FP7 Support Action - European Exascale Software Initiative

DG Information Society and the unit e-Infrastructures

EESI Final Conference

European Exascale Software Initiative

EESI vision and recommendations

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Agenda

- **European Strengths and weaknesses**
- EESI vision and recommendations
- Conclusions

EESI vision and recommendations

European Strengths (1/2)

- PRACE
- HPC already intensively used in academy thanks to PRACE and in industry: Energy (TOTAL, EDF), Aeronautic(AIRBUS), Finance, Defense&Security, …
- Applications (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
- In some of these domains Europe has shown its capacity to support long term and costly efforts (x100 man.years/code).

European Strengths (2/2)

- Hardware: Europe has all the competences to build an Exascale computer by the end of this decade with European technologies
- 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)

- Not clear how European ISV are preparing the coming of Exascale
- Europe: 30% HPC market, 1% of HPC revenue
- Simulation as a single program is not as strongly supported as observations and experiments (ITER, LHC)

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.
- Not enough participation in the definition of new standards for programming (MPI, OpenMP, C++, Fortran, …)

EESI vision and recommendations

European weaknesses (2/2)

- Lack of critical mass on some critical software domains: OS, compilers, MSG passing libraries, File system, hybrid core design
- Lack of unified data layer for Bio-Data, most of databases are non-European
- 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

Agenda

- European Strengths and weaknesses
- **EESI vision and recommendations**
- Conclusions

EESI recommendations

- **General statement**
- **Funding strategy and organization**
- **Funding targets**
  - Research and Development projects
  - co-design centers,
  - Technological transfer
  - Exascale hardware platform
  - Education and training in High Performance Computing
- **Budget**
- **European and international governance**

EESI vision and recommendations

EESI recommendations – general statement

Need for a sustainable, long term, coordinated effort

- **Fund** strategic projects where Europe is strong and able to federate significant critical mass
- Insure the coordination of 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
- Reinforce Multi-disciplinary HPC Centers providing support in terms of code development, porting and optimization as well as algorithm development
- Foster the development of 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
- Promote open source development while enabling commercial exploitation

EESI vision and recommendations

EESI recommendations – funding strategy and organization

Defining the right Work Programs, with the right agenda, funding the right teams with the right budget

- a **cross-thematic European program dedicated to Exascale**:
  - e-infrastructure, ICT research, DG INFSO
  - Weather, Climatology and Earth Sciences, DG CLIMA
  - Energy, Environment, DG ENERGY
  - Specific domains (Life science, Health, Fundamental sciences, Industrial technologies…), DG RESEARCH & INNOVATION

