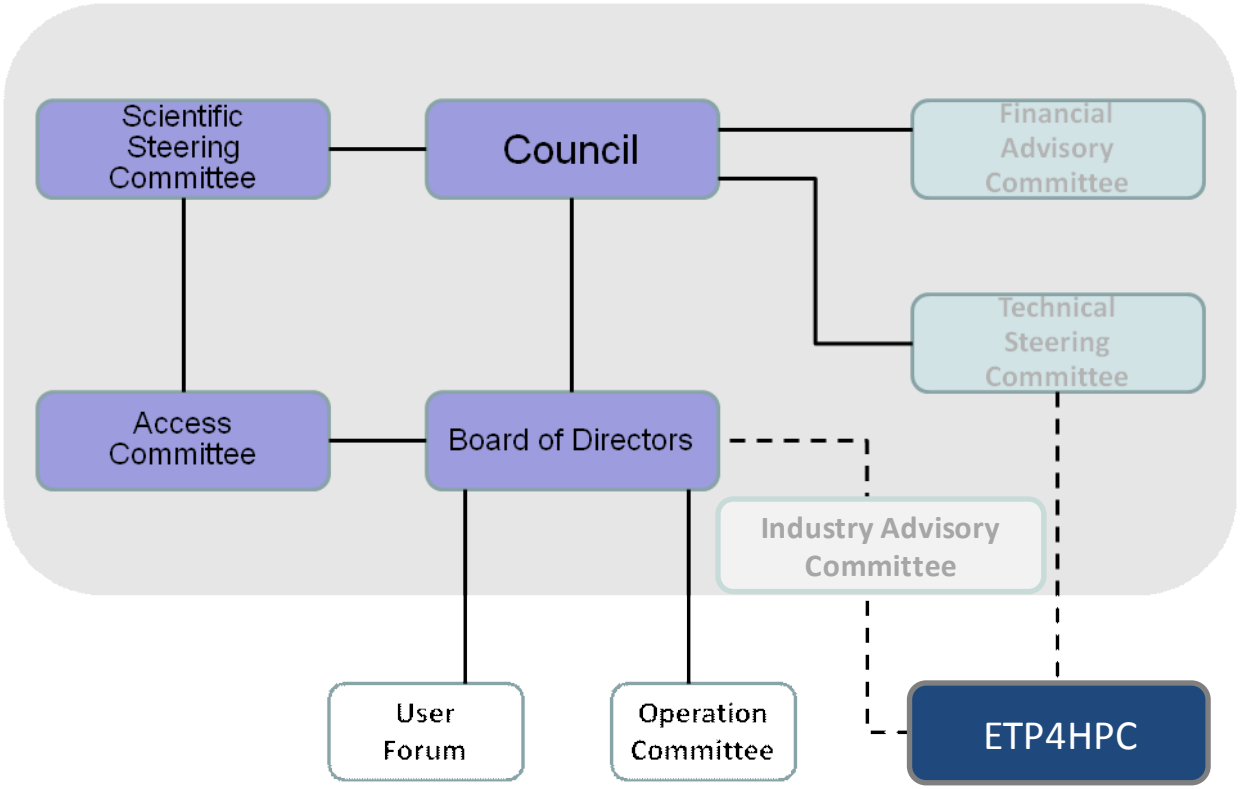
23.4. 2010 | PRACE Implementation Phase (1IP, 2IP, 3IP)

