# PARTNERSHIP FOR ADVANCED COMPUTING IN EUROPE
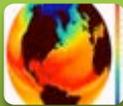
**PRACE the European HPC infrastructure: World Class HPC Services for Science**

Sergio Bernardi (CINECA), PRACE Board of Directors
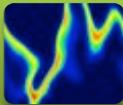Scalability Workshop, ECMWF, April 2014

# HPC Context in Europe: a strategic tool

## For Science

**Meteorology, climate, earth sciences**
- Measure global warming and climate evolution
- Anticipate climate events

**Astrophysics, Particle physics, Plasma physics**
- Understand the evolution of galaxies
- Explore advanced physics (LHC, ITER)

**Material sciences, Chemistry, Nanosciences**
- Design smart materials
- Understand better nanomaterial properties

**Life sciences**
- Explore biological systems
- Drug design

**Energy and engineering**
- Lower the energetic impact of industry
- Design tomorrow's power plants

## To support public policies

**Natural risks**
Modeling the progress of the seismic waves during the Sichuan earthquake

**Epidemiologic risks**
Modeling the spread of the H1N1 infection

**Public policies impact**
EDF: transport of sediments and saltiness in the Loire basin, on a time period of 10 to 20 years

**Security**
Search of virulence and resistance to antibiotics

## To boost Industrial innovation

**Solve instabilities in helicopter engines**
CERFACS
Shortens conception cycle (6 months)

**Speed-up airplane design**
AIRBUS
Saves money in wind-tunnel costs (20%)

**Increase efficiency of oil search and production**
Eni
Avoids useless drillings (80 M$ avg)

# PRACE : THE EUROPEAN HPC RESEARCH INFRASTRUCTURE

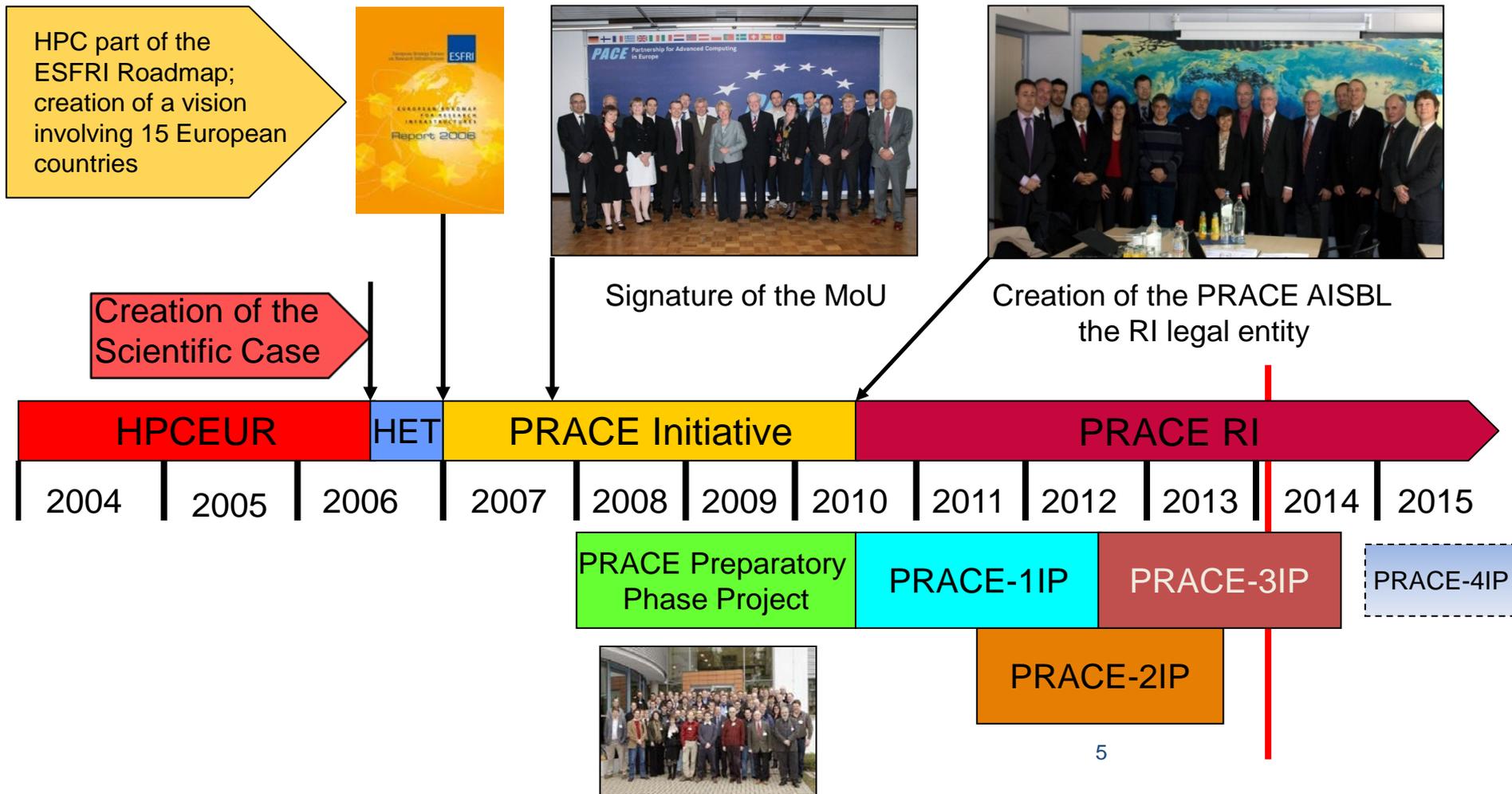# PRACE: *the* European HPC Research Infrastructure

