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Research Infrastructures**

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Performance Computing (HPC) service PRACE**



PRACE-1IP

PRACE First Implementation Project

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Updated Scientific Case for a European HPC Infrastructure

Final

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References and Applicable Documents

- [1] <http://www.prace-ri.eu>
- [2] <http://www.hpcineuropetaskforce.eu/>
- [3] [http://www.hpcineuropetaskforce.eu/files/Scientific case for European HPC Infrastructure HET.pdf](http://www.hpcineuropetaskforce.eu/files/Scientific_case_for_European_HPC_Infrastructure_HET.pdf)
- [4] High-Performance Computing: Europe's place in a Global Race, EC COM (2012)-45, Bruxelles, 15.2.2012
- [5] <http://www.eesi.eu>
- [6] <http://www.prace-ri.eu/Scientific-Case-Update>

List of Acronyms and Abbreviations

AISBL	Association Internationale Sans But Lucratif
BoD	Board of Directors (in this document usually referring to the PRACE AISBL BoD in particular)
CINECA	Consorzio Interuniversitario, the largest Italian computing centre (Italy)
EESI	European Exascale Software Initiative
FZJ	Forschungszentrum Jülich (Germany)
HET	High Performance Computing in Europe Taskforce. Taskforce by representatives from European HPC community to shape the European HPC Research Infrastructure. Produced the original Scientific Case (2007) and valuable groundwork for the PRACE RI.
HPC	High Performance Computing; Computing at a high performance level at any given time; often used synonym with Supercomputing
PRACE	Partnership for Advanced Computing in Europe; Project Acronym
PRACE-1IP	First Implementation Phase project of PRACE
SSC	PRACE Scientific Steering Committee

Executive Summary

In 2005 and 2006, an international panel produced a White Paper entitled ‘Scientific Case for a European Super Computing Infrastructure’ [3] that argued the case for High Performance Computing (HPC) to support European competitiveness. The document was published by the “HPC in Europe Taskforce” (HET) in January 2007 [2]. The initiative was instrumental to the establishment of PRACE – The Partnership for Advanced Computing in Europe – and the PRACE Research Infrastructure (PRACE-RI) in April 2010 [1].

Five years after the publication of the scientific case, the HPC landscape in Europe has changed significantly. This Deliverable represents the culmination of WP4 - Task 4.5 in the First Implementation Phase project of PRACE (PRACE-1IP) to create an update of the Scientific Case and capture the current and expected future needs of the scientific communities. It has involved the PRACE Scientific Steering Committee (SSC), the PRACE User Forum, the PRACE AISBL and many researchers from a variety of scientific domains.

This document describes in short the considerations and decisions that were made to define the process to update of the Scientific Case. The Scientific Case document itself is published separately and will be made available to a wide audience.

1 Introduction

Five years after the publication of the previous Scientific Case in 2007, [2], [3], the HPC landscape in Europe has changed significantly. The PRACE Research Infrastructure is providing Tier-0 HPC services to Europe, while the importance of HPC in solving the socio-economic challenges and maintaining Europe's competitiveness has become even more evident [1]. It is clear that the position of HPC has evolved since 2007 from a discipline crucial to the academic research community to a point where it is acknowledged as central in pursuing "Europe's place in a Global Race" [4]. The sidebar extract from the communication from the Commission to the European Parliament pays testimony to this position.

The primary objectives of the update to the Scientific Case are to identify the existing and new scientific areas for which PRACE is an important Research Infrastructure and the key challenges within these areas. In highlighting the crucial role of large-scale computer simulation, the Scientific Case document identifies the potential outcomes in science and engineering to be addressed through PRACE Petascale resources, and the impact of computer simulations on the economy and society in general. This impact is quantified through the production of a roadmap of expected achievements in the next 5-8 years.

The update to the Scientific Case was originally due in Month 14 (August 2011) of PRACE-1IP. However, during the initial discussions and activities to create the update in Task 4.5 of PRACE-1IP, it became clear that the update of the Scientific Case is a document that is of high strategic importance to PRACE and the European HPC communities. Therefore, a process that initially was considered and that would lead to a (minor) update of the Scientific Case document from 2007 would most likely not meet the expectations that several of the stakeholders had concerning a new Scientific Case document. The process was subsequently modified to involve all stakeholders, including the PRACE Scientific Steering Committee (SSC), the PRACE User Forum, the PRACE AISBL and, most importantly, the scientific communities. A major objective of the writing process for the Scientific Case should be to guarantee a good anchoring of the process in (i.e., active participation by) the scientific communities.