2009 2010 2011 2012 2013

PRACE

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

PRACE present … 2010 - 14

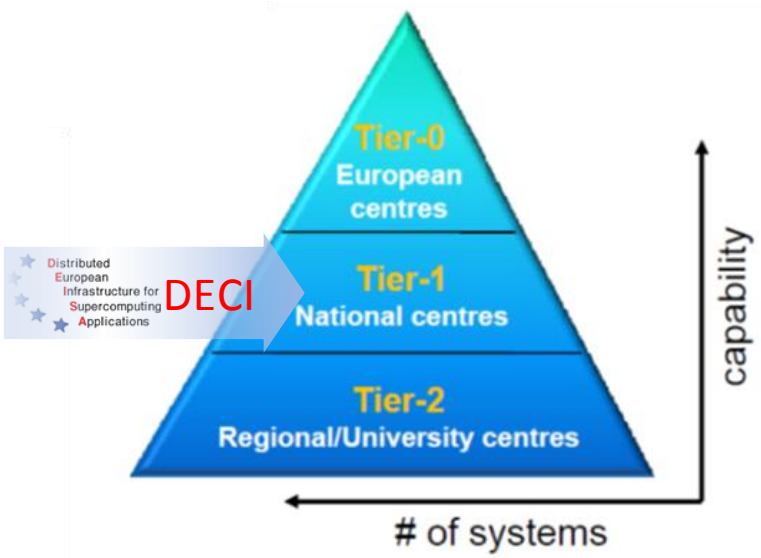


6 PRACE Advanced Training Centres

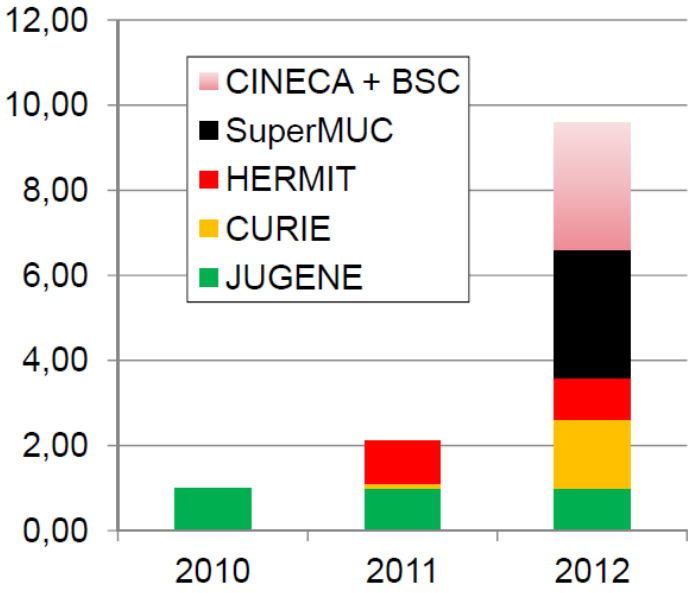
- BSC
- CINECA
- CSC
- EPCC
- GAUSS
- Maison de la Simulation

