FP7 Support Action - European Exascale Software Initiative

DG Information Society and the unit e-Infrastructures

European Exascale Software Initiative
EESI2

Towards exascale roadmap implementation

2nd IS-ENES Workshop on
"High-performance computing for Climate Models"

Toulouse, January 30&31, 2013

Philippe RICOUX (TOTAL)
EESI2 Coordinator

Agenda

- **EESI objectives, agenda, major achievements**
- From EESI to **EESI2**

EESI objectives

Build and consolidate a **vision and roadmap** at the European level, **including applications**, both from ***academia and industry*** to address the challenge of ***performing scientific computing*** on the new generation of super-computers, **hundreds of Petaflop/PBytes** in 2015 and **Exaflop/ExaBytes** in 2020

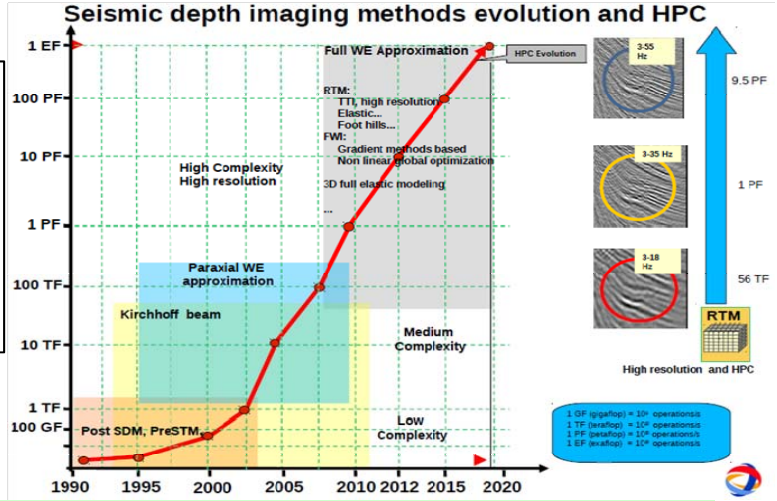
Toward EFFICIENT EXASCALE APPLICATIONS

Why Exascale?

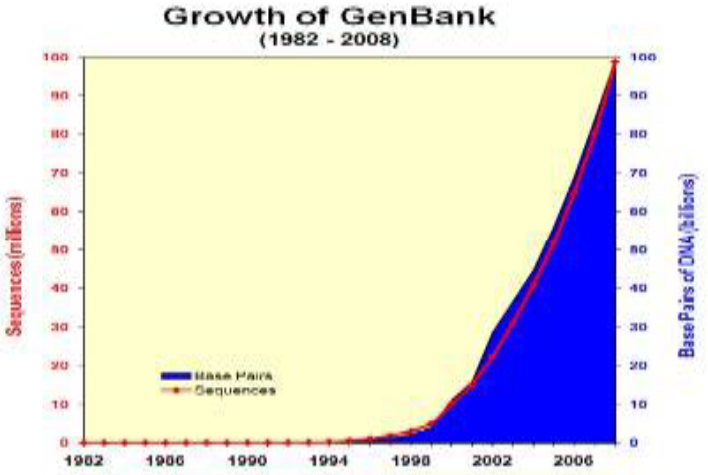
EXAFLOP (capability and capacity)

Oil & Gas Roadmap

HPC - Physics and Numerics



… and/or **ExaBytes**



Drug design: realistic cell membrane models, including **drug permeation and binding**

Oil&Gas: huge 3D seismic wave inversion, reservoir modelling, robust optimization

Materials: material properties identification

Aeronautics-Greening the aircraft

Astronomy: **Square Kilometre Array**,

Earth Sciences: Natural hazard mitigation

Fundamental Sciences, Life Sciences,

Engineering sciences (Turbulence, Combustion, acoustics, Mechanical, chemical engineering, …)

Climate: satellite sensors create floods of data (x 1000), leading to Exa-scale archives, ex. projected frequency of intense tropical cyclones in some region of the globe

Quantum Chemistry : discover a material and properties: ab initio databases of materials and molecular properties connected to existing databases of experimental properties

Industrial applications: management of data generated from micro/macro sensors and automated measurement devices

