

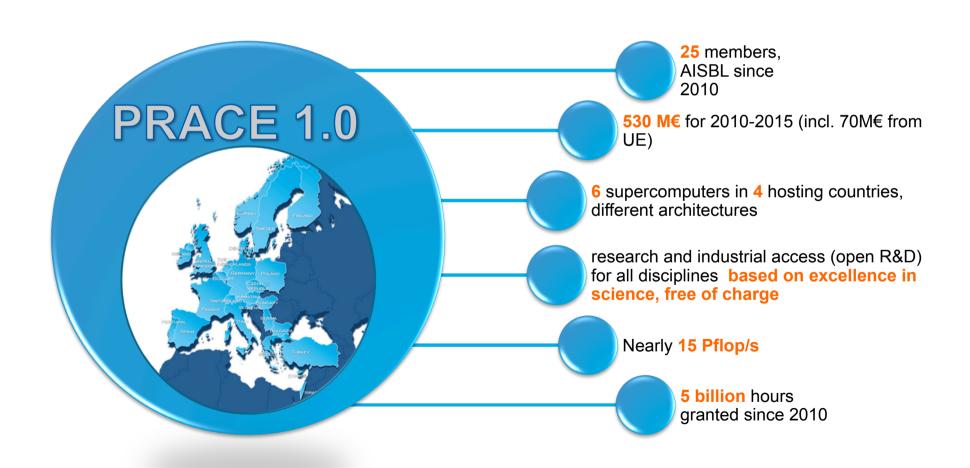
# PRACE Scientific Conference 2013 Sergi Girona

Chair of the Board of Directors and Managing Director

ISC, Leipzig, 16-June-2013



## The HPC European e-infrastructure (ESFRI)





### 25 members since 2010

PRACE has 25 members, representing European Union Member States and Associated Countries

#### **4 Hosting Members**

France: **GENCI** 

Germany: GCS - GAUSS Centre for Supercomputing

Italy: CINECA - Consorzio Interuniversitario

Spain: BSC - Barcelona Supercomputing Center

#### 21 General Partners

Austria: Johannes Kepler University of Linz

Belgium:

Direction générale opérationnelle de l'Économie, de

l'Emploi et de la Recherche

Bulgaria: NCSA
Cyprus: CaSToRC

Czech Republic: <u>VŠB - Technical University of Ostrava</u>

Denmark: <u>DelC - Danish e-Infrastructure Cooperation</u>

Finland: CSC - IT Center for Science Ltd.

Greece: GRNET
Hungary: NIIFI
Ireland: ICHEC

Israel: IUCC

The Netherlands: **SURFsara** 

Norway: SIGMA Poland: PSNC

Portugal: Universidade de Coimbra

Serbia: <u>IPB - Institute of Physics Belgrade</u>

Slovenia:

<u>University of Ljubljana, Faculty of Mechanical Engineering</u> <u>Sweden: Vetenskapsrådet – Swedish Research Council</u>

Switzerland: <u>ETH</u>
Turkey: <u>UYBHM</u>
UK: EPSRC



## PRACE's HPC resources in 2013

In 2013, PRACE is providing nearly 15 Pflop/s (Tier-0 competencies)

Universe Sciences

23%

**Fundamental** 

**Physics** 

18%

MareNostrum: IBM IDPX at BSC, >48 000 cores



JUQUEEN: IBM BlueGene/Q at GCS partner FZJ, >458 000 cores



FERMI: IBM BlueGene/Q at CINECA, >163 000 cores



SuperMUC: IBM IDPX at GCS partner LRZ, >147 000 cores

Biochemistry, **Bioinformatics** and Life sciences 10%

> Mathematics and Computer Sciences 2%

**Chemical Sciences** and Materials 21%

awarded since 2010

Earth System Sciences 12%

Engineering and Energy 14%

**CURIE:** Bull Bullx at **GENCI** partner CEA >90 000 cores.



**HERMIT**: Cray at GCS partner HLRS, >113 000 cores

# PRACE is a European infrastructure





# Financing: 530 M€ for 2010-2015 (incl. 70M € from UE)

### Contribution of Hosting Members (400 m€)

- TCO (total Cost Owner ship) of HPC systems
- Includes: HW, software, facilities, operations, energy,...