25 Member States

- Hosting members: France, Germany, Italy, Spain
- 100M€ each in kind



tier-0 capability

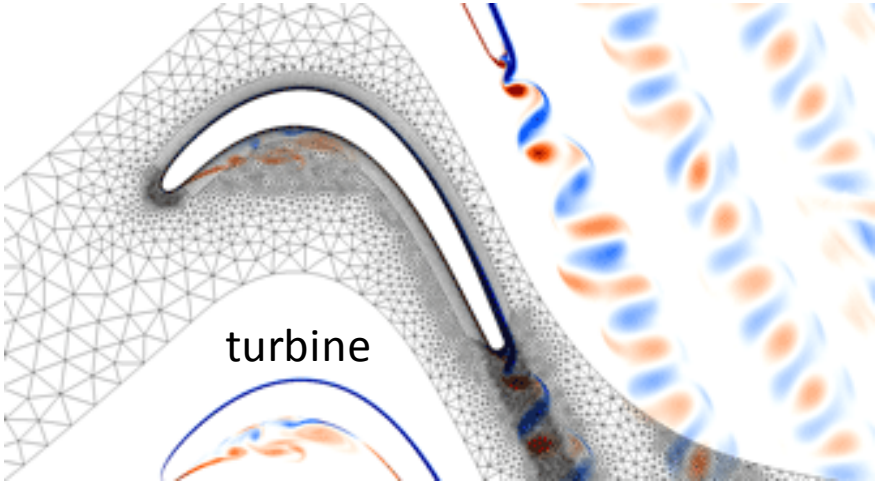


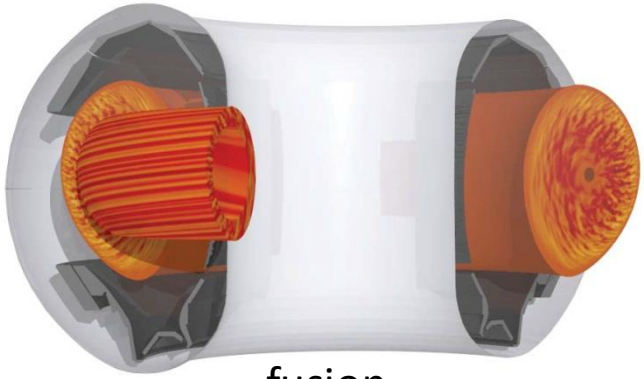
PRACE Scientific Steering Committee

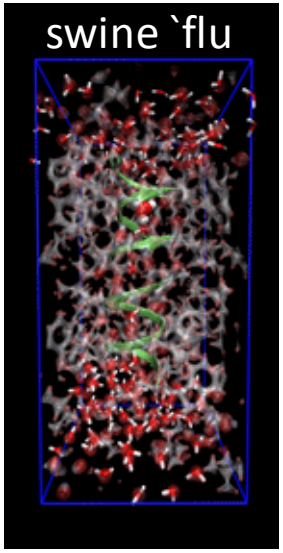
Paolo Carloni (life sciences, Germany)
Giovanni Ciccotti (materials science, Italy)
Christoph Dellago (materials science, Austria)
Sylvie Joussaume (environmental sciences, France)
Richard Kenway (particle physics, UK)
Christian Lang (particle physics, Austria)
Ben Moore (astrophysics, Switzerland)
Antonio Navarra (environmental sciences, Italy)
Risto Nieminen (materials science, Finland)
Modesto Orozco (life sciences, Spain)
Maurizio Ottaviani (plasma physics, France)
Olivier Pironneau (mathematics, France)
Thierry Poinsot (engineering, France)
Simon Portegies Zwart (astrophysics, The Netherlands)
Kenneth Ruud (chemistry, Norway)
Wolfgang Schröder (engineering, Germany)
Christof Schütte (life sciences, Germany)
Luis Serrano (life sciences, Spain)
Luis Silva (plasma physics, Portugal)
Joost VandeVondele (materials science, Switzerland)
Claudio Zannoni (materials science, Italy)

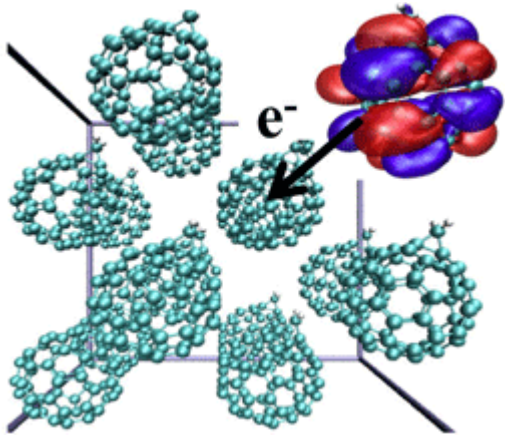
- vision
  - PRACE should support the best computational science in the world
- strategy
  - world-wide competition subject to best-practice peer review
  - projects with the greatest potential for new knowledge that are only possible at tier 0
  - all-or-nothing allocations
- first 2 years
  - 103 major projects
  - 3 billion core hours
- extending to open industry research in Europe
- … and multi-year projects

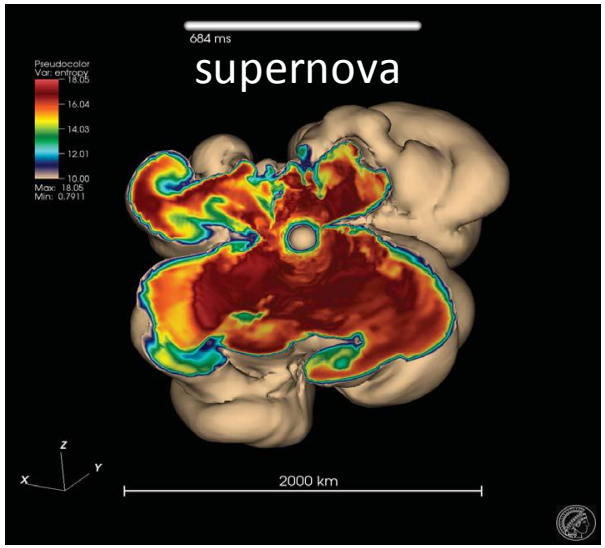
first results











PRACE future … 2015-19

EUROPEAN COMMISSION

Brussels, 15.2.2012
COM(2012) 45 final

COMMUNICATION FROM THE COMMISSION TO THE EUROPEAN PARLIAMENT, THE COUNCIL, THE EUROPEAN ECONOMIC AND SOCIAL COMMITTEE AND THE COMMITTEE OF THE REGIONS