- Enabling **world-class science** through large scale simulations

- Providing **HPC services** on **leading edge capability** systems

- Operating as a **single entity** to give access to **world-class supercomputers**

- **Attract**, **train** and **retain** competences

- **Lead** the **integration** of a highly effective **HPC ecosystem**

- Offering its resources through a **single** and **fair** pan-European **peer review process to academia and** industry

- **25** members, since 2010
- **6** supercomputers in **4** hosting countries, nearly **15 Pflop/s**
- Common operation procedure between **35** centers in Europe
- **22** prototypes evaluated
- **169** white papers produced
- **1500** communications from our users
- **166** Thesis
- HPC Community building: **183** events

- **8 billion** hours granted since 2010 (a system with 900k cores for 1 year)
- **303** scientific projects enabled from **38** countries
- More than **20 SME** and **industries** access in first year
- **360** PATC Training days
- **2734** Trained people
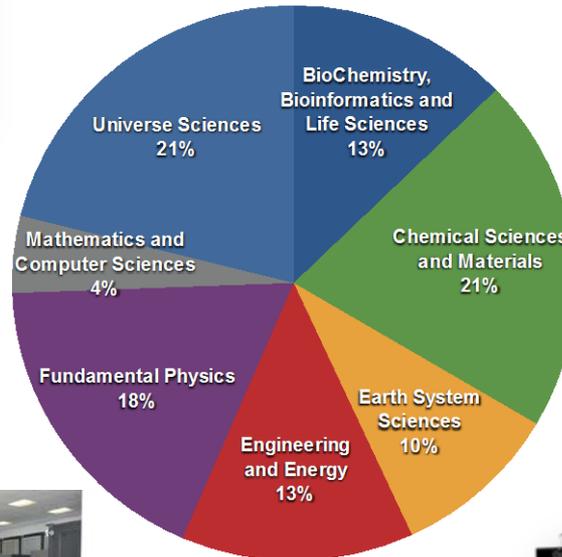- **170** applications enabled

# PRACE History: An Overview of a Success Story

HPC part of the ESFRI Roadmap; creation of a vision involving 15 European countries

Signature of the MoU

Creation of the PRACE AISBL the RI legal entity

Creation of the Scientific Case

| HPCEUR | HET | PRACE Initiative | PRACE RI |

2004 · 2005 · 2006 · 2007 · 2008 · 2009 · 2010 · 2011 · 2012 · 2013 · 2014 · 2015

