HPC Centres of Excellence Consultation Workshop

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The Communication argues that, in addition to PRACE, "an e-Infrastructure for HPC application software and tools needs to be put in place. This e-infrastructure should further consolidate the EU’s strong position in HPC applications by coordinating and stimulating parallel software code development and scaling, and by ensuring the availability of quality HPC software to users" (p. 9). Therefore, "Centres of Excellence should be established for the application of HPC in scientific or industrial domains that are most important for Europe (e.g. in the area of energy, life sciences and climate)". 
The challenges with HPC applications

- **Scalability of applications**
  - Implementation
  - Algorithmic
  - Big data input and output

- **True collaboration between researchers, computational scientists and HPC experts**
  - Maybe not yet promoted enough
  - Maybe not enough incentives

- **The real implementation of co-design with vendors involved**
  - Although the current European exascale projects are moving forward

- **How to advance science?**
The current situation (ecosystem if you wish)

> There already is/are:

- Individual users/code owners which
  - are often organized around applications
- National HPC centres which
  - are closest to the end user, and offer services and expertise
  - typically have at least Tier-1 hardware resources available
  - participate in PRACE
- PRACE which
  - aims to combine all expertise of its partners in the IP projects
  - aims to facilitate access to the largest (Tier-0) systems
- Organised scientific/industrial communities which
  - Consist of partners that collaborate on science themes and algorithm development
  - need to find ways to get access/support on large systems
- Suppliers/vendors/ISVs which
  - are organized around technology
Use existing strong pillars

> Huge human efforts are required to realise Europe’s ambitions on the application of HPC

> To achieve this:
  - Combine all current efforts in an effective way
  - Financially steer on improvements, new initiatives and incentives

> The model:
  - Use position of national HPC centres
    - Often already have expertise on certain scientific domains (history, experts originating from certain scientific fields)
  - Enable scientific/industrial communities to join forces with national HPC centres, and link to the European infrastructure (PRACE)
  - Stimulate the development of (virtual) CoEs around themes and/or specific expertise, using national HPC Centres and communities
  - Enable involvement of vendors/suppliers to get to co-design
Think of …

> **In practice:**

- Support scientific communities in the usual way (research), but also give incentives for collaboration with national HPC Centres to get to CoEs
  - More financial freedom, e.g., for access, expert support, training, …
- Monitor the current European Exascale projects, which bring together HPC Centres, communities, users and vendors – these look promising
- Stimulate joint future development plans of apps and technology by CoEs, and execute on a daily basis

> **And also:**

- Set up a European-wide HPC training program in which each HPC centre should participate (not only the PATC’s)
- Enable staff exchange programs:
  - HPC Centre staff, community scientists, current CoE staff, …