High-Performance Computing: Europe's place in a Global Race

The 2009 investment level of EUR 630 million per year[5] for acquiring high-end HPC resources across Europe is not sufficient to sustain HPC systems and services at a globally competitive level. It would need to double to some EUR 1.2 billion per year to bring Europe back as a major actor in the field of HPC[5]. Consultations with stakeholders have confirmed such an increased investment.

PRACE ensures the wide availability of HPC resources on equal access terms. It has to be further strengthened to acquire the competence to (i) pool national and EU funds, (ii) set the specifications and carry out joint (pre-commercial) procurement for leadership-class systems, (iii) support Member States in their preparation of procurement exercises, (iv) provide research and innovation services to industry, and (v) provide a platform for the exchange of resources and contributions necessary for the operation of high-performance computing infrastructure.

"Our partnership for advanced computing, PRACE, already makes supercomputer capacity available, for industry and academics to simulate and design. Why not make access to those platforms systematic, pervasive, available to every high-tech small company?"
Neelie Kroes, EC Vice-President for the Digital Agenda, 25 September 2012

enhancing economic competitiveness

- EC wishes to strengthen Europe's HPC technology industry
  - support R&D using Pre-Commercial Procurement (PCP)
  - exploit the opportunity for exascale technology development
- complementary roles
  - PRACE as major procurer of HPC technology
  - ETP4HPC setting industry's Strategic Research Agenda

- Member States are invited to carry out joint procurement activities and to use PCP to stimulate the development of advanced HPC systems and services. Each Member State should actively encourage the use of PCP and devote in the order of 10% of its annual HPC procurement budget to it.
- The Commission should contribute to the funding provided collectively by Member States for PCP of R&D on HPC systems services with an EU-level mission and with EU-wide availability.
- HPC e-Infrastructure projects receiving funding from the Commission should be encouraged to use PCP where relevant.
- EU Industry is encouraged to actively engage in advanced HPC and application development efforts in response to PCP.

ETP 4 HPC

European Technology Platform for HPC industry forum
"… to define Europe's research priorities to develop European technology in all the segments of the HPC solution value chain"

- tier-0 access for industry is not enough
  - local support structures (tiers 1 and 2): awareness raising, expertise, sharing best practice
  - ISV code development + licencing changes ("pay per use")
- PRACE actions
  - input user requirements to ETP4HPC
  - explore how PCP can support PRACE mission and co-design (trial project on energy-efficient HPC)
  - establish an Industry Advisory Committee

Hicham Lahlou, Xcelerit, receives the PRACE Award for the Most Innovative Industrial HPC Application in Europe

The Scientific Case for HPC in Europe 2012-2020

1 The need for HPC infrastructure at the European level

The scientific progress that has been achieved using HPC since the "Scientific Case for Advanced Computing in Europe" was published in 2007, the growing range of disciplines that now depend on HPC, and the technical challenges of exascale architectures make a compelling case for continued investment in HPC at the European level.

2 Leadership and management

The development of Europe's HPC infrastructure, its operation and access mechanisms must be driven by the needs of science and industry to conduct world-leading research.

3 A long-term committment to Europe-level HPC

Major experiments depend on HPC for analysis and interpretation of data, including simulation of models to try to match observation to theory, and support research programmes extending over 10-20 year timeframes.