PRACE Preparatory Phase Project

PRACE-1IP

PRACE-3IP

PRACE-4IP

PRACE-2IP

# PRACE operations after 4 years

> *15 Pflop/s provided*

**8 BILLION CORE HOURS awarded since 2010**

**MareNostrum:** IBM BSC Barcelona, Spain

1 PF

6 PF

**JUQUEEN :** IBM BlueGene/Q GAUSS/FZJ (Forschungszentrum) Jülich, Germany

3.2 PF

**SuperMUC:** IBM GAUSS/LRZ (Leibniz-Rechenzentrum) Garching, Germany

2 PF

**CURIE :** Bull Bullx GENCI/CEA Bruyères-le-Châtel, France
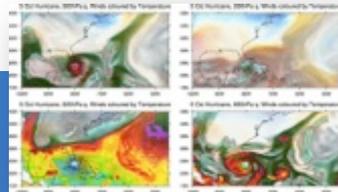
2 PF

**FERMI:** IBM BlueGene/Q CINECA Bologna, Italy

1 PF

**HERMIT :** Cray GAUSS/HLRS (High Performance Computing Center Stuttgart) Stuttgart, Germany

Pie chart:
- Universe Sciences 21%
- BioChemistry, Bioinformatics and Life Sciences 13%
- Chemical Sciences and Materials 21%
- Earth System Sciences 10%
- Engineering and Energy 13%
- Fundamental Physics 18%
- Mathematics and Computer Sciences 4%

# Scientific achievements: example

Academia

## FACING THE TEMPEST
**A three-year advance in developing new models**

→ **Possibility for the UK Meteorology Office to develop worldwide high-resolution climate models (12 km)**

- Largest allocation ever made on a single PRACE system
- UPSCALE Project
- Focused on tropical Atlantic storms

National Centre for Atmospheric Science
NATURAL ENVIRONMENT RESEARCH COUNCIL

**144 million core hours** on Hermit (Germany)

Team: **Prof. Pier Luigi Vidale** (NCAS-Climate, Dept of Meteorology, Univ. of Reading and UK Met Office, Exeter, UK)

## IMAGING A WHOLE SEISMIC AREA
**1st numerical mapping of the North of Italy**

INGV

→ **Estimate the effects of major earthquakes according to local geological structures, thus providing better foundations for decision-making processes**
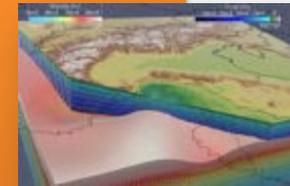
- SHAKEIT Project
- North of Italy = most active seismic area in Europe

**53,4 million core hours on SuperMUC (Germany)**

Team: **Dr. Andrea Morelli** – Instituto Nazionale di Geofisica e Vulcanologia, Italy

7

# Scientific achievements: example

Industry: SMEs

## ASSESSING NATURAL RISKS
**From a 27x27 to a 3x3 km resolution**

→ **Creation of a database to assess flood risks due to extreme weather events all over The Netherlands**

- Among the first SME granted on a PRACE system
- OASIS-ARIA-HPC Project
- Collaboration with academics within the Climate-KIC OASIS European project
- Ensemble simulation on 512 cores

**6 milion core hours**
on CURIE
(France)

ARIA TECHNOLOGIES

## USING HPC TO DISCOVER NEW THERAPIES

Dompé

→ **Creation of a database containing a comprehensive range of possible protein targets for every drug available**

- One of the first pilot of the "Open R&D" model
- Conducted between industry and academic researchers: Dompé/University of Parma/Cineca
- Systematical investigation of protein-drug interactions through massive docking studies
- **Unexpected result: a drug registered in 1981 for hypertension has an effect against prostate cancer**
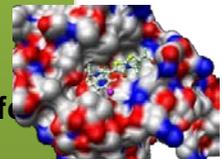
**200 000 core hours**
on CURIE
(France)

