HPC Centres of Excellence – Business Perspective

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informed through membership of
PRACE Scientific Steering Committee
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Why?

• the growing diversity of application requirements
  – “one size fits all” is not cost effective and can be a barrier to new applications
  – internationalisation of HPC is an opportunity to share costs and expertise
• increased productivity and competitiveness
  – well-maintained and validated community codes and data
  – scale and coherence to match/exceed other big players and meet societal challenges
• interdisciplinarity and innovation
  – bring together computer scientists, mathematicians and domain experts
  – exploit co-design to innovate effectively and keep ahead of the market
• stronger scientific leadership of e-infrastructure development
  – to keep pace with rapid technology advances and growth of applications
  – community ownership of, and engagement in, the infrastructure roadmap
• better skills retention and career structures
  – long-term persistence and scale to support career development
  – coordinated up-to-date training at all levels (according to domain needs)
Specific Needs – PRACE Scientific Case

• **Medicine & Life Sciences**
  – on-demand access to tier-0 capability for medical interventions
  – security for patient data
  – high bandwidth end-to-end data management for complex workflows
  – visualisation and computational steering
  – co-design involving academia and industry

• **Weather, Climate & Solid Earth Sciences**
  – system stability over 3-5 years for bit reproducibility
  – specific commercial architectures spanning tiers 0, 1 and 2 for capability and capacity jobs
  – big data, high bandwidth end-to-end data management, visualisation
  – coordination of community codes, simulations, data

• **Industrial Applications & Engineering Science**
  – consultancy and pilot projects providing an ‘on-ramp’ via tier 2/cloud, particularly for SMEs
  – exascale co-design, particularly for large industry
  – on-demand access and security for codes and data
  – ISV codes

• **Astrophysics, High-Energy Physics & Plasma Physics**
  – dedicated specialised architectures via co-design for low-cost/high performance
  – highly optimised community codes
  – algorithm development
  – 10-20 year timescales to match experiment/observation
Scientific Case Recommendations

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 commitment 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.
Centres of Excellence for Science

Topical
- new technologies
- ETP4HPC + vendors
- co-design
- hardware
- community
- services
- data
- users
- scientific community

PRACE
- shared facilities
- ETP4HPC
- tier 0
- tools
- software
- training
- peer review
- users
- global HPC ecosystem

new applications

HPC CoE Workshop, 18 Oct 12
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Competence Centres for Industry

Competence
- new technologies
- ETP4HPC + vendors
- co-design
- ISV codes
- consultancy
- cloud
- tier 2
- on demand
- security
- services

PRACE
- best practice
- ETP4HPC
- tier 0
- services
- software
- tier 1
- tools
- training
- users
- topical
- peer review
- global HPC ecosystem

New businesses
New applications

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Structure & Governance

• virtual vs physical
  – generally, both, according to function
  – physical location for topical facilities and core staff
  – regional role for CCs
  – virtual structure for some domain-specific staff and users

• science/industry led
  – science/industry sets the direction and objectives
  – users in partnership with providers
  – innovating, globally competitive and ahead of the market

• organising mechanism
  – one overarching body interfacing to EC and member states, or many autonomous centres?
  – minimally, coordination across CoE/CCs and PRACE, eg Coordinating Committee of Centre Directors
  – also ETP4HPC, EGI, EUDAT, GÉANT, ...
CoE Funding and Sustainability 1

- two main funding streams
  - science/exploitation through users
  - infrastructure through PRACE

- PRACE provides baseline funding and services
CoE Funding and Sustainability 2

- two main funding streams
  - science/exploitation though users
  - infrastructure through both CoEs and PRACE

  - autonomous CoEs
CC Funding and Sustainability

• funding
  – EC/government: infrastructure + support for awareness raising, training, expertise sharing, ISV licences, pilot projects → business propositions
  – industry: in-kind effort
  – partnership with a major company?

• sustainability
  – autonomous regional CCs, or an overarching organisation?
  – sustained public funding needed to keep ahead of the market
  – services can provide income, but should migrate to the commercial market