4 Algorithms, software and tools

Most applications targeting Tier-0 machines require some degree of rewriting to expose more parallelism and many face severe strong-scaling challenges

5 Integrated environment for compute and data

Most application areas foresee the need to run long jobs (for months or years) at sustained performances around 100 Pflop/s to generate core data sets and very many shorter jobs (for hours or days) at lower performances for pre- and post-processing, model searches and uncertainty quantification. A major challenge is the end-to-end management of, and fast access to, large and diverse datasets, vertically through the infrastructure hierarchy. Most researchers seek more flexibility

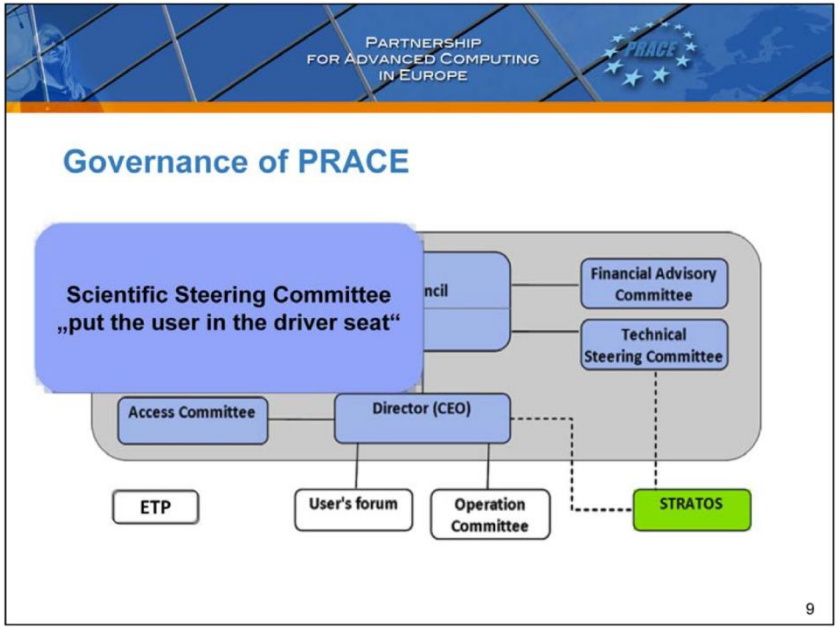
6 People and training

There is grave concern about HPC skills shortages across all research areas and, particularly, in industry.

7 Thematic centres

Organisational structure is needed to support large long-term research programmes, bringing together competences to share expertise. This could take the form of virtual or physical Thematic Centres which might support community codes and data, operate dedicated facilities, focus on co-design, or have a cross-cutting role in the development and support for algorithms, software, or tools. While some existing application areas have self-organised in this way, new areas such as medicine might achieve more rapid impact if encouraged to follow this path. **Thematic Centres should be established to support large long-term research programmes and cross-cutting technologies, to preserve and share expertise, to support training, and to maintain software and data.**

who drives?



Achim Bachem, SC11

e-IRG White Paper 2011

1.4 Recommendations

- Establish a user-community-centric approach in strategic e-Infrastructure governance.

- scientific opportunities and requirements are evolving fast
- many paths lead from here … many are dead ends
- new leadership … users and providers in partnership … co-design + co-lead