Industrial Roadmaps

Wing prototypes: **77**

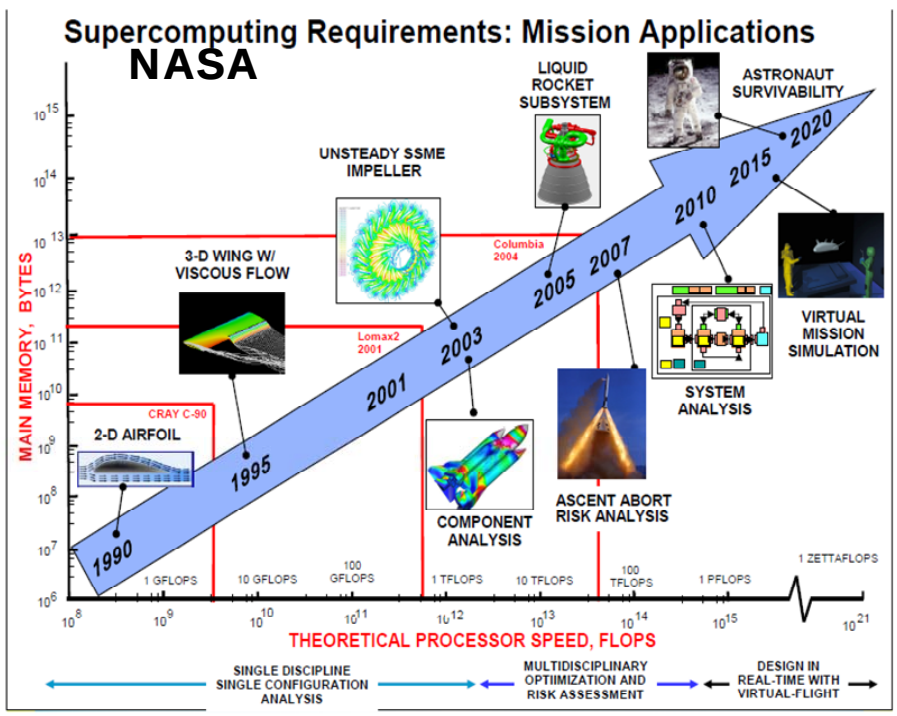
Boeing From 767 to 787

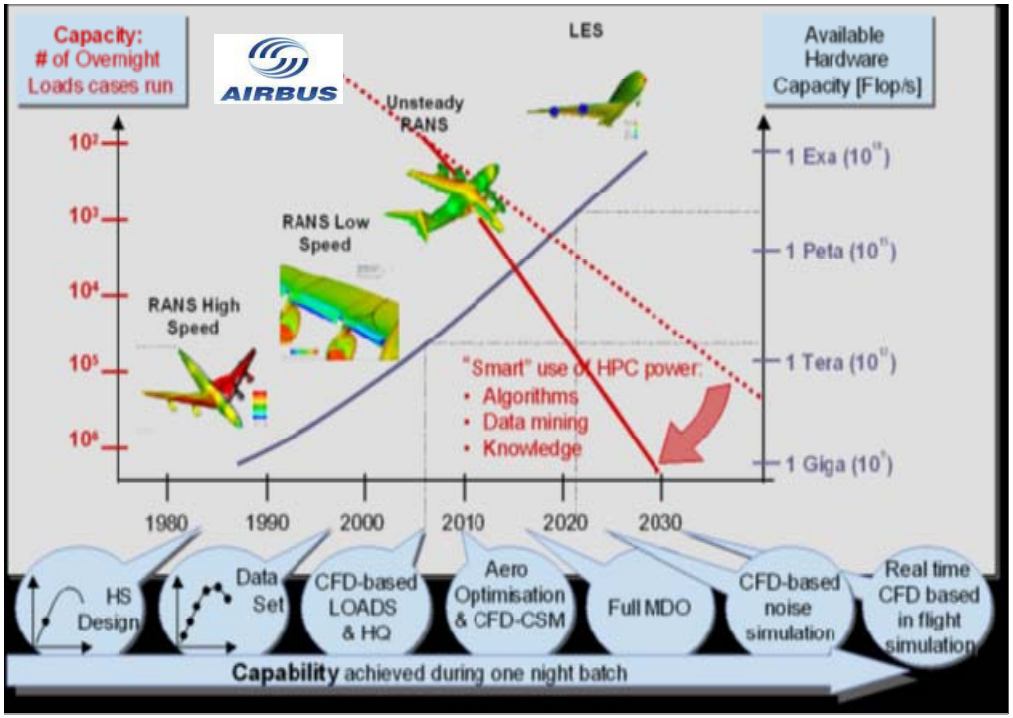
- **40 %** less **wind-tunnel days**
- **25 %** saving in aerodynamics **development time**
- **20 %** saving on wind-tunnel **tests cost**

Thanks to HPC-enabled CFD runs, especially in high-speed regime, even providing better representation of aerodynamics phenomenon turned into better design choices.

But … Digital Aircraft will require at least 1 ZetaFlop !

Wing prototypes: **11** (2008) → **7** by new methods and HPC (2015)

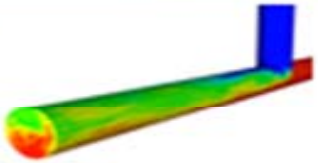
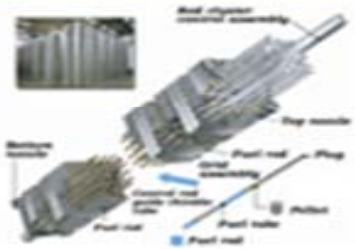
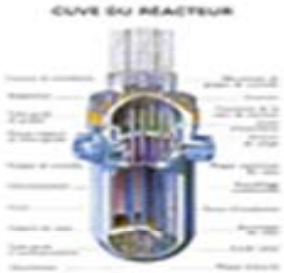




Industrial Roadmaps

American Nuclear Plant vision

Computational Challenges and Needs for Academic and Industrial

2003	2006	2007	2010	2015
Consecutive thermal fatigue event Computations enable to better understand the wall thermal loading in an injection. Knowing the root causes of the event ⇒ define a new design to avoid this problem.	 Computation with an L.E.S. approach for turbulent modelling Refined mesh near the wall.	 Part of a fuel assembly 3 grid assemblies	9 fuel assemblies No experimental approach up to now Will enable the study of side effects implied by the flow around neighbour fuel assemblies. Better understanding of vibration phenomena and wear-out of the rods.	The whole vessel reactor 

Computations with smaller and smaller scales in larger and larger geometries
⇒ a better understanding of physical phenomena ⇒ a more effective help for decision making
⇒ A better optimisation of the production (margin benefits)