Team: Dompé/University of Parma

## CAPABILITY & CAPACITY SIMULATIONS

# PRACE supports international collaborations on climate

**Example: Earth System Sciences**

**38 million** (5th Call) **+ 50.44 million** (7th Call) **core hours on MareNostrum (Spain)**

In HiResClim we use a seamless multi-model climate modelling approach, which, as well as being the most efficient way to **utilise the most advanced HPC systems of today** and improve the realism of climate simulations, is also the only path to providing robust and actionable estimates of climate changes.
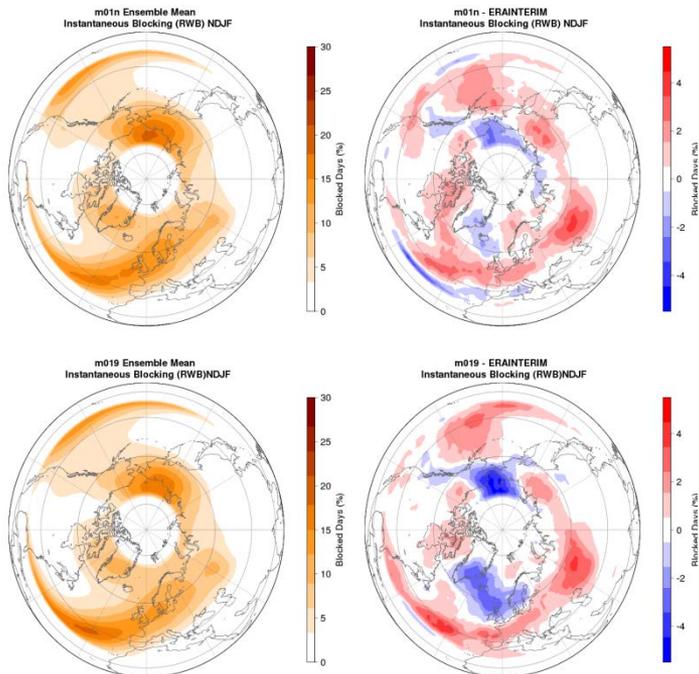


**Team: Dr Colin Jones** - Swedish Meterological and Hydrological Institute (SMHI) (5th Call) and **Dr. Francisco Doblas-Reyes** - Institut Catal de Cincies del Clima, Spain (7th Call)

