



FP7 Support Action - European Exascale Software Initiative

DG Information Society and the unit e-Infrastructures



# European Exascale Software Initiative

## IESP meeting

### April, 6-7 2011

WP3 Application Grand Challenges

WP4 Enabling Technologies for Exaflop Computing

Speakers: Stephane Requena (GENCI)

Bernd Mohr (JSC)

# WP3 Organisation



## □ Application Grand Challenges (GENCI)

- Identify the apps drivers for Peta and Exascale
- Needs & expectations of scientific applications
- Economic impact & European competitiveness
- Build a European vision and a roadmap

## □ 4 working groups

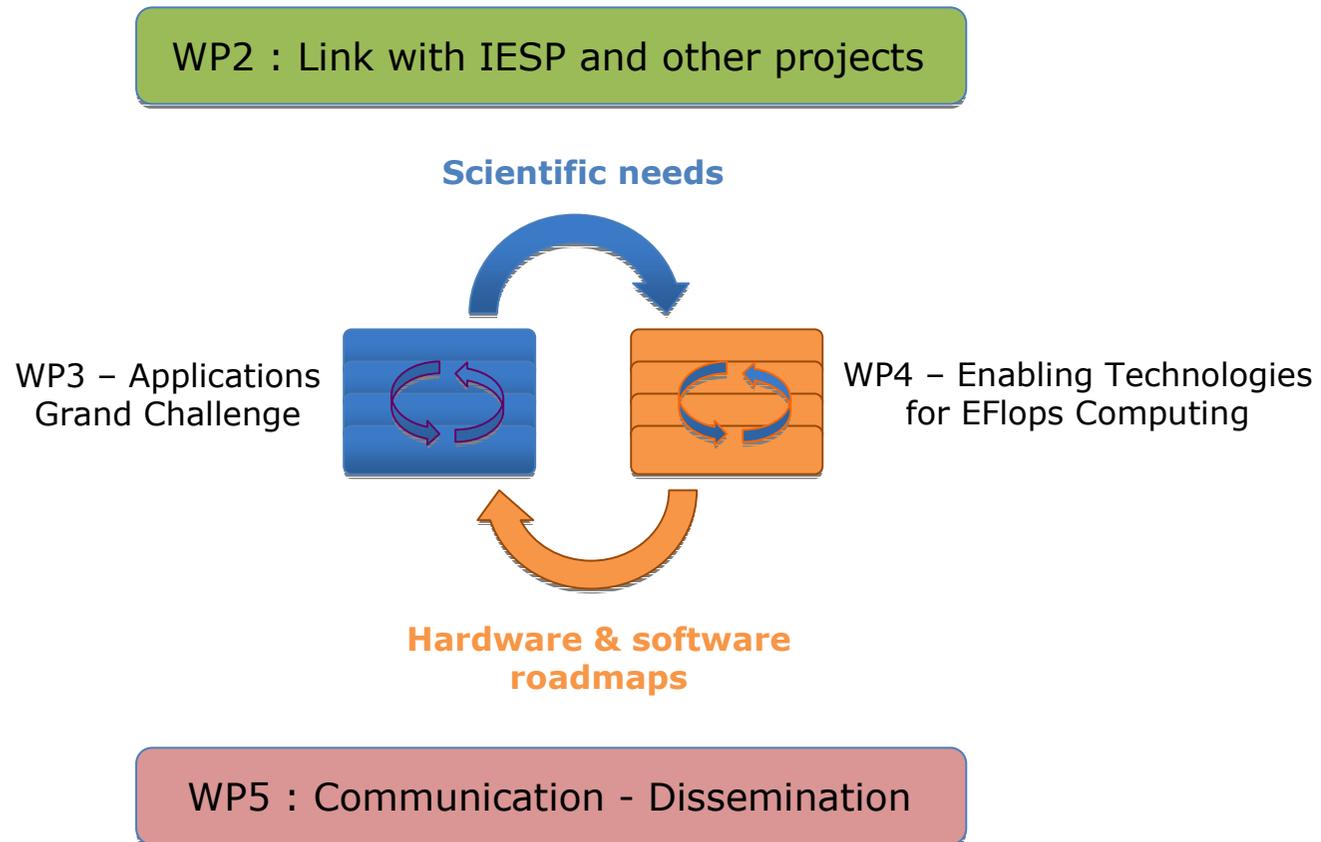
- WG 3.1 : Industrial & Engineering Apps (Transport, Energy)  
P. Ricoux (Chair, Total) & JC. André (Vice Chair, CERFACS)
- WG 3.2 : Weather, Climatology and Earth Sciences  
G. Aloisio (Chair, ENES-CMCC) & M. Cocco (Vice Chair, INGV)
- WG 3.3 : Fundamental Sciences  
G. Sutmann (Chair, CECAM-JSC) & JP. Nominé (Vice chair, CEA)
- WG 3.4 : Life Sciences and Health  
M. Orozco (Chair, BSC) & J. Thorton (Vice Chair, EBI)