10^8 cells 3.10^{13} operations	10^7 cells 6.10^{14} operations	10^8 cells 10^{16} operations	10^9 cells 3.10^{17} operations	10^{10} cells 5.10^{18} operations
Fujitsu VPP 5000 1 of 4 vector processors 2 month length computation	Cluster, IBM PowerS 400 processors 9 days	IBM Blue Gene/L « Frontier » 20 Tflops during 1 month	600 Tflops during 1 month	10 Pflops during 1 month
# 1 Gb of storage 2 Gb of memory	# 15 Gb of storage 25 Gb of memory	# 200 Gb of storage 250 Gb of memory	# 1 Tb of storage 2,5 Tb of memory	# 10 Tb of storage 25 Tb of memory
Power of the computer	Pre-processing not parallelized	Pre-processing not parallelized Mesh generation IESP/Application Subgroup	... Ibid. ... ... Ibid. ... Scalability / Solver	... Ibid. ... ... Ibid. ... ... Ibid. ... Visualisation

EESI Motivations and Organization

Origins of EESI: IESP (Jack Dongarra)

www.exascale.org

Build an international plan for developing the next generation open source software for scientific high-performance computing

IESP meetings

Nov 2008

Apr 2009

Jun 2009

Oct 2009

Nov 2009

EESI proposal

Apr 2010

EESI start

Oct 2010

Nov 2010

Apr 2011

www.exascale.org

EESI Motivations and Organization

Exascale, a technological breakthrough

- Compare to Petascale computers: **memory per core 1/10, CPU heterogeneity, total node interconnect BW & node memory 1/10, concurrency *10**
- ***Software layer and applications** need to exploit these new hardware trends **by existing software stack that** cannot be handled*
- ***Community codes unprepared*** **for sea change in architecture while:**
  - designing and developing a new generation of Scientific Applications **takes 5 to 10 years,**
  - lifetime of Scientific Applications are **several decades**

EESI: 150 experts, 100 entities

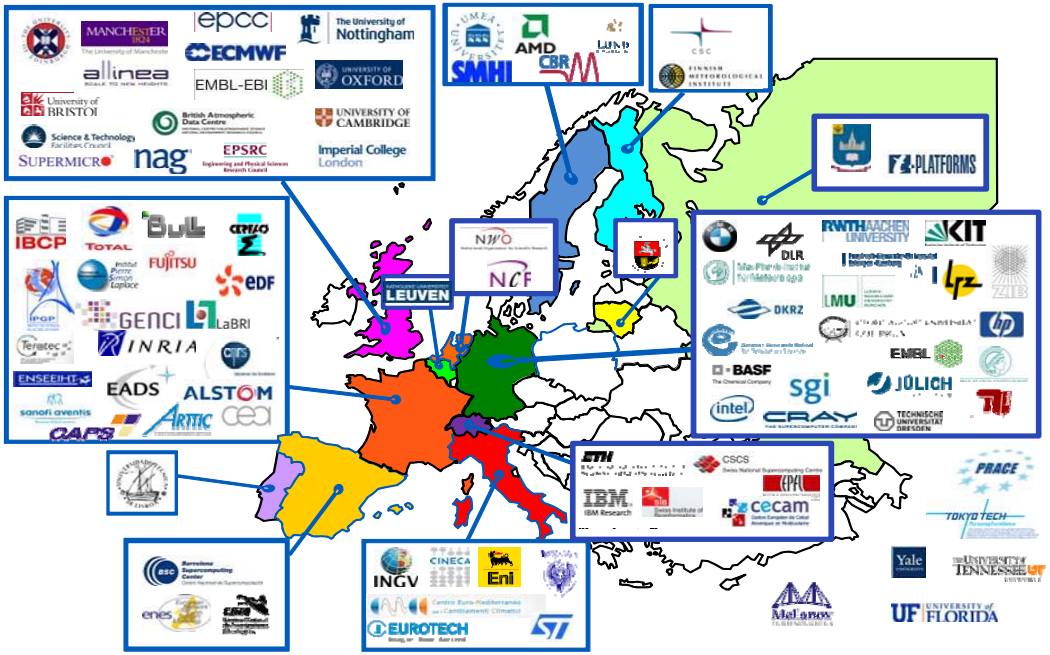
Leader : Dr. Jean Yves BERTHOU

8 contractual partners

Large support of TOTAL

14 countries covering Europe

Participation of 2 US, 1 Israeli and 1 Lithuanian



EESI Motivations and Organization

It is time NOW to

- **Evaluate the key missing components in the software stack**
- **Coordinate hardware development with software and applications communities**
- **Engage the redesign and development of the new generation of software stack and applications**

A several decades program(s)

Main goals:

- investigate how Europe is located, its strengths and weaknesses, in the overall international HPC landscape and competition
- identify priority actions
- identify the sources of competitiveness for Europe induced by the development of Peta/Exascale solutions and usages
- investigate and propose programs in education and training for the next generation of computational scientists
- identify and stimulate opportunities of worldwide collaborations

EESI Main Challenge

Academy and industries, are looking for multi-peta and exaflopic computing resources

not only the next supercomputers themselves

but also and mainly the ways to know how programming on millions cores machine.

Industrial and academic applications are in fact expecting for the **best coupling between**

Architecture / Algorithm / Application,

in order to address and solve crucial issues in many fields.