=> Comparable in size and time span to LHC or ITER programs

- a coordination between EC and National European funding agencies

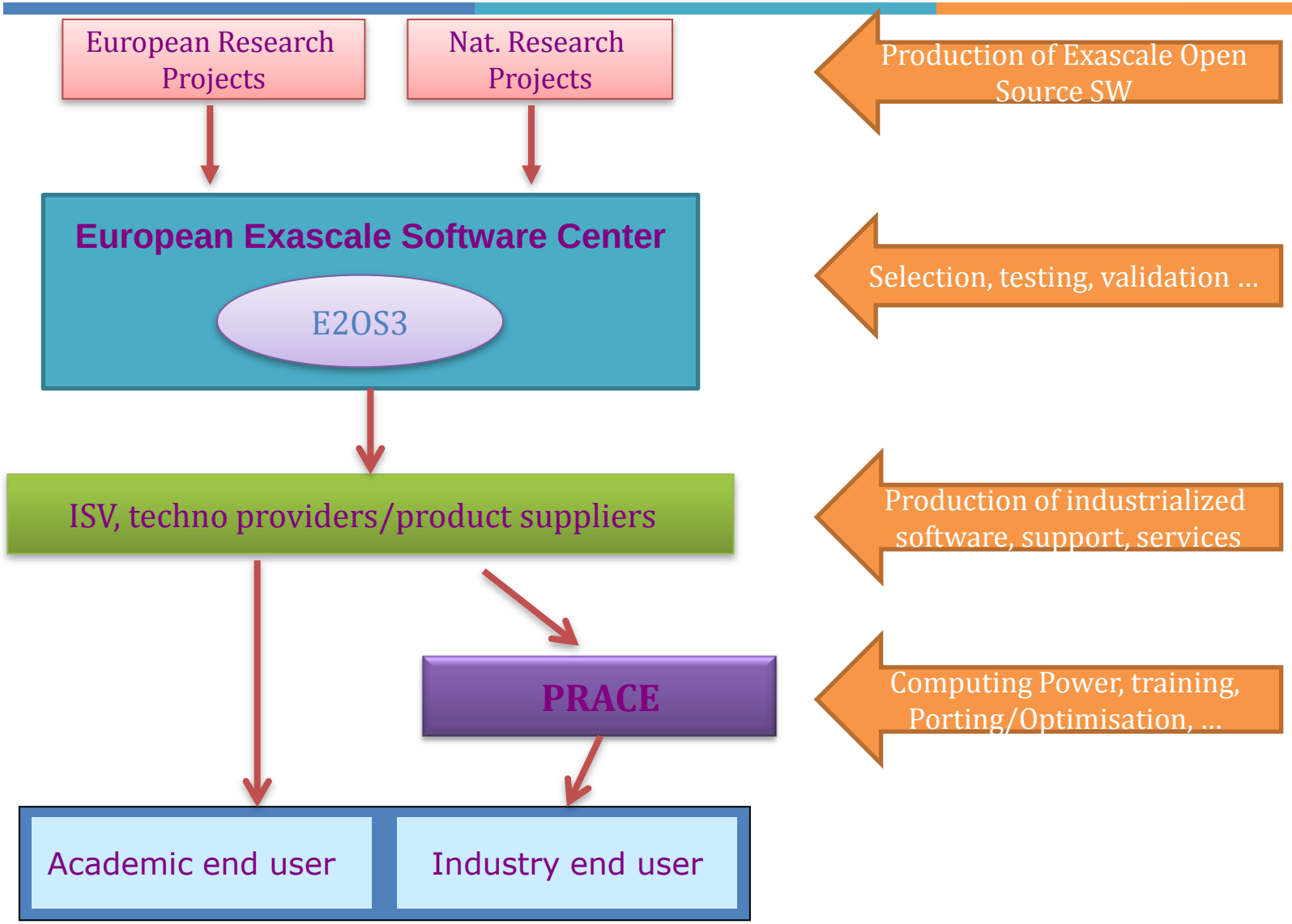
A 20 years agenda

EESI vision and recommendations

EESI recommendations – funding targets

- **Fund Research and Development projects** implementing the EESI/IESP Technological Exascale roadmap, both hardware and software items, **monitored and coordinated** by a High level European body dedicated to HPC-Exascale.
- **Fund co-design program**, mixing vendor-application community-CS&MA specialists, targeted **Grand Challenge Applications**
- **Fund**, organize and monitor the **technological transfer** of Exascale projects into products through a European Exascale Software Center

A European Exascale eco-system



EESI recommendations – funding targets

- **Fund** 2 to 3 R&D projects **each** aiming at delivering one Exascale hardware platform in Europe
- **Fund** Education and Training in High Performance Computing

EESI vision and recommendations

EESI recommendations – funding targets

R&D projects

- **System software:**
  - Where Europe is leading and having critical mass: programming model & runtime, performance, validation & correctness tools,
  - Strategic areas but Europe lack of critical mass: resilience, OS, compilers, msg passing libraries, File system, hybrid core design, energy efficiency,, programming models, Cloud
- **Unified Multiscale/Multiphysics simulation framework,** enabling coupling of (parts) legacy and new generation (parts of) codes/librairies, component based architecture
- **Pre and post treatment tools and Big DATA management:** meshing (up to x100 billions cells, adaptive, automatic refinement, …), visualization (of large data set, of statistical data, measured or computed), data mining, unified data layer for Bio-data

EESI vision and recommendations

EESI recommendations – funding targets

R&D projects

- **Code redesign, rewriting for Exascale:** ex. Materials/Molecular Mechanics, Climate models, Life Science (molecular dynamics, Quantum Chemistry, Sequence Analysis, Protein docking,/3D strucure, Chemoinformatics)
- **Applied mathematics:** scientific libraries, innovative algorithmic developments and numerical methods (ultra-scalable, multi-level and type of parallelism, fault tolerant, memory thrifty), e.g iterative methods for handling resilience issue
- **Verification&Validation, Uncertainty Quantification, Data Assimilation** (climate, emerging in earth science and engineering apps), probabilistic and stochastic models (earth science), coupling between stochastic and deterministic methods

EESI recommendations – funding targets

Co-design program

Fund co-design program, between 5 to 10 projects targeted Grand Challenge Applications, mixing hardware specialist-application community-Computer Scientist &Applied Mathematics specialists (relaying on the so called tiger teams (IDC report)):