This Deliverable describes briefly the considerations and decisions that were made by PRACE to define the process to update the Scientific Case document. The new Scientific Case document itself is published separately and is made available to a wide audience. The electronic version of the document will be available on the PRACE RI web site for final public consultations [1].

The target audience for the Scientific Case document includes policy makers, national funding agencies as well as the European Commission, and the research communities for which the PRACE RI is an important infrastructure (or of potential interest).

2 Definition of the Process

After the decision on the new focus on the Scientific Case update, a meeting was held in November 30, 2011, at the PRACE AISBL premises in Brussels to kick-start the process that led to the update of the Scientific Case. The meeting was organized by WP4-IIP Task 4.5 in conjunction with a meeting of the SSC. The meeting was attended by 25 people, including members of the SSC, the PRACE AISBL, the PRACE-IIP Project Management and candidate members of the PRACE User Forum.

At that meeting, a number of topics were discussed and/or proposed as presented below in this section.

2.1 Additional Objectives for the Scientific Case Update

- The main target audiences for the Scientific Case are the policy makers and the funding agencies.
- The update should put more emphasis on socioeconomic challenges, business, and innovation than the original Scientific Case from 2007.
- If possible, the updated Scientific Case should include success stories, demonstrating the impact of the new PRACE-RI on the quality of science in Europe; and include statements and/or success stories from industry to make the case for the importance of HPC for European development and growth.
- The new Scientific Case should be used to strengthen the link between the PRACE RI and its users.
- The update should cover the period up to 2020. With this timeframe, the Scientific Case will have to address Exascale and the need for (re)writing application software and corresponding needs for training and education.
- The Scientific Case should ideally be provided early enough to provide input to the discussion on Horizon2020 (EU's framework for research and innovation for 2014-2020).

2.2 Anchoring in the Scientific Communities

The European Exascale Software Initiative (EESI) produced in 2011 a report of similar scope [5]. It must be ensured that the update of the Scientific Case will not be a repetition of the EESI report. The EESI report focuses more on the technical aspects of Exascale computing rather than the scientific ones. A combination of the existing Scientific Case and the results from EESI will provide a good basis for the update.

It was therefore proposed to include members of the panels that were active in EESI in the work for the update of the Scientific Case. This should be complemented by members of the five scientific panels that were active for the previous Scientific Case.

2.3 Grouping of the Scientific Areas in the Scientific Case

- New areas with high societal and economic importance should be added to the Scientific Case. This includes adding medicine as a new topic to the Life Science area and addressing industrial applications.

- For the update, it needs to be ensured that the scientific panels that will contribute to the update of the Scientific Case are not smaller than those for the previous Scientific Case (with 10-15 persons), but have a broader inclusion of countries. A further way to increase involvement is to publish intermediate versions of the Scientific Case.
- In general, the scientific panels should work independently and only be loosely interacting. At least one workshop (per panel) is needed. To simplify the organization, these workshops could be co-scheduled, also giving the opportunity for global sessions. In addition to the panel members, these workshops should be open to others (openness is key to the credibility of the updated Scientific Case). Scientific communities from all European countries need to be able to contribute (and be listed as contributors in the document), to make it their document. Endorsement of the Scientific Case by these scientific communities is important.
- The SSC and the PRACE User Forum must have a role in the update of the Scientific Case, ideally taking ownership of the document.

2.4 Responsibilities and Organization of the Writing Process

- The appointment of a single main editor (Martyn Guest) was crucial for the success of the original Scientific Case. A similar solution should be adopted also for the update.
- A Group of four members is suggested to steer the update process: a representative each from the SSC, the User Forum, PRACE-1IP and the AISBL. The role of this group is to identify panel chairs, help setting up the panels, and contribute to the introductory and conclusion section of the updated Scientific Case.
- Candidates for panel chairs would be the panel chairs of the original Scientific Case, the chairs of the four EESI scientific panels and SSC members.
- The workshop should ideally be held in February 2012, considering the limited time to complete the update (June 2012). Travel expenses for the panel members and EESI representatives need to be covered. Travel costs for other participants should be covered by national funding.