EESI vision and recommendations

European Strengths

- **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): 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***, ***combustion*** codes, ***bioinformatics*** tools for data mining, ***Full Wave Inversion*** (seismic)
- **Applied math**.: dense and sparse Solvers, direct or iterative (i.e AMG)
- **Software**: programming models, validation & correctness, performance tools design and development, system design, simulation frameworks/coupling tools, meshing tools

EESI vision and recommendations

European weaknesses

- 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 development of HPC software, i.e developed within Europe **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, …), of OS, compilers, File system, hybrid core design
- Lack of data management (most of databases are non-European)
- Applications in various areas where European has a leadership position, will **need to be redesigned**, i.e Climate models, Life Science (molecular dynamics, Sequence Analysis, …), engineering structural mechanics …

These applications represent X1000 man.year of development

EESI vision and recommendations

R&D projects

- **System software:**
  - Europe 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 codes, 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
- **Code redesign, rewriting for Exascale:**
  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 high degree of freedom, in earth science and engineering apps lower dof but accurary, optimal sensors network, probabilistic and stochastic models (earth science), coupling between stochastic and deterministic methods, robust optimization, data validation and reconciliation

Common main issues to be addressed

- **At the level of the simulation environment:**
  - Unified Simulation Framework and associated services: CAD, mesh generation, data setting tools, computational scheme editing aids, visualization, etc.
  - Multi-physics simulation: establishment of standard coupling interfaces and software tools, mixing legacy and new generation codes
  - common (jointly developed) mesh-generation tool, automatic and adaptive meshing, highly parallel
  - Standardized efficient parallel IO and data management (sorting memory for fast access, allocating new memory as needed in smaller chunks, treat parts of memory that are rarely/never needed based on heuristic algorithms, …)

- **At the level of codes/applications:**
  - New numerical methods, algorithms, solvers/libraries, improved efficiency
  - coupling between stochastic and deterministic methods
  - Numerical scheme involving Stochastic HPC computing for uncertainty and risk quantification
  - meshless methods and particle simulation
  - Scalable program, strong and weak scalability, load balancing, fault-tolerance techniques, multi-level parallelism (issues identified with multi-core with reduced memory bandwidth per core , Collective communications, Efficient parallel IO)
  - *Development of standards* programming models (MPI, OpenMP, C++, Fortran, …) handling multi-level parallelism and heterogeneous architecture

- **Human resources, training (what level?)**

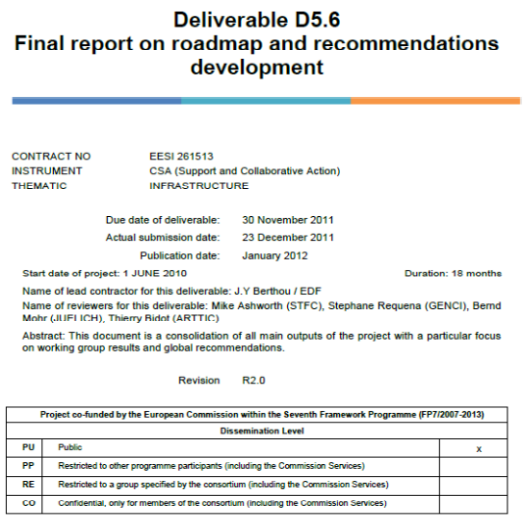
EESI Conclusions

- **EESI recommendations – general statement**
  - Fund strategic projects and, whenever Europe lacks critical mass, coordinate European efforts with those of the rest of the world
  - Reinforce multi-disciplinary HPC Centers and foster the development of community organizations
  - Promote open source development while enabling commercial exploitation.
- **EESI recommendations – funding strategy and organization**
  - Funding of Exascale projects should not be limited to DG INFSO but supported by relevant Directorates
  - These efforts should be coordinated with national funding agencies in Europe.
- **EESI recommendations – funding targets**
  - Fund R&D projects according to the EESI/IESP Technological Exascale roadmaps coordinated by a High level European body dedicated to HPC-Exascale
  - Reinforce multi-disciplinary HPC Centers
  - Fund co-design programs
  - Create a European Exascale Software Center in charge of increasing the status of the funded R&D projects.
- **EESI recommendations – budget**
  - 2,5 to 3,5 billion euros over the next 10 years.

EESI Documents

- All documents on EESI
  - WP, WG Reports
  - All Final Reports
  - Final Roadmap, Vision & Recommendations
  - Available on :

  http://www.eesiproject.eu/pages/menu/homepage.php



Deliverable D5.6
Final report on roadmap and recommendations development

CONTRACT NO EESI 261513
INSTRUMENT CSA (Support and Collaborative Action)
THEMATIC INFRASTRUCTURE

Due date of deliverable: 30 November 2011
Actual submission date: 23 December 2011
Publication date: January 2012

Start date of project: 1 JUNE 2010 Duration: 18 months

Name of lead contractor for this deliverable: J.Y Berthou / EDF
Name of reviewers for this deliverable: Mike Ashworth (STFC), Stephane Requena (GENCI), Bernd Mohr (JUELICH), Thierry Ridel (ARTTIC)

Abstract: This document is a consolidation of all main outputs of the project with a particular focus on working group results and global recommendations.