#### Membership fee, all members (7,5 m€)

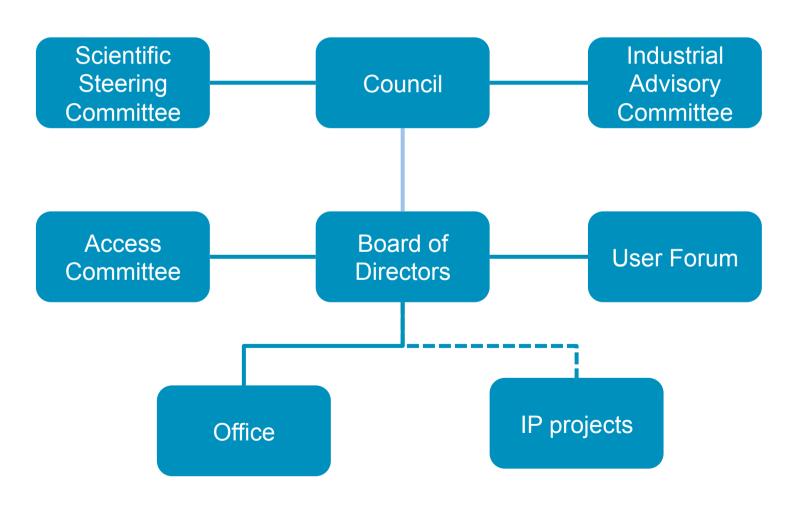
• Office operation: peer review, dissemination, legal

### Projects: PP, 1IP, 2IP, 3IP (122,5 m€)

- Legal support
- Dissemination
- Training
- Operation
- Application enabling
- Market watch
- Prototypes
- PCP, Pre-Commercial Procurement

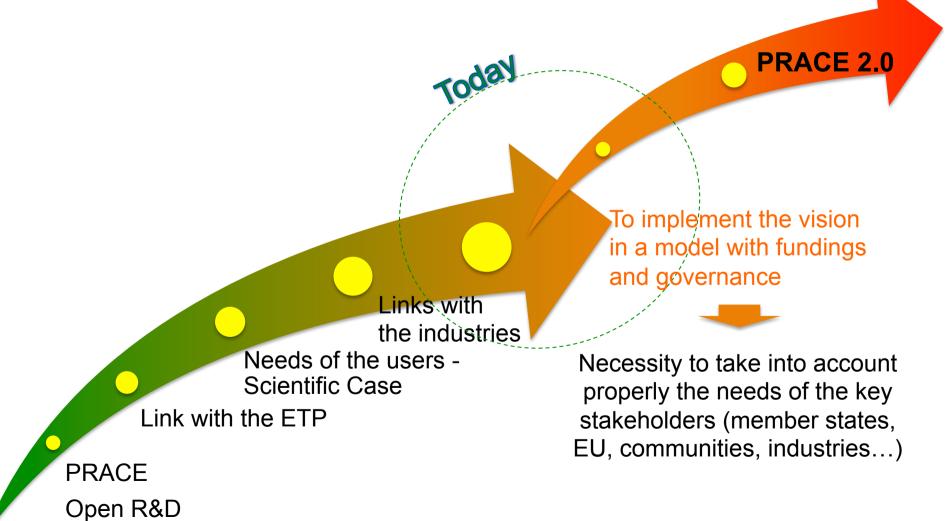


## Governance



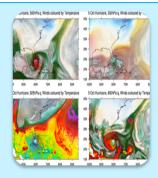


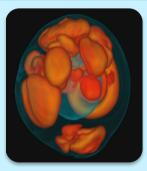
## What will be done between 2013 and 2015?

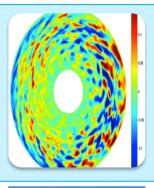




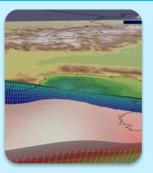


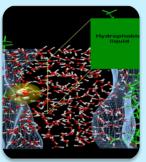












#### Climate

144 million core hrs on Hermit (DE) for UK - UB

PRACE will give to UK Met a 3 years advance in the development of their models (high resolution global weather & climate models).

#### Astrophysics

million core hrs: 98 on CURIE (FR) -49 on SuperMUC (DE) for Germany

This PRACE grant is one of the biggest worldwide allocation in this domain. Without this huge computational resources this project would not have been carried out in a reasonable time.

#### Energy

30 million core hrs on SuperMUC (DE) for Finland

PRACE resources enable the first European direct comparison of first-principles simulations to multi-scale experimental data for fusion energy (Link ITER).

#### Chemistry

59,8 million core hrs on JUQUEEN (DE) for Switzerland

Simplified models would not give reliable or meaningful results: Only PRACE systems are large enough to allow these computational models to be calculated.

#### Seismology

53.4 million core hrs on SuperMUC (DE) for Italy

The massive allocation of computing resources awarded via PRACE can be used to explore the non-linearity involved in the dependence of local ground shaking on geological structure.