- Enabling technologies for Exaflop computing (JSC)
  - Assess novel HW and SW technologies for Exascale challenges
  - Review IESP roadmap and discuss in broader EU context
  - Economic impact & European competitiveness
  - Build a European vision and a roadmap
  
- 4 working groups
  - WG 4.1 : Hardware roadmap, links with Vendors  
H. Huber (Chair, STRATOS/LRZ) & R. Brunino (Vice Chair, CINECA)
  - WG 4.2 : Software eco-systems  
F. Cappello (Chair, INRIA) & B. Mohr (Vice Chair, JSC)
  - WG 4.3 : Numerical libraries, solvers, and algorithms  
I. Duff (Chair, SFTC) & A. Grothey (Vice chair, Univ. Edinburgh)
  - WG 4.4 : Scientific software engineering  
M. Ashworth (Chair, STFC) & A. Jones (Vice Chair, NAG)

# WP3 and WP4 Interactions



## □ EESI General framework



# Common Guidelines for Group Activity



- Common templates in order to
  - Facilitate exchanges between WP3 and WP4
  - Identify and classify key issues (**What-Who-Where-When-How much**)
    - Description of the scientific and technical perimeter of the WG (\*)
    - Social benefits, societal, environmental and economical impact (\*)
    - Scientific and technical hurdles
    - Address cross cutting issues : Resilience, Power Mngt, Programmability, Performance and Reproducibility of the results, ...
    - European strengths and weaknesses in the worldwide competition
    - Sources of competitiveness for Europe
    - Needs of education and training
    - Potential collaborations outside Europe
    - Existing funded projects and funding agencies
    - Timeline, needs of HR, provisional costs, ...
    - Building an (or several) exa-scale prototype in Europe? By when?
  - Facilitate elaboration of intermediate and final reports