Revision R2.0

Project co-funded by the European Commission within the Seventh Framework Programme (FP7/2007-2013)		
Dissemination Level		
PU	Public	x
PP	Restricted to other programme participants (including the Commission Services)	
RE	Restricted to a group specified by the consortium (including the Commission Services)	
CO	Confidential, only for members of the consortium (including the Commission Services)	

- EESI also largely participated to the new

  PRACE Scientific Case Update (2012 - 2020), available on:

http://www.prace-ri.eu/PRACE-The-Scientific-Case-for-HPC

Lead Author:
Martyn Guest – Cardiff University, UK

Panel Chairs:
From EESI
- Giovanni Aloisio – University of Salento and ENES-CMCC, Italy
- Stefan Blügel – Forschungszentrum Jülich, Germany
- Modesto Orozco – Institute for Research in Biomedicine, Spain
- Philippe Ricoux – TOTAL, France
- Andreas Schäfer – University of Regensburg, Germany

Agenda

- EESI objectives, agenda, major achievements
- **From EESI to EESI2**

From EESI to EESI2

EESI roadmaps, vision and recommendations ***need to be monitored, updated, on a dynamical way***

Key issues to be addressed are pointed out in EESI1 … Now EESI2 must recommend R&D actions how to tackle them

- **Extend, refine, and update** Exascale cartography (**directly in the dedicated WG for better analysis of each WG)** and **roadmaps** from HPC community, on software, tools, methods, R&D and industrial applications**, ...**

new *With a Gap Analysis.*

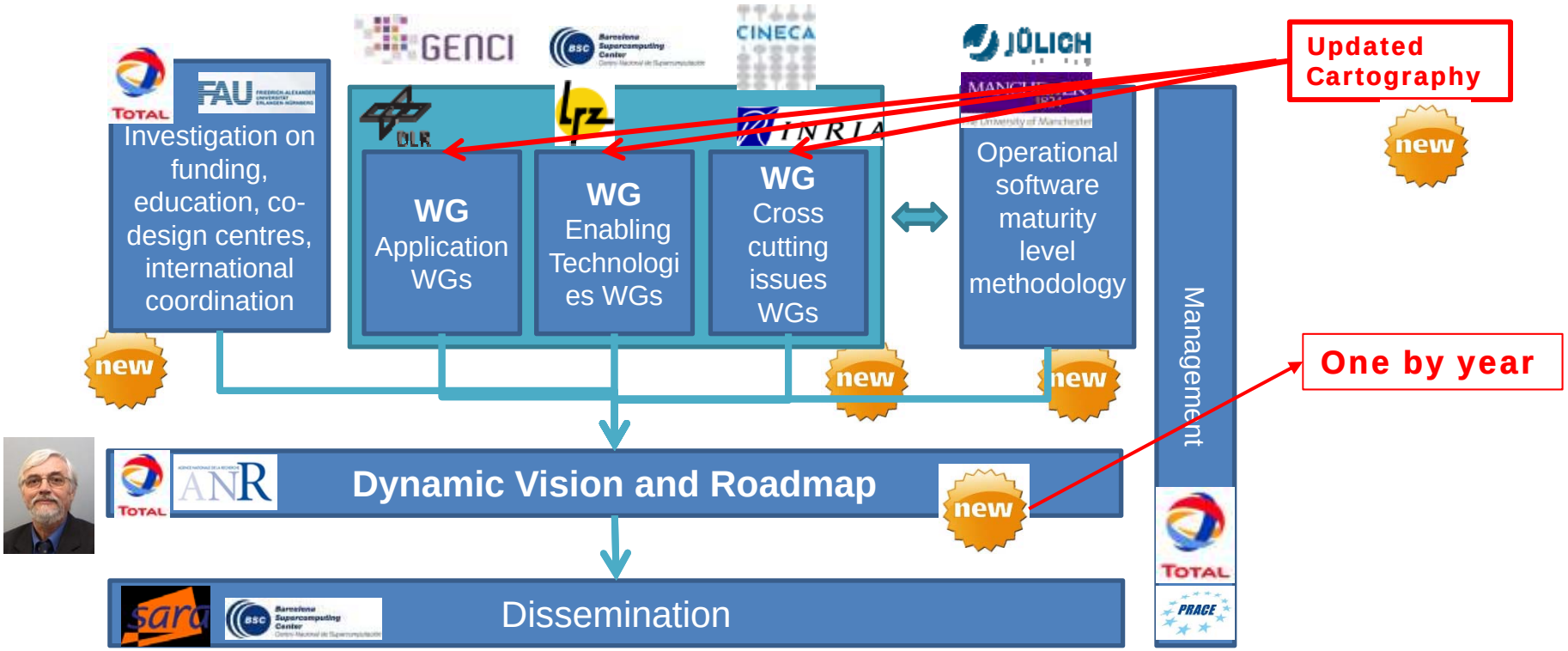
new Including WG on ***disruptive technologies***

new **Address "Cross Cutting issues":** Data management and exploration, **Uncertainties - UQ&VQ**, Power & Performance, Resilience, Disruptive technologies

new **Investigation on** funding scheme and opportunities, education, co-design centres, international coordination

new Operational **Software maturity** level methodology, evaluation

EESI2 general picture



Contractual partners: TOTAL (coordinator), PRACE AISBL (acting for third parties LZR, GENCI, BSC, CINECA, EPCC, SARA…)

Contributing partners, involved in the management of EESI2 tasks but not associated to PRACE AISBL: INTEL, DLR, EDF, ANR, CERFACS, …

