



# PARTNERSHIP FOR ADVANCED COMPUTING IN EUROPE

## How does the PRACE Scientific Steering Committee (SSC) work?

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*University of Barcelona*

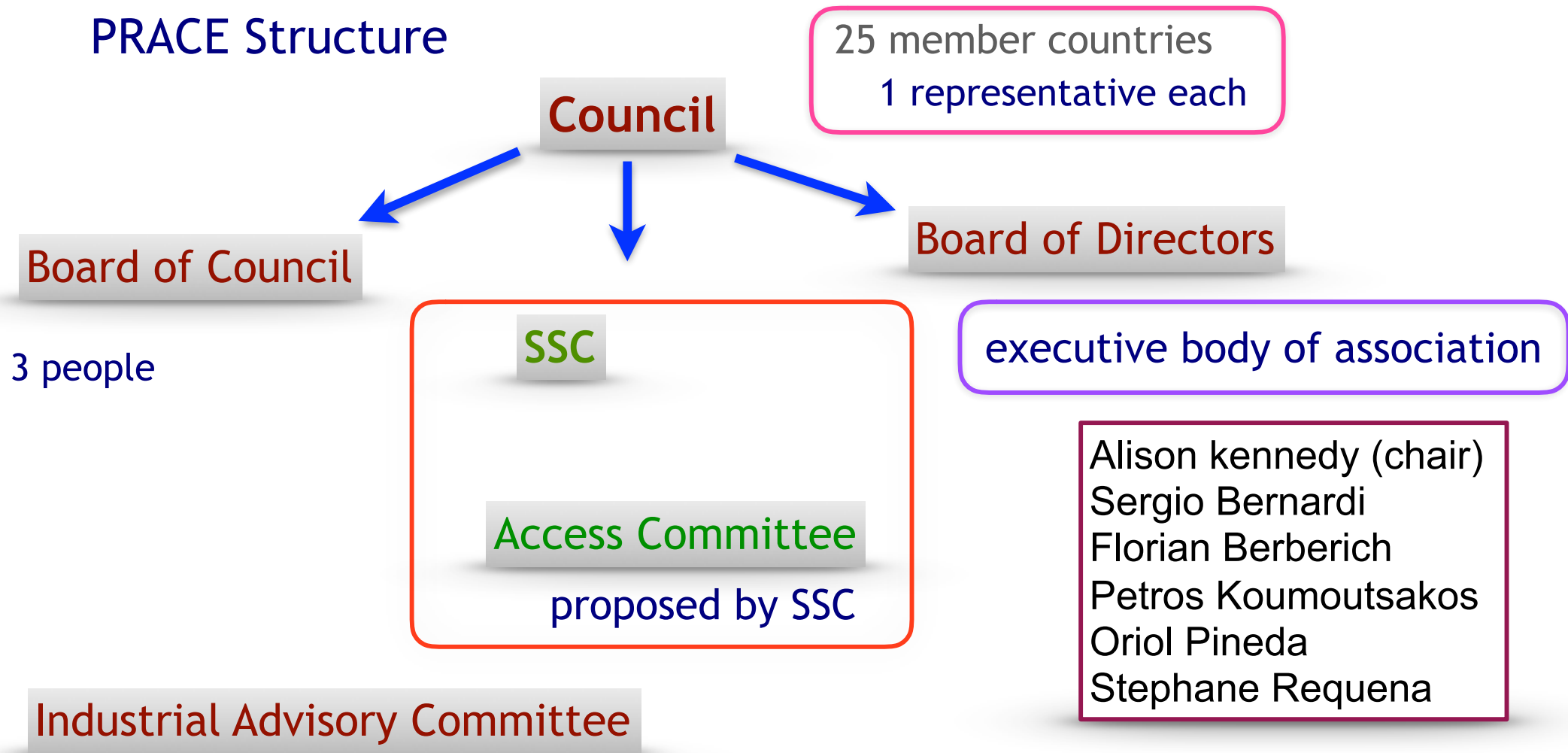
05/03/2015





# PARTNERSHIP FOR ADVANCED COMPUTING IN EUROPE

## PRACE Structure





## Role of SSC

Advice / guidance

scientific / technical matters associated to scientific work in PRACE

Active role to ensure the scientific quality of PRACE projects

Contributes to set long-term agenda in HPC in PRACE

liase with users

develop scientific case

Provides input for hardware required from scientific needs



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## Identify european infrastructure

Tier 0 unprecedented capabilities European scientists  
experience in new types of machines  
technologically competitive: keep up scaling-up resources