*(\*) for Application WGs, description in terms of Application Grand Challenges*

# Role of the Experts

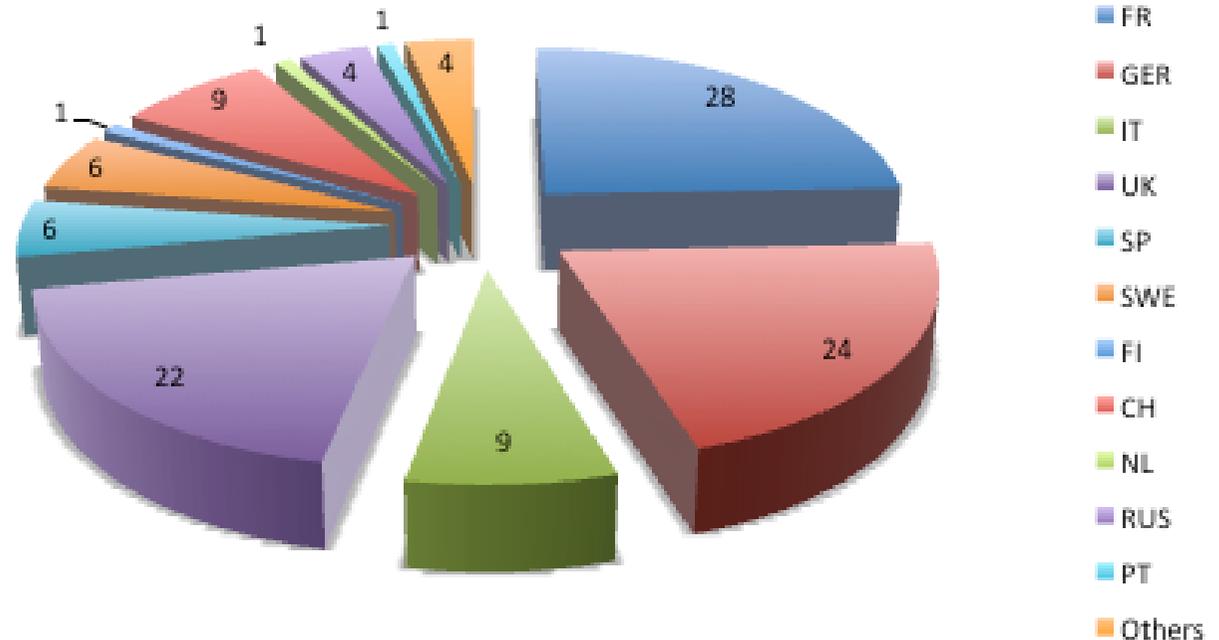


- Main contributors in the 2 work packages
- Complementary with IESP experts
  
- Status : about 15 experts / group
  - Includes experts from Switzerland and Russia
  - Non EU members if the expertise was missing in Europe
  - Ensured good “geographical” coverage
  - Ensured good coverage of all the topics