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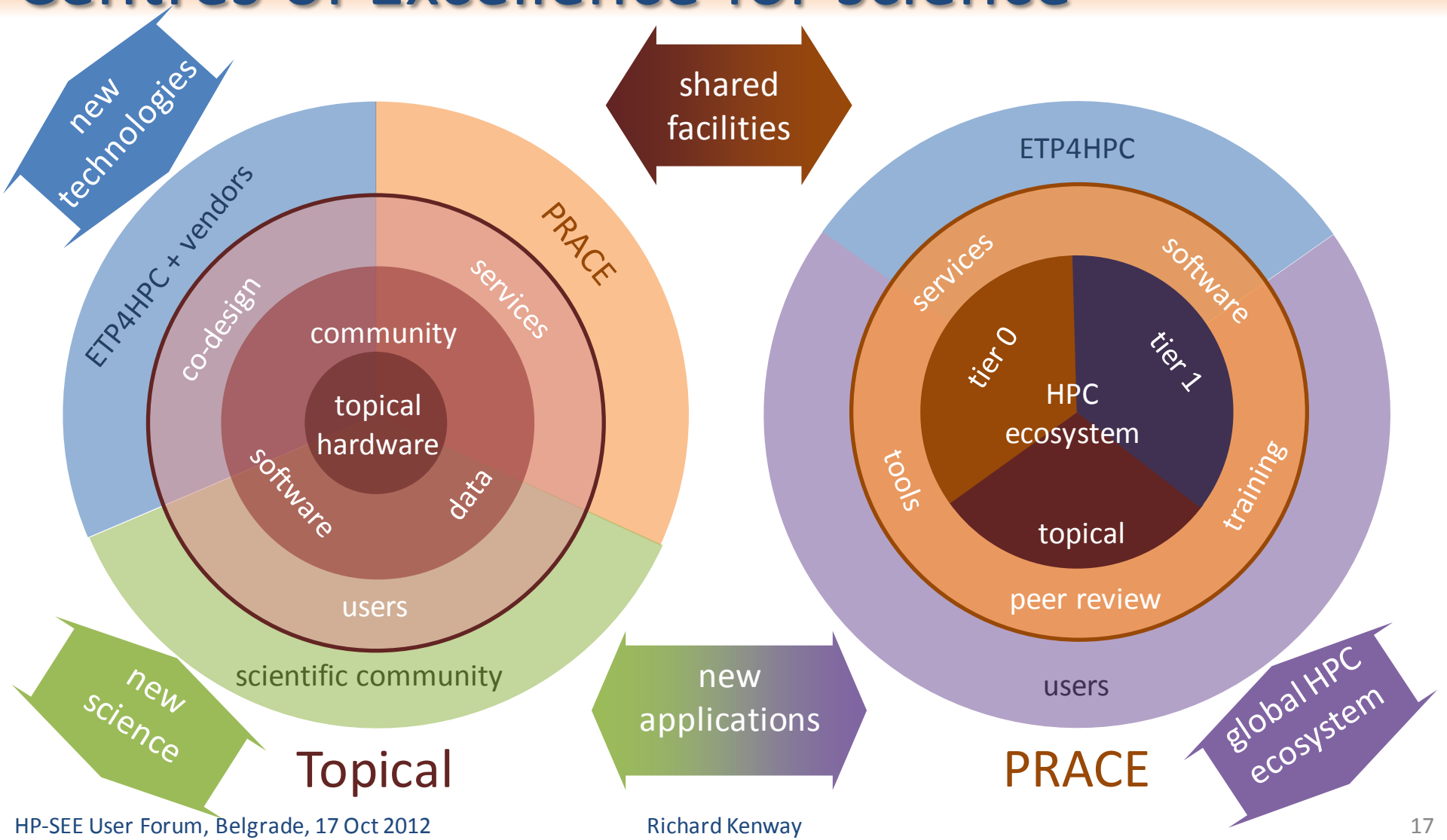
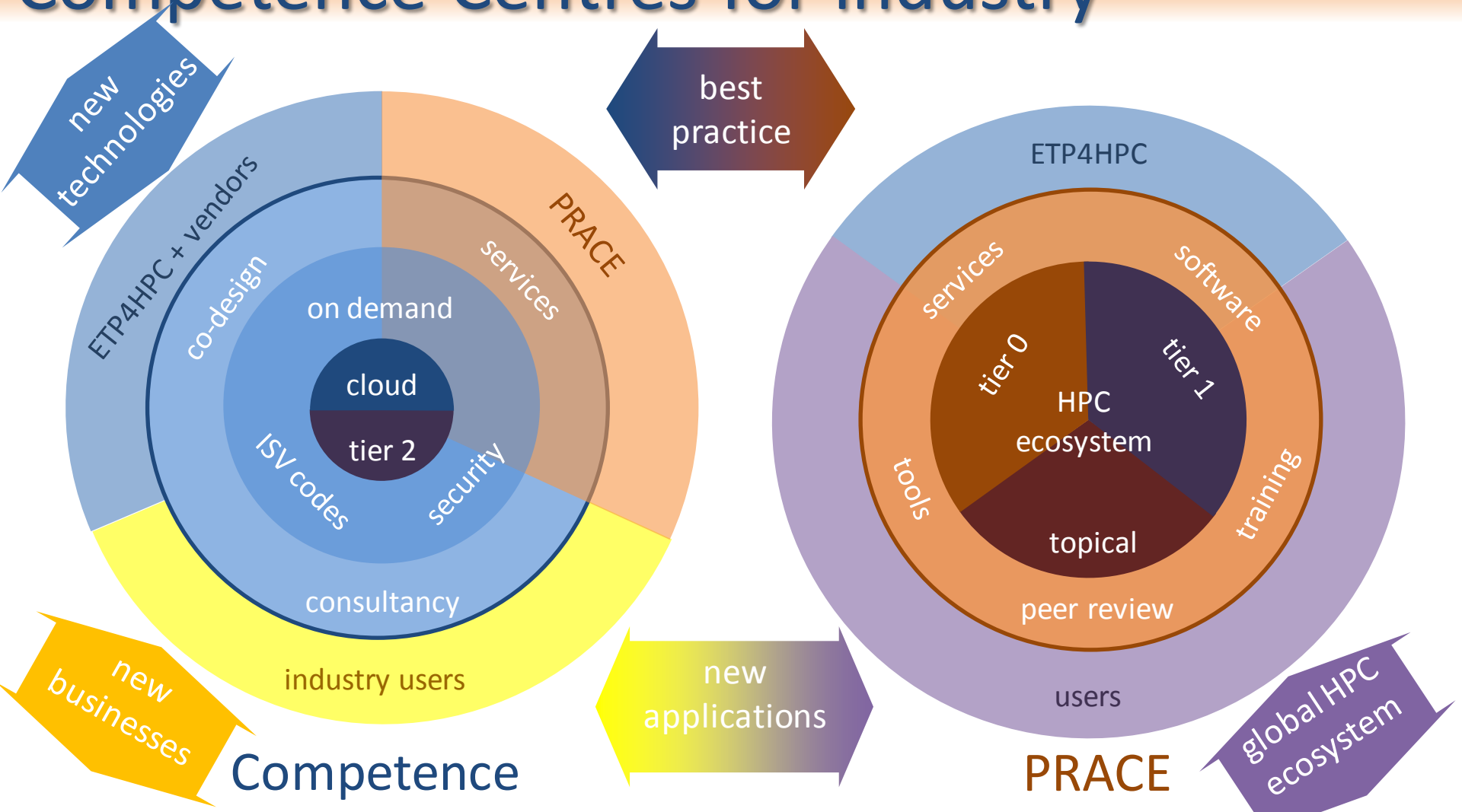
Centres of Excellence for science