**Collaborators**: Catalan Institute of Climate Sciences, Spain; Linkoping University, Sweden; CERFACS, France; the Royal Netherlands Meteorological Institute (KNMI); and the Swedish Meterological and Hydrological Institute (SMHI)
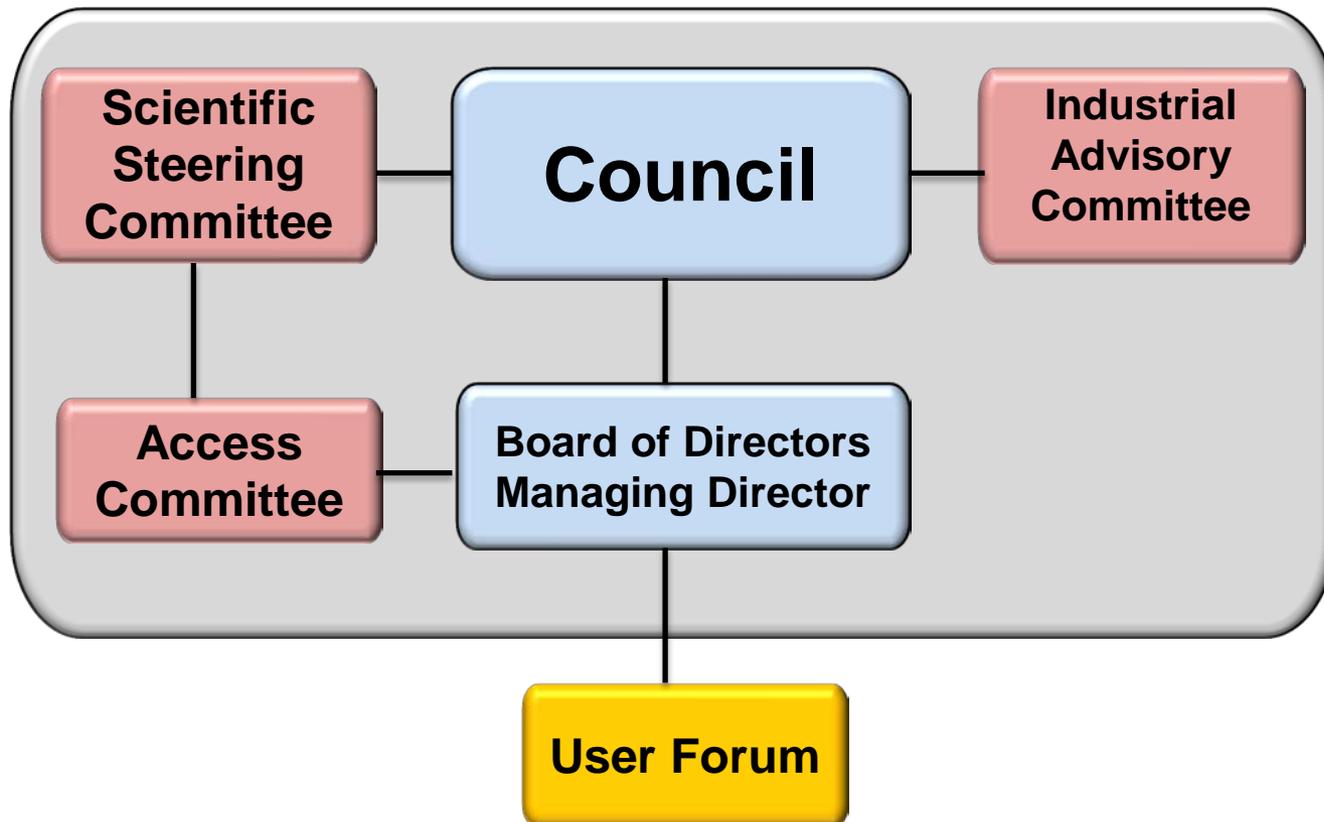
**Goal:** HiResClim aims to make major advances in the science of estimating climate change and formulating climate predictions . This will be achieved by addressing the dual requirements of increased climate model resolution and increased number of ensemble realizations of future climate conditions over a range of time scales and for a set of plausible socio-economic development pathways.

Blocking index (Rossby wave breaking) from four-month EC-Earth3 simulations with T255/ORCA1 (top) and T511/ORCA025 (bottom) resolution. November start dates over 1993-2009 using ERA-Interim and GLORYS initial conditions. – **Copyrighted image**

*InfraStructure for the European Network for Earth System Modelling*

is-enes

# PRACE GOVERNANCE AND ORGANIZATION

# User and communities in the governance

❑ **Scientific Steering Committee**

- Responsible for giving opinions on all matters of a scientific and technical nature
- Proposes the members of the Access Committee
- Examples
  - Guides Peer Review Process
  - Steered Creation of Scientific Case
  - Gave advice on Programme Access, Cooperation with XSEDE, …
  - SSC Chair is member of the Board of Directors

❑ **Industrial Advisory Committee**

- Similar role for industrial users and their requirements

# User and communities in the governance (2)

❑ **Access committee**

- Giving opinions on the scientific use of Tier-0 Infrastructure
- Providing recommendations on the allocation of PRACE resources based on the Peer Review process

❑ **User Forum**

- Open to all (potential) PRACE users from academia and industry
- Main communication channel between HPC users and PRACE AISBL
- Interaction with members of the PRACE AISBL
- Discussion and issuing recommendations to PRACE AISBL
- Promoting HPC usage
- Fostering collaborations between user communities

# An access model focused on the sole criterion of scientific excellence

❑ Free at point of use, need to publish results at the end of the grant period

❑ Three types of resource allocations for scientists

- **Preparatory Access**
  - optionally with support from PRACE experts
  - Prepare proposals for Project Access

  **50 or 200k CPU hours/ proposal**

- **Project Access** (every 6 months)
  - For a specific project, grant period ~ 1 year
  - For individual researchers and research groups (no restriction of nationality for both researcher and centers)