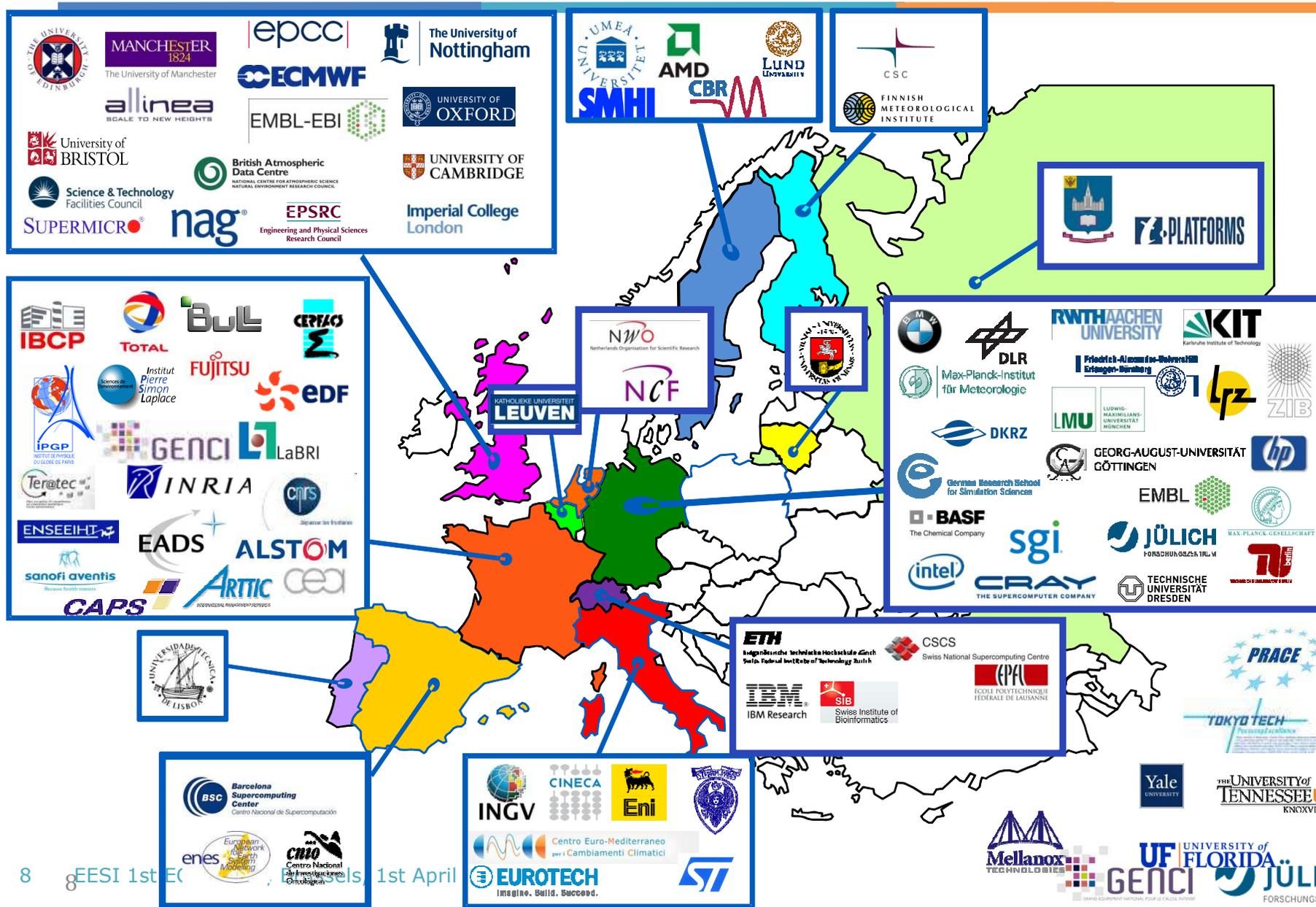
# Expert Distribution



- 118 experts excluding Chairs/Vice chairs
  - 14.7 experts/group av without Chairs/Vice Chairs
- 15 countries, good European coverage
- Participation of 3 US and 1 Israeli experts



# EESI participants



# Meeting Timeline



When	Where (who)	Purpose	Participants
2. Jul 2010	Paris (EDF)	Kick-off	ALL
18/19 Oct 10	Mauai (IESP)	IESP meeting	IESP invitees
9/10 Nov 10	Amsterdam	EESI Initial Workshop	ALL
Dec 10/Jan 11	? (C)	1 <sup>st</sup> Work Meeting	Each WG separate
9/10 Feb 2011	Bologna (WP34)	WG Coordination Meeting	WP34, C, some experts
Mar/Apr 2011	? (C)	2 <sup>nd</sup> Work Meeting	Each WG separate
5/7 Apr 2011	SFO (IESP)	IESP Meeting	IESP invitees
29/30 Jun 2011	Paris (Ter@tec)	Internal Workshop	WP34, C, experts
Sep 2011		Final Report Coordination	WP34, C
Oct 11	Cologne (IESP)	IESP Meeting	ALL
10/11 Oct 11	Barcelona (BSC)	Public Conference	ALL

NOW →

WP34: Work package 3 + 4 leaders (Stephane, Bernd)  
 C: Working group chair and vice chair  
 ALL: Everyone interested (on own money?)

# WP3 Summary and Future Work



- WP3 well on track
  - Engaged an impressive set of 58 enthusiastic applications experts from 12 countries → few more to enroll
  - Scientific and Technical status quo and technical hurdles clearly identified → need to work on costs, agenda and cross cutting issues
  - Draft reports (covering the 11 key issues) in preparation for the 2<sup>nd</sup> working group meetings
- Next steps
  - May 11: Produce working reports
  - Jun 11: Produce WP3 report
  - Jun 11: Final overall synchronization at June meeting

# WP4 Working Group Meetings



## □ 1<sup>st</sup> Meeting

Working Group	Where	When	No. of Experts
WG 4.1	Bologna, IT	Jan 21 <sup>st</sup> , 2011	13 of 17
WG 4.2	Paris, FR	Jan 7 <sup>th</sup> , 2011	15 of 16
WG 4.3	Edinburgh, UK	Feb 2 <sup>nd</sup> -4 <sup>th</sup> , 2011	11 of 13
WG 4.4	Daresbury, UK	Feb 2 <sup>nd</sup> +3 <sup>rd</sup> , 2011	12 of 15