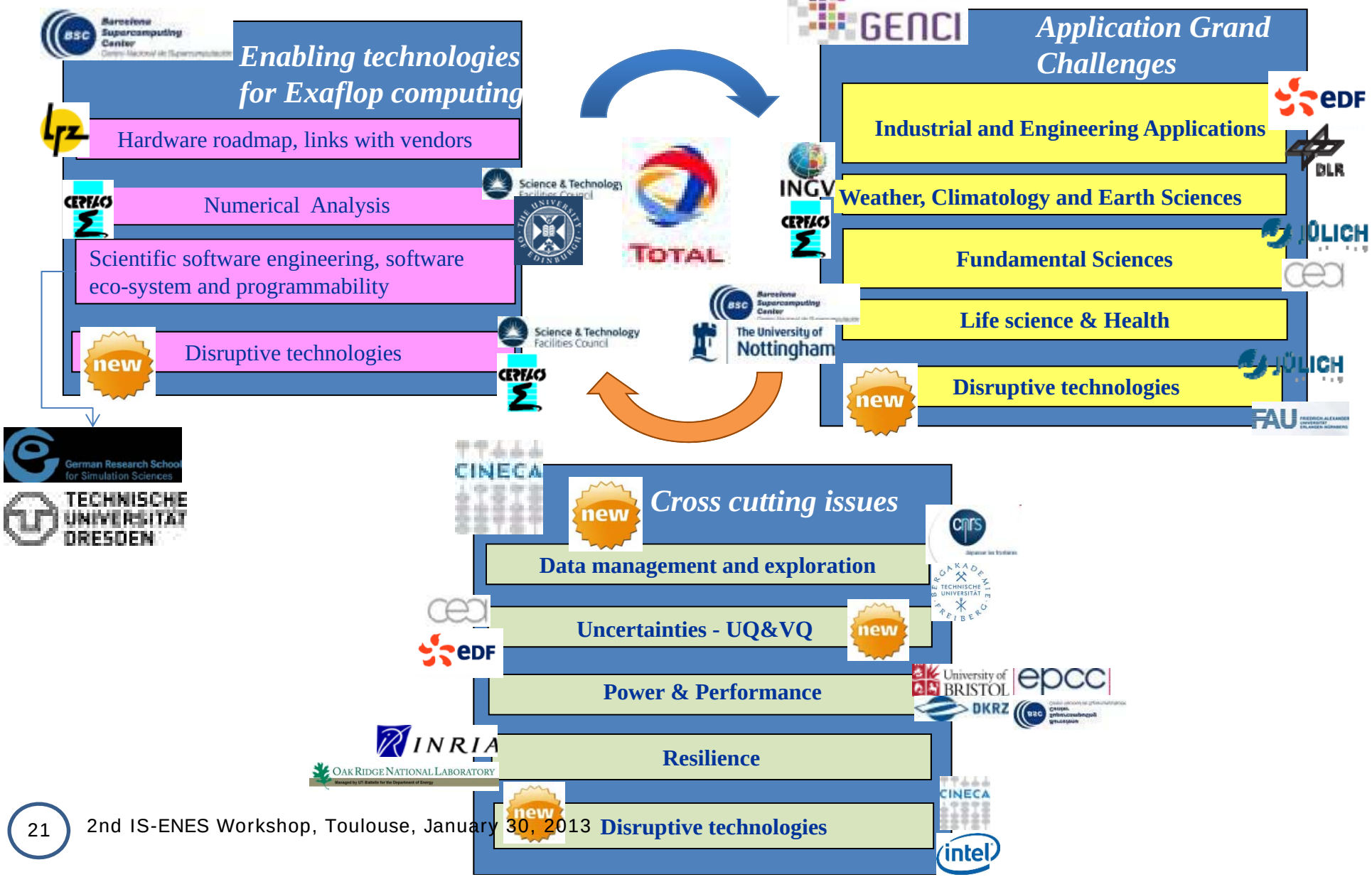
Supporting partners : more than 50 letters of Support

EESI2 proposal submitted in November to INFRA-2012-3.3: *Coordination actions, conferences and studies supporting policy development, including international cooperation, for e-Infrastructures*.

Requested funding: 1.5 M€ → 1.36 M€ accepted by EC

Duration: 30 months, Start 1st September 2012 - kick off 18th September 2012

EESI2 Working Groups



EESI2 WP brief tasks (1/2)

Education, strategic scientific coordination:

- State-of-the-art, trends, and future needs in HPC training and education.
- Recommendations for EU co-design centers in the area of Exascale computing.

Application Work Groups:

- Key application breakthroughs, and performing a gap analysis and integrating international cartography
- R&D activities, especially in applications redesigning and development of multiscale/multiphysics frameworks;
- Assessing the feasibility of setting up Applications Co Design Centers
- structuring of scientific communities at the European level.

Enabling technologies Work Groups:

- Numerical analysis, with aspects such as dense linear algebra, graph and hypergraph partitioning, sparse direct methods, Iterative methods
- Disruptive technologies and Integration of international cartography

Cross cutting issues Work Groups:

- Data management and exploration specific issues roadmap
- actions and follow up of projects on uncertainties and roundings
- power management impact on the system design and on programmability
- achieve the best coupling Architecture-Algorithm-Application
- fault tolerance at system and application level
- Survey new hardware and software technologies

EESI2 WP brief tasks (2/2)

Operational software maturity level methodology, WP6 :

- **D**evelop and document a methodology for estimating the level of maturity of Exascale software components
- Identify 3 software stack components from existing and near future European Exascale projects and apply the defined methodology

ALL previous WP will converge in WP7

- **EESI2 vision and roadmap**
- **Annual recommendations synchronized with EC R&D projects decision agenda**

Dissemination, WP8

- Organization of technical workshops
- Organization of European Exascale conference
- Information Dissemination
- *EESI in Europe and world-wide*
- Involvement in International community workshops