- **Programme Access**
  - Available to major European projects or infrastructures that can benefit from PRACE resources
  - Planned for 2 years allocation

# Peer review

## ❑ Peer review process

- A single process for evaluating proposals
- Expert assessment
- Transparency and confidentiality
- Right to reply
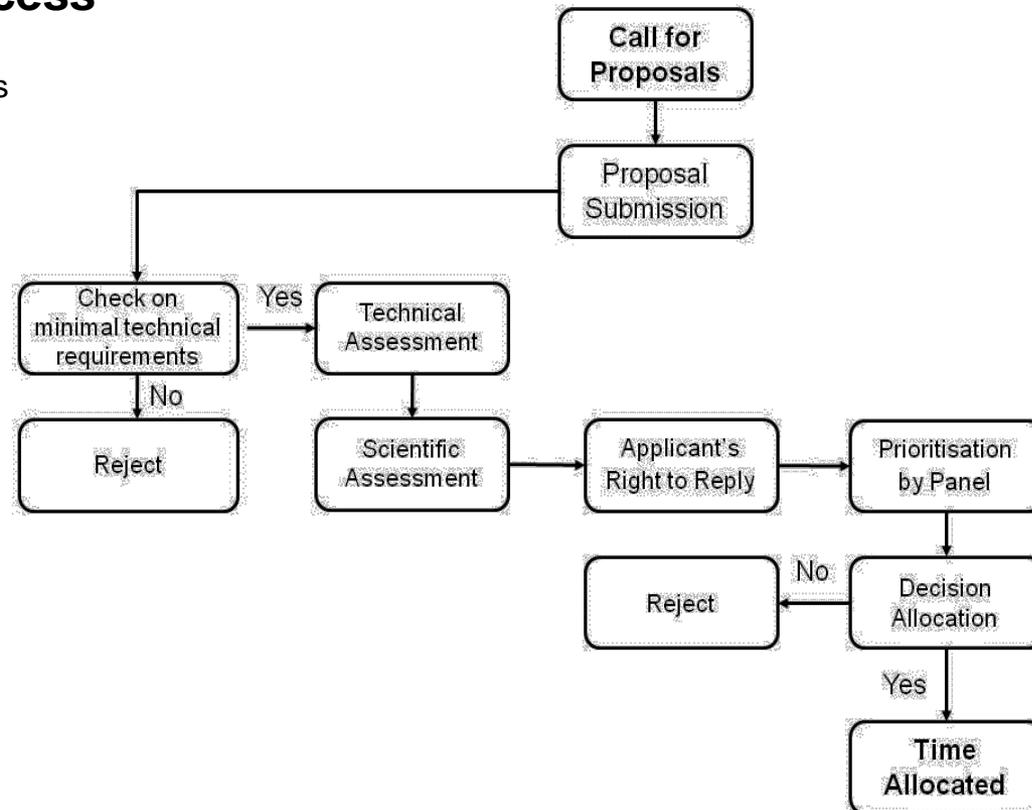
# Types of Access

| | Preparatory | Project | Programme |
|---|---|---|---|
| **Technical Assessment** | Yes | Yes | Yes |
| **Scientific Assessment** | No | Yes | Yes |
| **Mid-term Review** | No | No | Potentially |
| **Duration** | 6 months | 12 months | 24 months |
| **Final Report** | Technical | General | General |

# How PRACE is addressing a key challenge: Training
## 71 PATC courses per academic year



### SYLLABUS FOR AUG.–DEC. 2012

**August**

27.08.–29.08. • FEM Workshop [CSC]

28.08.–30.08. • GPU Programming with CUDA and OpenACC [EPCC]

**September**

03.09.–07.09. • Parallel Programming with MPI and OpenMP and Advanced Parallel Programming [GCS]

11.09.–13.09. • Fortran 2003/2008 [CSC]

11.09.–14.09. • MPI + MPI–IO [MdS]

17.09.–21.09. • Advanced Fortran Topics

24.09.–26.09. • Introduction to Parallel Programming with MPI & OpenMP [CSC]

