"HIGH PERFORMANCE COMPUTING – CENTRES OF EXCELLENCE“

Some EESI recommandations

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**Enabling technologies for Exaflop computing**

- Hardware roadmap, links with vendors
- Software eco-systems
- Numerical libraries, solvers and algorithms
- Scientific software engineering

**Application Grand Challenges**

- Industrial and Engineering Applications (Transport, Energy)
- Weather, Climatology and Earth Sciences
- Fundamental Sciences (Chemistry, Physics)
- Life science, Health, BPM
EESI: 150 participants, 100 entities
EESI Recommendations

- Most HPC system software components have to be substantially adapted or newly developed. The different Exascale system architectures should not be visible at the level of the programming model... But all experts consider that the only chance of success of Exascale applications is to develop the best coupling between architecture, algorithm, and application (physics).

- So, Multidisciplinary teams must be developed to ensure this best coupling and also an inter-link between Industrial laboratories and Academic researchers: for HPC, there must be an unprecedented level of collaboration between these experts and researchers who will use it to tackle fundamental questions in earth sciences, life sciences, energy, fusion energy, biomass, biology, engineering, safety, …where generally several physics are active at different scales. 

  - This close partnership is the essence of center of excellence, The center must be very practical due the very high level of complexity of the systems we have to face.

  - Computer designers, applied mathematicians, programmers and hardware specialists, have to tackle crosscutting issues for Exascale, but centers of excellence must involve now different science (physics, chemistry, electromagnetism, analytics, …) communities in order to create exascale-capable applications in specific disciplines.

  - Climate - Ocean / Atmosphere
  - Earth Sciences: Seismics, Tectonics, ...
  - Turbulence: Turbulent flows, turbulent combustion,
European Strengths (1/2)

- **Applications** in Europe (2011 IDC survey):
  - 83% developed in Europe, 66% of IP in Europe
  - Leader in various scientific fields, supported by community organizations (CECAM, ENES, ELIXIR/European Bioinformatics Institute): astrophysics/cosmology, fusion research, materials sciences, life science, i.e. Ab initio, astrophysical, molecular dynamics, Large Eddy Simulation, combustion codes, bioinformatics tools for data mining

- **Applied math.** Europe has one of the best scientists in applied mathematics, many existing scientific libraries either developed in Europe or significant European input to US-led/international projects

- **Software:** Europe has leading position in some software areas: programming models, validation&correctness, performance tools design and development, a long-standing activity in runtime design, system design (mobile, network, energy efficiency), simulation frameworks/coupling tools, meshing tools
EESI vision and recommendations

European weaknesses (1/2)

From a technical point of view:

- Lack of coordination in the development of HPC software, i.e., often few isolated centres within Europe developed scientific libraries which are integrated in US de facto standard.

- Lack of critical mass on some critical software domains: OS, compilers, MSG passing libraries, File system, hybrid core design

- Applications in various areas where European has a leadership position, will need to be redesigned, i.e., Materials/Molecular Mechanics, Climate models, Life Science (molecular dynamics, Quantum Chemistry, Sequence Analysis, Protein docking, 3D structure, Chemo-informatics), some engineering domains (structural mechanics).

These applications represent X1000 man.year of development
EESI vision and recommendations

Needs for HPC Centres of Excellence

- **Reinforce** Multi-disciplinary HPC Centers providing **support** in terms of code development, porting and optimization as well as algorithm development
- **Organize and monitor** the **technological transfer** of Exascale projects into products through a European Exascale Software Center
- **Educate and train**, needs for **co-education centers** for training scientists to acquire a deep knowledge in scientific disciplines, in software design and hardware architectures, extend the formation with the complementary aspect of system -design and -engineering
- **Promote open source** development while enabling commercial exploitation
- **Coordinate** European efforts with the **rest of the world**, in particular:
  - on strategic areas where Europe lack of critical mass and,
  - in World wide initiatives in those that Europe has more value

Should rely on community organizations (CECAM, ENES, EBI…), forming networks between scientific groups, disseminating knowledge within specific scientific domains and identifying demanding and grand challenge problems in the domains and ensure their link with community specific co-design centers
Agenda

Annex

EESI Final Conference, 10-11 Oct. 2011, Barcelona
EESI recommendations – funding targets

Technological transfer

- **Fund**, organize and monitor the technological transfer of Exascale projects into **products** through a European Exascale Software Center:
  - Testing (maturity), validation, eventually rewrite, … the European Exascale Open source software production
  - Specifying, developing, promoting API shared at the international level
  - Promote, organize links with vendors, ISV and service providers

- **Fund** support action for providing credible support and maintenance structure, constant adaptation of libraries, codes, simulation framework to hardware (r)evolution and user needs
  - Encourage the widest dissemination of the produced software libraries and tools among the academic and industrial communities,
  - Favor collaborations aiming at their continuous improvement, thus growing the original investment made in producing these tools
  - Preserve the rights of each of the parties involved in their production (e.g. LGPL license)
A European Exascale eco-system

- European Research Projects
- Nat. Research Projects

European Exascale Software Center

- ISV, techno providers/product suppliers

- Production of Exascale Open Source SW
- Selection, testing, validation ...
- Production of industrialized software, support, services
- Computing Power, training, Porting/Optimisation, ...

- Academic end user
- Industry end user