UE

EESI2 Main Resouces

Working Package	Working Group	Title	Chair	Vice Chairs		
WP1		*Management*	*Philippe RICOUX TOTAL FR*	*Jean Yves BERTHOU ANR FR*		
	T1.1	Project Global Management	Philippe RICOUX TOTAL FR			
		Project	Philippe RICOUX			
WP3		*Application Work Groups*	*Stephane REQUENA GENCI FR*	*Norbert KROLL DLR GER*		
	T3.1	Industrial and engineering applications	Stephane REQUENA GENCI FR	Ange CARUSO EDF FR	Norbert KROLL DLR GER	
	T3.2	Weather, Climatology and Earth Sciences	Giovani ALOISIO Salente Univ. IT	Jean Claude ANDRE CERFACS FR		
	T3.3	Fundamental Sciences	Godehard SUTMANN JSC GER	Romain TEYSSIER CEA FR		
	T3.4	Life Science & Health	Modesto OROZCO BSC SP	Charles LAUGHTON Birmingham Univ. UK		
	T3.5	Disruptive technologies	Godehard SUTMANN JSC GER	Ulrich RUEDE Erlingen Univ. GER		
	T3.6	Coordination	Stephane REQUENA GENCI FR	Norbert KROLL DLR GER	Per OSTER CSC FIN	

NEW in EESI2

Specific Funding allocated

All WP can request International External Expertise
(Out of initial partners and third parties)

- **Specific overview document**
- **Specific Scientific expert**
- **…**

Center of excelle

Need External Expertises

KEY ISSUE

	WP4		***Enabling technologies Work Groups***	***Rosa Maria BADIA BSC SP***		***Herbert HUBER LRZ GER***		
Open …		T4.1	Numerical analysis	Andreas GROTHEY Edinhburg Univ. UK		Iain DUFF STFC UK		
		T4.2	Scientific software engineering, programmability	Felix WOLF GRS GER		Mathias MUELLER Dresden Univ. GER		
Need External Expertises		T4.3	Disruptive technologies	Iain DUFF STFC UK		Serge GRATTON CERFACS FR		**KEY ISSUE**
Open …		T4.4	Hardware and operating software vendors	Herbert HUBER LRZ GER		Lee MARGETTS Manchester Univ. UK		
		T4.5	Coordination	Rosa Maria BADIA BSC SP		Herbert HUBER LRZ GER	Per OSTER CSC FIN	
	WP5		***Cross cutting issues Work Groups***	***Giovanni ERBACCI CINECA IT***		***Franck CAPELLO INRIA FR***		
		T5.1	a management and exploration	Jean Pierre VILOTTE CNRS FR		Christian HASSE Frieberg Univ. GER		
Open …		T5.2	Uncertainties	Vincent BERGEAUD CEA FR		Alberto PASANINI EDF FR		**KEY ISSUE**
		T5.3	Power & Performance	Simon McINTOCH-SMITH Bristol Uinv. UK		Jesus LABERTA BSC SP	Thomas LUDWIG DKRZ GER	Mark BULL EPCC UK
		T5.4	Resilience	Franck CAPELLO INRIA FR				
Need External Expertises		T5.5	Disruptive technologies	Carlo CAVAZZONI CINECA IT		Karl SOLCHENBACH INTEL GER		**KEY ISSUE**
		T5.6	Coordination	Giovanni ERBACCI CINECA IT		Franck CAPELLO INRIA FR	Per OSTER CSC FIN	

WP6		***Operational software maturity level methodology***	***Bern MOHR JSC GER***	***Lee MARGETTS Manchester Univ. UK***		
	T6.1	Evaluation methodology set up	Bern MOHR JSC GER	Francois BODIN CAPS Entre. FR		
	T6.2	Perform evaluation on 3 components,	Lee MARGETTS Manchester Univ. UK	Andrew JONES NAG UK		
WP7		***EESI2 vision and roadmap***	***Philippe RICOUX TOTAL FR***	***Jean Yves BERTHOU ANR FR***		
	T7.1	Vision and roadmap.	Philippe RICOUX TOTAL FR	Franck CAPELLO INRIA FR		
	T7.2	recommendations to European	Philippe RICOUX TOTAL FR	Jean Yves BERTHOU ANR FR		
WP8		***Dissemination***	***Peter MICHIELSE SARA NL***	***Sergi GIRONA BSC SP***		
	T8.1	Organization of technical workshops	Philippe RICOUX TOTAL FR	Giovanni ERBACCI CINECA IT	Herve MOUREN TERATEC FR	
	T8.2	Organization of European Exascale conference	Peter MICHIELSE SARA NL	Jean Yves BERTHOU ANR FR		
	T8.3	Information Dissemination	Sergi GIRONA BSC SP	Philippe RICOUX TOTAL FR		
Open …	T8.4	EESI in Europe and world-wide	Franck CAPELLO INRIA FR	Peter MICHIELSE SARA NL		

EESI2 Outputs (1/2)

Based on detailed cartographies and roadmaps shared by the EU HPC community on key issues challenges:

- A **detailed evaluation** of how Europe is located, its strengths and weaknesses, in the overall international HPC landscape and competition, including: Identification of main HPC European actors and users, Identification of main European and international HPC existing or planned initiatives and strategies, Links with funding agencies, Links with vendors, ISV and service providers, for leading to