**October**

01.10.–04.10. • C/C++ Multicore Application Programming [MdS]

08.10.–10.10. • Introduction to Parallel Programming and Message Passing Paradigm (MPI) [CINECA]

11.10. • Introduction to OpenMP Programming [CINECA]

12.10. • Introduction to Hybrid Programming MPI+OpenMP [CINECA]

16.10.–19.10. • 10th VI–HPS Tuning Workshop [GCS]

19.10. • Hybrid Programming for Material Science [CINECA]

24.10.–26.10. • Usage of CURIE@CEA–TGCC Tier–0 Supercomputer and Related Best Practices [MdS]

29.10.–31.10. • Advanced Parallel Programming [CSC]

**November**

05.11.–08.11. • Cray XE6 Optimization Workshop [GCS]

12.11.–13.11. • HPC Surgery: debugging, profiling and optimization of a scientific code [CINECA]

19.11.–21.11. • Programming on GPUs [MdS]

20.11.–22.11. • Cray Systems Workshop [EPCC]

26.11.–27.11. • Large Scale Data Visualization with Visit [MdS]

26.11.–28.11. • HPC Enabling of OpenFOAM for CFD Applications [CINECA]

26.11.–30.11. • Parallel programming Workshop (BSC)

**December**

03.12.–04.12. • Tools and techniques for scientific programming on BG/Q (Fermi) [CINECA]

04.12.–05.12. • Software Carpentry [EPCC]

10.12.–11.12. • Software Development Tools [MdS]

13.12.–14.12. • Introduction to simulation environment for earth sciences [BSC]
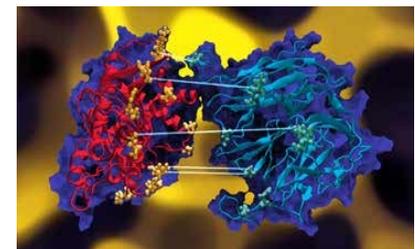
# PRACE AND THE COMMUNITY OF CLIMATOLOGY AND WEATHER

# How PRACE presently supports the climate community



- Support to large scale international research projects
  - More than 400 million core hours for 12 projects:
    - 5% of the total number of resources and 4% of the total number of projects
  - Projects from academia and industry:
    - P.L Vidale (NCAS, UK) : High resolution global climate models applied to extreme events – 144 Mh on Hermit (HLRS@GCS) ➔ First ever in the domain
    - ARIA Technologies (France) : risk assessment applied to extreme rainfall conditions and flooding– 6 Mh on CURIE (TGCC@GENCI)
    - Colin Jones (SMHI, Sweden): HiResClim aims to make major advances in the science of estimating climate change and formulating climate predictions – 38 Mh on MareNostrum (BSC)
    - Francisco Doblas-Reyes (Institut Catal de Cincies del Clima, Spain): HiResClim second proposal – 50 Mh on MareNostrum (BSC)
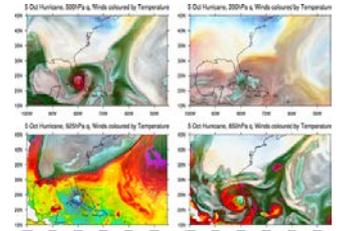
# How PRACE presently supports the climate community