- Life Science&Health, focus on tissue simulation, molecular dynamics, cell Simulation, genome sequencing and personalized medicine, expected impact on cancer, heart, diabetes, kidney, bone, blood, etc…
- Climate and earth Science
- Engineering
  - Energy applications (Oils&Gas, renewable, Nuclear)
  - Transport (Aeronautics & Automotive)
- Fundamental Science
- General algorithmic support and libraries

EESI recommendations – funding targets

Technological transfer

- **Fund**, organize and monitor the technological transfer of Exascale projects into products through a European Exascale Software Center (could be an ETP)**:**
  - 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)

EESI recommendations – funding targets

Education and training in High Performance Computing

- **Technical :** new programming schemes, efficient mapping of algorithms to hardware and knowledge of memory hierarchies and data access over different levels of hardware implementations, porting and optimization or re-design of simulation codes for a specific exa-scale machine, data management(data analysis, visualisation), (use of/development of) scientific libraries, benchmarking/performance analysis
- **Strategic**: train the next generation of computational scientists and engineers, attract and retain young scientists
- **Type**: educational programs in terms of master or PhD programs and training of scientists on the postdoctoral or senior scientist level.
- **Format: co-education centers**, need for scientists who have both a deep knowledge in scientific disciplines, in software design and hardware architectures, extend the formation with the complementary aspect of system -design and -engineering

EESI recommendations – funding targets

European Exascale hardware platforms

Fund 2 to 3 R&D projects **each** aiming at delivering one Exascale hardware platform in 2020, because:

- **need for different kind of architectures for different kind of needs**: weak and strong scaling, capacity/capability, big data oriented computers, field dedicated architectures-*Anton like machine for Molecular Dynamics*(?)
- **Exascale computing is a technological breakthrough compared to Tera and Petascale**, several technological options will have to be addressed
- **need competition between different providers** in order to have (at least) a world class vendor in Europe

Proposal:

- One platform built in Europe, integrated by a European vendor, with mainly European technology.

Should not only target a prototype but a product

- One or two platforms developed in collaboration with non European partners (US, Japan, China, Russia, …) and possibly assembled in Europe

EESI recommendations – budget

Global estimated budget : 2,5 to 3,5 billion euros over the next 10 years

- **Research and Development projects:** 1000 Meuros during 10 years
- **Co-design program**: between 500 to 1000 Meuros for 5 to 10 co-design centers, during 10 years
- **Exascale hardware platforms:** , between 500 to 1000 Meuros for 2 to 3 platforms, during 10 years
- **Technological transfer** through a European Exascale Software Center: 500 Meuros during 10 years

EESI recommendations – European and international coordination

Goals:

- Insure the **coordination** of European efforts **inside Europe** and with the **rest of the world**
- Should contribute to implement the what, be sustainable, should look at precedence for the forums, such as OGF, OSS, FSIO, Linux, MPI

EESI vision and recommendations

International Exascale Software Initiative
US-Europe-Asia coordination

IESI Steering Committee

- European Steering Committee
- US Steering Committee
- Asia Steering Committee

- Exascale roadmap update
- International project cartography
- International Exascale Software Stack monitoring
- Managing WGs on specific subjects (MPI, resilience, ...)
- Training & education
- Dissemination

Internationals projects: G8, Japan/France, ...

Regional software stack

EESI vision and recommendations

Consequences for **not implementing** the EESI recommendations

- world leaders in their field will contribute to non European frameworks, maybe US, certainly China in the future
  - Ex: Scientific libraries, performance tools, …
- Not prepared when Exascale technology will be available, **lost of leadership in some scientific fields** (Climate, Bio, Material science…) and **lost of competitiveness in industry**, some of them are world leaders, e.g drug design, aeronautics, nuclear energy, Oil&Gas, automotive
- Best European researchers will collaboration with leading teams, non localized in Europe, risk of losing young researchers to US, Japan, China

Do not engage the right efforts, at the right time with the right budget is this acceptable for strategic fields, such as Security and Defense?

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EESI Conclusions

- Europe need for a **sustainable, long term and coordinated** effort

- Europe is still well positioned to be part of the few player worldwide deploying and exploiting Exascale technology but action is needed now

- A 2,5 to 3,5 billions euros total budget over 10 years, supported by EC, National European funding agencies, industry, … **a several decades** engagement

EESI Conclusions

- Scientific Computing at Exascale, from a computing and data intensive point of view are **strategic** for maintaining and developing both **European Scientific Excellence and Industry Competitiveness**

- **International** collaboration is required

- Europe should encourage the development of **Open Source solutions** to foster international collaborations and the emergence of international *de facto* standards, enabling commercial exploitation


Thank you