  Periodic Exascale VISION and ROADMAP, RECOMMENDATIONS

- A cartography of existing **education** courses and **training** needs and **proposition for new programs adapted to Exascale**

- **A complete overview of existing worldwide Co-design centres (New from EESI1) and recommendations for Europe on such structures**

  Real Actor in very new EC "Centres of Excellence" program

- A **methodology to evaluate the maturity of results of projects that implement software components (New from EESI1)**

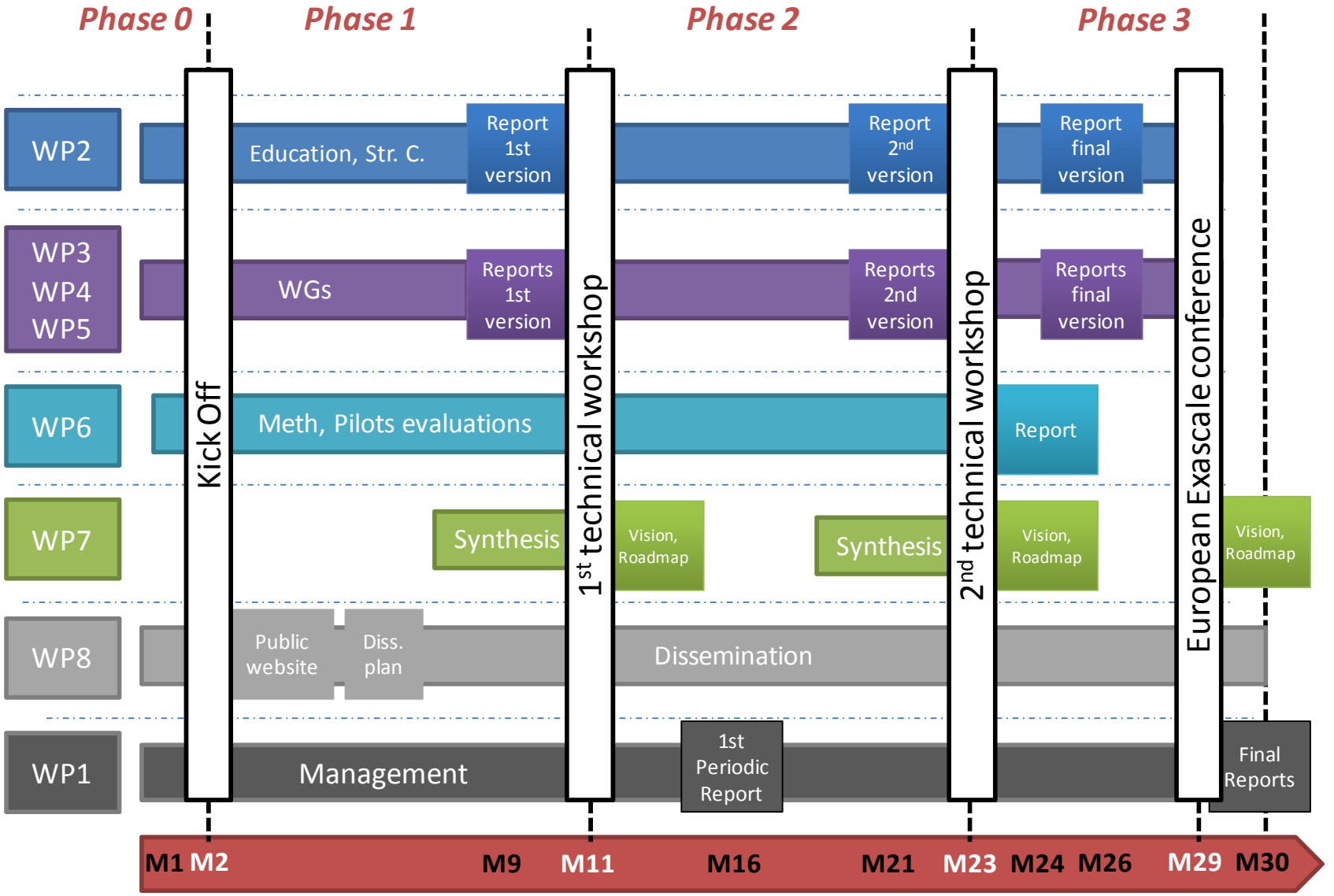
EESI2 Outputs (2/2)

- Detailed periodic roadmaps on the key challenges identified in EESI1, including:
  - **Gap analysis, Breakthroughs, (New from EESI1)** , Identification of priority actions, Identification of the main sources of competitiveness for Europe
  - Uncertainties propagation, roundings calculation model

- Dissemination actions, including:
  - Meeting with Funding agencies, A public web site, 2 large public international conference

- Strengthening of worldwide collaborations, including:
  - Representing Europe in the international Exascale community
  - Contribution to the International dialogs between US, Europe and Asia including EU organisations, the European commission and IESP.
  - **Contributing to build an international Exascale software Organization**

EESI2 Work Plan



EESI2 FOCUS

- **Scientific key issues to be tackled**
  - **Fundamental, Industrial, Engineering, eco software, …**
  - **Cross Cutting**
  - **Funding specific expertises**
  - ***Not only need or objectives but technical propositions***

- **Detailed periodic roadmaps** on the key challenges, including:
  - **Gap analysis,**
  - ***Breakthroughs*,**
  - **Identification of priority actions,**
  - ***Recommendations* to R&D project**

- **Define educational programs for Exascale**

- **Contributing to build an international Exascale software Organization**

EESI2