- Support to application development
  - Preparatory Access for porting and scaling out of climate apps
  - Co-development (software refactoring, development of new algorithms) - PRACE-2IP WP8 « Community code scaling »
- Training
  - 6 PRACE centers (PATCs) 71 courses in 2013
  - Support to specific actions : « 2nd European Earth Systems & Climate modeling school »
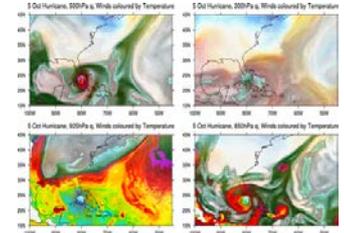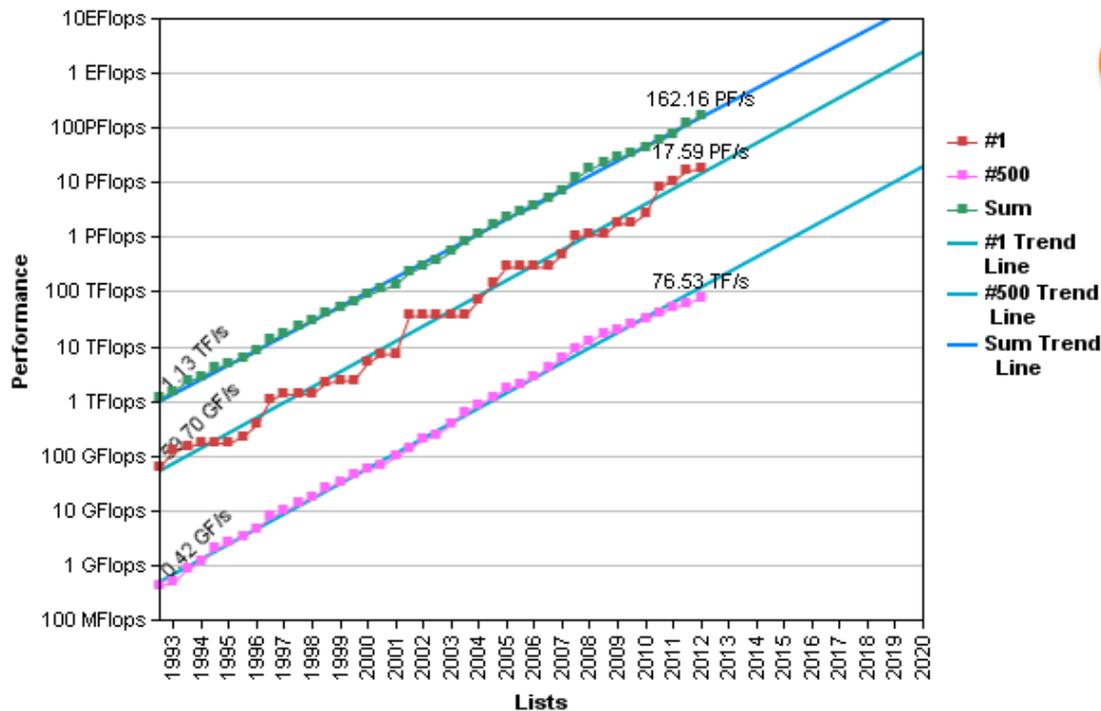
# FUTURE CHALLENGES AND NEXT STEPS

# Technology cycle: A challenge in itself is the road to exascale and beyond



Strong issues in :
- ✓ Power consumption
- ✓ Data management
- ✓ Heterogeneity, …

But the real challenge = How to best use these machines in the future !

# The HPC European e-infrastructure: persistency, long term sustainability

**Scope of the EC H2020 HPC support**

- Provision of seamless and efficient Tier-0 services adapted to the needs of different user classes
- Activities that build on national Tier-1 capabilities (training, service prototyping, software development etc.)

- Governance, business models and long term financial sustainability
- Strategy for deployment of world-class HPC environment

- Openness to new user communities and new applications, and Industrial take-up of HPC services in particular by SMEs

- Work in synergy with:
  - Centres of Excellence
  - European Technology Platform for HPC by providing specs for future exascale prototypes and systems

- Training and skills development


Tier0 European Centres
National Centres
Tier2 Regional Centres / Universities
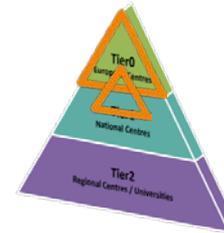
- Infrastructure based on 50 Pflop/s systems (minimum)
- 100 M€ minimum TCO

**Services/Ecosystem**
- Training
- Mobility program to users
- Code porting, application enabling
- Communication, dissemination
- New types of access

PRACE 2.0

23

# CONCLUSION

**Our next frontier:** supercomputing for all

**Priority**: To extend the use of HPC, especially among SMEs

**Aim**: To support the scientific communities for future global challenges

**Necessity**: To improve the collaboration with end-users, ISV, open source communities…