## Scientific/engineering case

plasma physics	: grid size	... plasma turbulence
particle physics	: increase physical volumes	... excited states
climate modeling	: increase resolution ..	improve predictive capabilities
fluid dynamics	: explicit resolution of turbulence	

## Heterogeneous architectures

particle physics	
chemistry	weak communication between nodes

climate	
fluid dynamics	high level communication

needs of storage /capacity



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## **Essential to progress on science and innovation**

- Larger size of domains, more complex physical, chemical and biological systems
- Gain experience on new types of machines

## **Importance of the HPC ecosystem: national & European**

Tier 0, European: High-end experiments; Much larger allocations than at national level

Tier 1, National: smaller problems, more production runs (larger number of simulations), new developments ...

## **International competition**

- Need for larger allocation: several 100s M core hours
- Support to prepare codes

## **Range of architectures**

- Independent processes or particles (weak communications, limited memory per node)
- Fluid dynamics (higher level of communication and more memory per node)
- Some domains require a high storage capacity (climate ...) ;
- Emerging needs to analyse enormous data volumes (e.g. astronomy)





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## SSC Composition

European leading researchers

Cover relevant areas

science  
engineering  
supercomputing

Balance gender  
geography

Odd number up to 21

Serve two year term  
+ extension

Appointed by Council

Last Name	First Name	Field	Country
Bécoulet	Marina	Plasma physicists / Fusion	France
Casciola	Carlo Massimo	Engineering/CFD	Italy
Drury	Luke	Universe sciences	Ireland
Filipe	Claudia	QMC developer	The Netherlands
Grigori	Laura	Numerical mathematics, HPC	France
Komatitsch	Dimitri	Computational earth sciences	France
Koumoutsakos	Petros	Computation Science and Engineering	Switzerland
Lindahl	Erik	Life sciences	Sweden
López	Núria	Computational Chemistry	Spain
Navarra	Antonio	Environmental sciences	Italy
Pagonabarraga	Ignacio	Computational physics	Spain
Payne	Mike	Computational Physics	United Kingdom
Praprotnik	Matej	Chemistry, Multiscale Modeling	Slovenia
Ramos	Maria João	Computational biochemistry	Portugal
Ryan	Sinéad	Particle physics, mathematics	Ireland
Schütte	Christof	Life sciences	Germany
Stenström	Per	Computer science, HPC	Sweden
Yeomans	Julia	Physics: Soft and Biological Matter	United Kingdom
Zannoni	Claudio	Material sciences	Italy



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## SSC Functioning

Biannual meeting  
One in conjunction with PRACE days  
One in headquarters

Analyse access to HPC scientifically  
Scientific needs  
European scientific competitiveness



Types of access  
Needs of communities

Tier0      Above national resources  
Identify the niche for PRACE proposals

INCITE?

PRACE as an infrastructure  
How to manage users needs?



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## Access Committee

### Advice BoD on resource allocation

Experience researchers  
Cover relevant areas  
science  
engineering  
supercomputing

Odd number

Serve two year term  
+ extension

Last Name	First Name	Field	Country
Audit	Edouard	Universe	France
Braconnot	Pascale	Earth/Climate	France
Delgado	Rafael	Condensed Matter/ Materials	Spain
Hochgreb	Simone	Engineering I	United Kingdom
Koumoutsakos	Petros	Computer Science/Math/HPC	Switzerland
Plaat	Aske	Data Sciences	The Netherlands
Rovira Virgili	Carme	Chemistry/Biology	Spain
Zanoni	Claudio	Condensed Matter/Chemistry/Materials	Italy
Hartumt	Wittig	Quantum Monte Carlo	Germany





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## Access Committee

In charge of proposal management

Selects reviewers

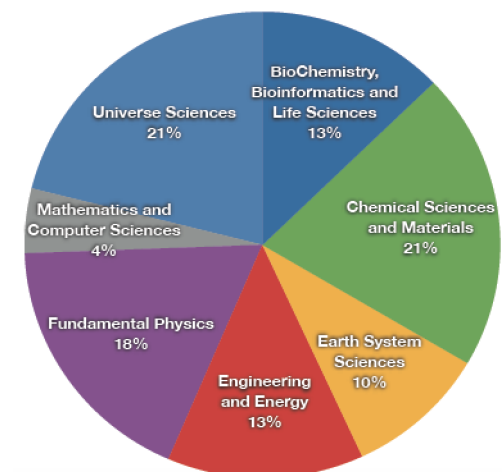
Organized in panels

Ranks proposals  
decides funded projects

Number of proposals  
Area distribution  
Hours requested

Head presents decisions at SSC

Closer collaboration AC/SSC





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## PRACE proposals

Strict format  
extension  
content

Personel  
Summary  
Computer resources  
What has been done with the code  
suitability for architecture/parallelism  
Dissemination / Knowledge transfer