#### Life Science

40 million core hrs on JUGENE (DE) for Germany

A single standard PC would need 5.000 years to do what JUGENE did in 100 days (40 million core hours) Only a PRACE system can offer enough resources to accomplish such a computationally intensive project.





## Recommendations from PRACE Scientific Case



# The need for HPC infrastructure at the European level

Europe should continue to provide a world-leading HPC infrastructure to scientists in academia and industry, for research that cannot be done any other way.



#### Leadership and Management

Leadership and management of HPC infrastructure at the Europe level should be a partnership between users and providers.



#### A Long-Term Commitment to Europe-Level HPC

A commitment to Europe-level HPC infrastructure over several decades is required to provide researchers with a planning horizon of 10–20 years and a rolling 5-year specific technology upgrade roadmap.



## Algorithms, software and tools

There is an urgent need for algorithm and software development to be able to continue to exploit high-end architectures efficiently to meet the needs of science, industry and society.



# Integrated Environment for Compute and Data

Europe-level HPC infrastructure should attach equal importance to compute and data, provide an integrated environment across Tiers 0 and 1, and support efficient end-to-end data movement between all levels. Its operation must be increasingly responsive to user needs and data security issues.



#### People and training

Europe's long-term competitiveness depends on people with skills to exploit its HPC infrastructure. It must provide ongoing training programmes to keep pace with the rapid evolution of the science, methods and technologies, and must put in place more attractive career structures for software developers to retain their skills in universities and associated institutions.

# 7

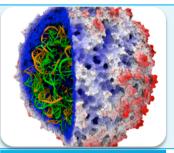
#### **Thematic Centres**

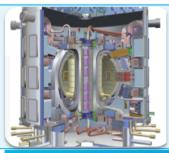
Thematic centres should be established to support large long-term research programmes and crosscutting technologies, to preserve and share expertise, to support training and to maintain software and data.





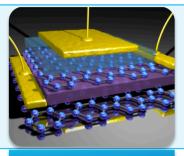
## Future challenges and scientific needs











## Personalised Medicines

- •Beyond the Omics revolution
- Rational drug design and systems biology

Scientific Case for HPC in Europe 2012-2020

 Reduce drug development costs (1.2B\$/drug), make test with humans safer and avoid animal testing (REACH)

### Renewable/sustainable

#### energy supply

- Design reliable and performant fusion reactors (ITER in 2019)
- Improve combustion and reduce greenhouse gases
- •Perform viable H<sub>2</sub> generation, storage and use on cars

# Managing the environmental change

- Towards a full global earth system for high resolution climate and weather / air quality forecast
- Early warning systems for earthquake ground motion simulation and seismic hazard

## Understanding the human brain

- Toward a full model of brain behaviour
- •Better understanding of the rise of serious diseases - Alzheimer -Parkinson
- •New chips and networks « brain inspired » → economic impact on the ICT market

## Improving Industrial processes

- breakthrough insights that dramatically accelerate and streamline R&D and engineering
- Improvement of business processes
- •Shorter product development duration, reduced total cost
- « green » supply chain

#### Agenda setting leading edge HPC capability

# Needs

- Higher resolution, longer timescale, multi-scale, multi-physics coupled models
- Validation, verification and uncertainty quantification
- ·Big data management, novel workflows
- •(re)development of applications, algorithms and software to efficiently exploit capabilities
- Co-design by multidisciplinary integrated teams
- Increasing capability, capacity, diversity of architectures
- Training and user support



# Links with the industry

# PRACE's Industrial Advisory Committee (IAC)

- To gather strategic expectations of industries
- To advise PRACE on the directions that best suit industrial needs
- To help to stimulate the use of HPC and numerical simulation by industry
- 1st meeting before October 2013

#### Specific initiatives

- PRACE: interactions with ETP4HPC
- Initiative towards SMEs: SHAPE (SME HPC Access Programme in Europe)
- Initiative towards large Companies: High-level executive meeting with industrial users
  - Airbus EADS, Rolls Royce, TOTAL, ENI (Feb. 8th)

#### Examples:

### EDF Energy (UK)

20.8 Mh on Hermit (HLRS, Germany)
6th call PRACE (March'13 to March'14)

**Objective:** by LES methods, modeling flow in a rotor of type « Magnus » or Turbosail

alternative-Concept for diesel engines



More ecological marine propellers

A. Revel (Univ Manchester)

#### RENAULT (France)

42Mh on CURIE (TGCC, France) 6th call PRACE (March'13 à March'14)

**Objective:** Improve the safety of vehicles by leveraging the simulation parameters of crashes

Unattainable ambition with internal resources of Renault



Anticipate new security regulation (EuroNCAP6 in 2015)

M. Pariente, Y. Tourbier (Renault)

# **Amplify services beyond Open R&D**

- □ Pre-Competitive R&D
  - Like an Open R&D model, but with more time to publish results (2 or 3 years), so to gain competitive advantage in the meantime
  - Possibility to not publish at the end and pay for the compute hours used



Pilot with interested companies?