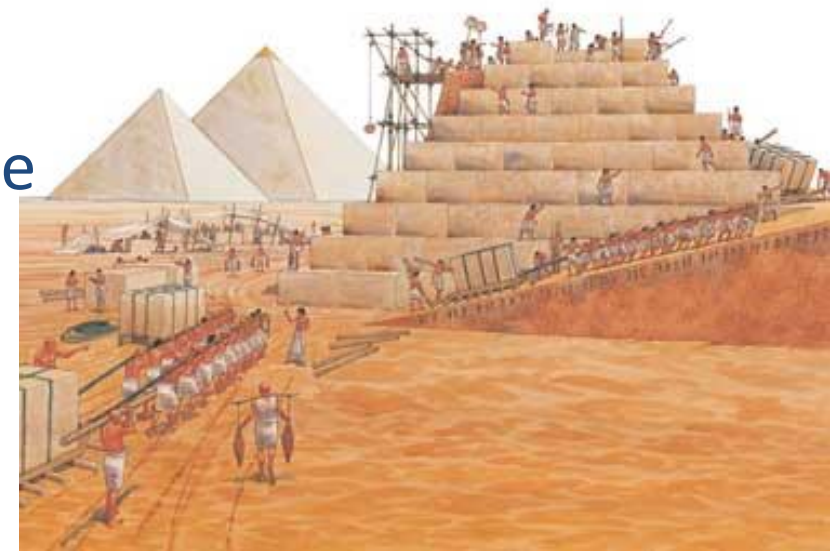


Competence Centres for industry



building a bigger pyramid

- opportunities for international collaboration
  - HPC has joined the ranks of “big science”
  - ambition + costs will drive it towards a global project
- tier-0 facilities open to academics worldwide
  - solely based on excellence
  - best-practice peer review
  - to ensure world-leading research
- Centres of Excellence/Competence
  - globally competitive
  - engaging new industry users
- Interconnect all tiers
  - build a functioning ecosystem



HPC global ecosystem