Project name	
Research field	

Project leader	
Title	
Last name	
First name	
Organisation name*	
Department*	
Group*	
Country	

Feedback from referees  
Possibility to improve proposal



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## PRACE Final report

### Summary

### Description of the results

scientifically  
future perspectives  
benefits society

### Expected future work

### Dissemination / Knowledge transfer

### Presentations / talks

### Images / movies

## 1. General information

1.1. Proposal ID

1.2. Type of proposal granted: Project Access

1.3. Period of access to the PRACE facilities

1.4. Name of the PRACE facility assigned

1.5. Name of the Principal Investigator



# PARTNERSHIP FOR ADVANCED COMPUTING IN EUROPE

## PRACE Final report

Summary  
Description of the results

### 1. General information

1.1. Proposal ID

1.2. Type of proposal granted: Project Access

1.3. Period of access to the PRACE facilities

**2.5. Description of the results obtained from the scientific point of view, future perspectives, benefits to our society, and the benefits of using computer resources.** *(Maximum of 1000 words)*

**2.6. Expected future work in the area**

**2.7. Images of the results including description or caption** *(Minimum resolution of 300 dpi)*



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## PRACE Final report

Feedback from center

Use of computer time

Future interest in PRACE

### **3. Feedback and technical deployment**

**3.1. Feedback on the centers/PRACE mechanism** *(Maximum 500 words)*

**3.2. Explanation of how the computer time was used compared with the work plan presented in the proposal. Justification of discrepancies, especially if the computer time was not completely used.** *(Maximum 500 words)*

**3.3. Please, let us know if you plan to apply for a PRACE project access? If not, explain us why.** *(Maximum 500 words)*





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## Role of SSC on PRACE projects

Overviews the selection process  
Analyzes issues and proposes changes to Access committee  
Evaluates project reports

## Ongoing discussion

Quality indicators  
objectives measures?



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## Role of SSC on PRACE projects

Stronger control on final report

Delay in publications

Ensure proper use of computational resources

Identify successful proposals

Increase awareness of need of HPC

Show relevant outcome

Need to structure results ?

relevant/impact stories to general public?

Contribute to PRACE days





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whereas particle physics and chemistry afford to use parallel computers with weak communications between nodes, climate and fluid dynamics problems require much higher level of communication. Domains also differ in their need for storage capacity, which is particularly demanding for weather and climate.

For example in plasma physics, the grid size is essential to carry out significant simulations of plasma turbulence and the ensuing energy losses in the ITER device. In particle physics, the physical volumes are still small, in particular for the simulations of excited states and composite objects like nuclei, and the lattices should be less coarse for a better control of the continuum limit, and only continued availability of high performance computing power will allow to continue towards a better control and precision results. In climate modelling, better understanding and improving predictive capabilities call for further increased resolution and more complexity, with important societal implications to help prepare for adaptation to climate change. Fluid dynamics in engineering will highly benefit from explicit resolution of turbulence as well as from a more statistical approach to deal with uncertainties, improving not only science but also industrial product



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## PRACE proposals

**1.** *Describe your research project. Include discussion of the scientific questions that you are planning to address and the overall scientific goals of the project. It is important that you describe the novelty, impact and timeliness of the proposal*

**2.** Describe how you will manage the resources requested? Use a Gantt chart or equivalent to illustrate this. (1 page).

#	Name	Mth1	Mth2	Mth3	Mth4	Mth5	Mth6	Mth7	Mth8	Mth9	Mth10	Mth11	Mth12
0													
1													
2													
3													
4													
5													





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## PRACE proposals

*3. Describe the numerical methods and algorithms that you are planning to use, improve, or develop, the codes, packages or libraries that you need to undertake the project, and how these will enable the research to be achieved. (1 page)*

*4. Explain why this project needs to run on a Tier-0 system, why the machine you have requested is suitable for the project and how the use of the system will enable the science proposed. You should describe the architecture, machine/system name and the problem sizes that have been used to test for scaling and provide supporting evidence.*

*5. Describe your experience of using HPC resources in the past and how you will manage using a Tier-0 system. What other experience do you and your team bring to this project? (1 page).*

Feedback from referees  
Possibility to improve proposal