- ☐ SHAPE : SMEs HPC Adoption Programme for Europe
  - In complement of national initiatives in France, Germany, Italy, UK, ...
  - Evangelize SMEs who want to engage in numerical simulation and HPC
  - Support them with services up to a proof-of-concept :
    - Training in PRACE centers
    - Expertise, both in HPC and in domain-specific problems
    - Access to resources to demonstrate a real industrial case



Pilot with supply chains in one or two selected fields?



#### **PRACE Advanced Training Center**

- 6 Centers: BSC, CINECA, CSC, EPCC, Gauss Center for Supercomputing, Maison de la Simulation
- Joint Curriculum, with 71 PATC courses in 2012-13
  - Message Passing (9)
  - Threading (8)
  - Mixed-mode Parallel Programming (7)
- Performance Analysis, Optimisation, Debugging (14)
- Scientific Programming and Computing (8) Software Engineering (8)
- Numerical Libraries (2)
- Scientific Visualisation (3)
- Accelerators (10)
- PGAS Programming (5)
- I/O Optimisation and Parallel I/O (7)
- Domain-specific courses (6)

#### Success Story: May 2012 - March 2013

- 60 Courses
- 176 Training days
- 1394 participant
- 24 PRACE countries, rest of Europe, Africa, Asia, N & S America.
- On average per course, ~23 participants and ~16% "visiting".
- 8.5/10: Average overall course rating, from 658 feedback forms collected from 47 courses



# PRACE 2.0 strategy: Meeting Europe's ambitions with HPC (1/4)

Provide an infrastructure for science and industry

- To maintain Europe as an agenda setting science contributor
- By offering access to leading edge HPC platforms
- opened to all disciplines and countries in Europe

Attract, train and retain competences

- To attract, train and retain highly skilled and innovative workforce in science and engineering
- To share knowledge and expertise

Provide an high quality service

- With at least one supercomputer in each major architectural class
- To support world-leading science

Lead the integration of an highly effective HPC ecosystem

#### Including:

- A) scientific and industrial communities,
- B) national HPC centres and their support for the PRACE systems
- C) training and software development efforts



# PRACE 2.0 strategy:

Principles (2/4)

To serve scientific excellence

To serve economic and technological competitiveness

To reinforce partnership between users and PRACE

To develop a **persistent** e-infrastructure

To aim at subsidiarity

To take a fair account of past contributions

To ensure transparency on information, access,...

To pursue the solidarity among members

To strive to openness



# PRACE 2.0 strategy:

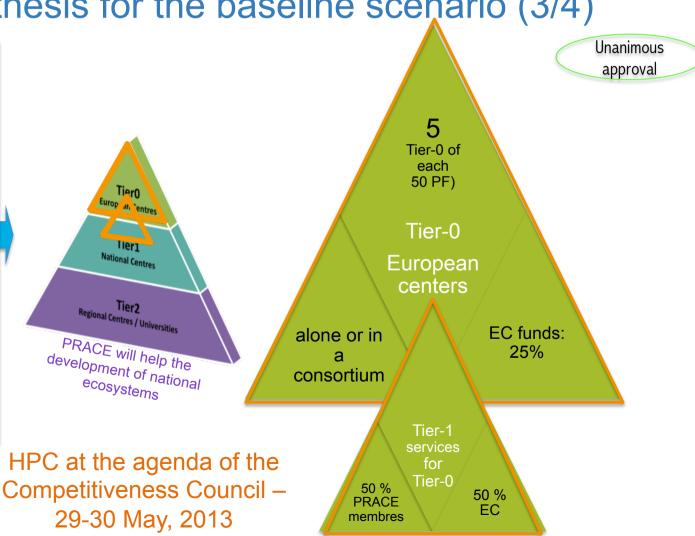
Hypothesis for the baseline scenario (3/4) **Ambitions** 