## □ 2<sup>nd</sup> Meeting

Working Group	Where	When	No. of Experts
WG 4.1	Munich, DE	Mar 3 <sup>rd</sup> +4 <sup>th</sup> , 2011	?? of 17
WG 4.2	Aachen, DE	Mar 24 <sup>th</sup> +25 <sup>th</sup> , 2011	11 of 16
WG 4.3	Toulouse, FR	Apr 4 <sup>th</sup> -6 <sup>th</sup> , 2011	
WG 4.4	Lund, SE	Apr 18 <sup>th</sup> +19 <sup>th</sup> 2011	

# WG 4.3 Numerical Libraries, Solvers and Algorithms



□ Chair:  
Iain  
Duff  
(STFC)

□ Vice-Chair:  
Andreas  
Grothey  
(EPCC)

Expert Name	Field of Expertise	Organisation	Country
Jack Dongarra	HPC. Numerical linear algebra	Manchester/Tennessee	UK/USA
Mike Giles	GPU. CFD/Finance	Oxford University	UK
Gerard Meurant	HPC. PDE solution	ex-CEA Paris	FR
Volker Mehrmann	Linear algebra. HPC applications	TU Berlin/Matheon	DE
Torsten Koch	Combinatorial Optimization	Berlin	DE
Peter Arbenz	Eigenvalues. HPC	ETH Zurich	CH
Bo Kågström	Dense Linear Algebra	Ulmea	SE
Julius Žilinskas	Global optimization	Vilnius University	LT
Salvatore Filippone	HPC. Numerical software	Tor Vergata, Rome	IT
Luc Giraud	Iterative and hybrid methods	INRIA Bordeaux	FR
Patrick Amestoy	Direct methods. Solvers	ENSEEIH-IRIT, Toulouse	FR
Karl Meerbergen	Preconditioners	KU Leuven	BE
Francois Pellegrini	Mesh, load balancing	Bordeaux University, INRIA lab LABRI	FR



### □ Objectives

- Identify challenges for numerical libraries, solver and algorithms
- Develop research roadmap for the development for Exascale systems

### □ First results

- Discussed in detail scope of report and relation to other WGs
- Discussed requirements on support software including MPI
- Discussed cross-cutting themes
- Circulated internal discussion draft of working group report
- Next, experts will complete their parts of the report in preparation for the next meeting

# WG 4.4 Scientific Software Engineering



□ Chair:  
Mike  
Ashworth  
(STFC)

□ Vice-Chair:  
Andrew  
Jones  
(NAG)

Expert Name	Field of Expertise	Organisation	Country
Sebastian von Alftan	HPC algorithms and optimisation	CSC	FI
John Biddescombe	scientific visualisation	CSCS	CH
Ian Bush	HPC algorithms and optimisation	NAG	UK
Iris Christalder	HPC software frameworks	LRZ	DE
Rupert Ford	HPC algorithms and optimisation	University of Manchester	UK
Yvan Fournier	HPC algorithms and optimisation	EDF	FR
Joachim Hein	HPC algorithms and optimisation	Lund University	SE
Mohammed Jowkar	HPC algorithms and optimisation	BSC	ES
Peter Michielse	HPC algorithms and optimisation	NWO	NL
Stephen Pickles	HPC algorithms and optimisation	STFC	UK
Felix Schuermann	Blue Brain project	EPFL	CH
Stephane Ploix	Visualisation	EDF	FR
Christopher Greenough	Software engineering	STFC	UK
Ash Vadgama	Performance Modeling	AWE	UK



## □ Objectives

- Identify issues for Exascale application development
- Develop roadmap for an Exascale application development process

## □ First results

- Five themes were proposed and accepted:
  - Application frameworks and workflows
  - Visualization and data management
  - Fault tolerant algorithms
  - Application design
  - Software engineering
- Each theme was investigated and extensively discussed
- Cross-cutting issues were identified

# WP4 Summary and Future Work



- WP4 well on track
  - Engaged an impressive set of 60 enthusiastic European HPC SW experts
  - Scientific and Technical status quo and technical hurdles clearly identified
  - Draft reports (covering the 11 key issues) in preparation for the 2<sup>nd</sup> working group meetings
- Next steps
  - May 11: Produce working reports
  - Jun 11: Produce WP4 report
  - Jun 11: Final overall synchronization at June meeting