Provide an infrastructure for science and industry

Attract, train and retain competences

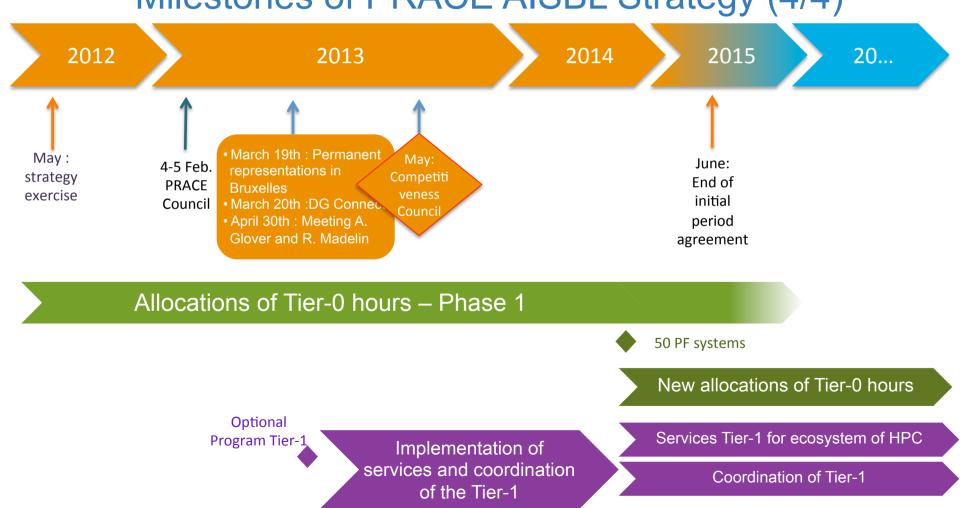
Provide an high quality service

Lead the integration of an highly effective HPC ecosystem





# PRACE 2.0 strategy: Milestones of PRACE AISBL Strategy (4/4)







## COUNCIL OF THE EUROPEAN UNION

Brussels, 31 May 2013

10322/13

RECH 218 COMPET 379 IND 170 TELECOM 149

#### **OUTCOME OF PROCEEDINGS**

From: Council

To: Delegations

No. Cion Prop.: 6596/12 RECH 56 COMPET 96 IND 31 TELECOM 32

No. Prev. doc.: 9808/13 RECH 182 COMPET 325 IND 161 TELECOM 133

Subject: - Communication from the Commission on "High Performance Computing: Europe's place in a Global Race"
- Council conclusions





# Highlights of Competitiveness Council Conclusions

- WELCOMES the attention brought to the issue of High Performance Computing
- STRESSES its strategic importance to the EU's industrial and scientific capabilities
- RECOGNISES the achievements of PRACE in pooling leadership-class computing systems and making them available to all researchers in the EU and associated countries, on the basis of, and in order to enhance, scientific excellence and innovation and the need to maintain this approach
- EMPHASIZES the **strength of the EU** in applications, low-power computing and integration
- ACKNOWLEDGES the efforts of HPC stakeholders to support the implementation of an EU- level HPC strategy, in particular PRACE as an independent actor on the scientific side and the industry-led European Technology Platform for HPC (ETP4HPC)

- RECOGNISES the need for an EU-level policy in HPC addressing the entire HPC ecosystem: world-class and sustainable HPC infrastructure; HPC use by Science and by industry, including SMEs; HPC industrial supply for development of exascale computing; excellence in HPC software, methodology and applications; and achieving a level-playing field for EU companies;
- 9 INVITES Member States, the Commission, and industry to ensure appropriate investments in HPC
- INVITES Member States and the Commission to step up the efforts to substantially increase the supply of scientists and engineers with HPC skills, through adequate training and educational programmes addressed to industry and academia;
- ASKS the Commission to explore funding possibilities and instruments to support the development of leadership-class HPC capabilities in Europe as well as the acquisition of world-class HPC systems on the global market on the basis of open competition to address the needs of various HPC user communities
- 15 INVITES the Commission to develop and elaborate its plans for HPC



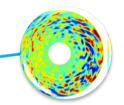


## Conclusion

Involving PRACE is a necessity

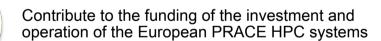
Sustainability for 2015-2020 and beyond

EC and member states acting together

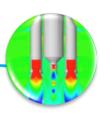


Recognize the achievements of PRACE to pool leadership-class computing systems and make them available to all researchers in all scientific communities on the basis of their scientific excellence

Support the development of PRACE as THE sustainable e-infrastructure to address societal and scientific challenges and for stimulating innovation in Science and industry



Support the European dynamic via a coherent and cooperative program for three pillars strengthening science, industry and the technology supply chain



Build on existing expertise, while raising the HPC skills and competencies through training and educational programs open to academia and industry



# Thank you very much for your attention!

#### **PRACE** aisbl

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