2.5 Recommendations from the Brussels Meeting

Based on the discussions summarized above, the following conclusions and recommendations were made at the meeting in Brussels on November 30, 2011.

- The organization of the process should be managed by a board of four people (the Managing Group) composed by:
 - **Maria Ramalho** (Chairman of the Board of Directors PRACE AISBL);
 - **Richard Kenway** (Chairman of the Scientific Steering Committee);
 - **Thomas Lippert** (Chairman of PRACE 1IP);
 - **Turlough Downes** (Chairman of the User Forum Programme Committee).
- The Managing Group proposes the panel chairs, helps identifying the panel members and the main editor. Panel chairs of the original Scientific Case, EESI panel chairs and SSC members are candidates for chairing the new panels.
- A main editor will be appointed and funded to make the editorial work.

- A (single) workshop for all panels, open to other participants/contributors, will be organized; PRACE-1IP should fund participation of panel members; other participants should be funded through national sources.
- Task 4.5 PRACE-1IP will assist the Managing Group in all the technical aspects of the organizing process.
- The updated Scientific Case should
 - cover the period 2012 – 2020;
 - include the same panels and scientific areas as the original one, with medicine added explicitly to life science;
 - put more emphasis on socioeconomic challenges, business, and innovation than the original Scientific Case;
 - address Exascale and the need for (re)writing application software and corresponding needs for training and education;
 - leverage the results from EESI: the findings of the original Scientific Case and the EESI report jointly constitute a good basis for the updated Scientific Case;
 - report on the establishment of the PRACE RI as a success in implementing the recommendations of the original Scientific Case;
 - structure the report such that success stories from Tier-0 usage can be added in future versions and report on Tier-0 allocations and early results.
- It will be essential that the updated Scientific Case has broad support from the scientific community. The following aspects should be considered to ensure this:
 - The PRACE partners should spread the information on the Scientific Case widely and encourage participation to the workshop(s) and the document itself;
 - The writing process should be organized in an open fashion, publishing also intermediate results on the web and asking for comments from the community.

3 The Update of the Scientific Case

The recommendations from the Brussels Meeting (and the necessary funds) were approved by the PRACE-1IP Management Board on December 16, 2011.

After the PRACE AISBL's BoD approval, the editor for the previous Scientific Case, Professor Martyn F. Guest (*Director of Advanced Research Computing at Cardiff University*), was contacted proposing him to act again as the editor of the update. Prof. Guest accepted to be the main editor for the update of the Scientific Case.

Supported by the PRACE-1IP project, the Managing Group steered the overall process.

Task 4.5 PRACE-1IP guided by the WP4 leader (Giovanni Erbacher) supported the Management Board and the Main Editor in the remainder of the activity.

3.1 The Scientific Panels

The Managing Group proposed the chairs of the five panels and together proposed the members for each panel. The following chairs were appointed for five scientific panels:

Weather, Climatology and Solid Earth Sciences:

- Chair Giovanni Aloisio, University of Salento and ENES-CMCC, Italy;

Astrophysics, High Energy Physics and Plasma Physics:

- Chair Andreas Schäfer, University of Regensburg, Germany;

Materials Science, Chemistry and Nanoscience:

- Chair Stefan Blügel, FZJ, Germany;

Life Sciences and Medicine:

- Chair Modesto Orozco, Institute for Research in Biomedicine, Spain;

Engineering Science and Industrial Applications:

- Chair Philippe Ricoux, TOTAL, France.

The members of the five Scientific Panels are listed in **Annex A**.

Furthermore, representatives from each PRACE partner were appointed as national contact points to disseminate the activity and identify scientists in their countries that could also contribute to the process. The members of the national contacts are listed in **Annex B**.

The Management Group supported by Task 4.5 members organised a workshop in Dublin with all the panels to start the updating activity.

Task 4.5 prepared a mailing list for each panel with the email address of the panel participants:

- scientific-case-wce@fz-juelich.de (Weather, Climatology & Earth Sciences);
- scientific-case-ahp@fz-juelich.de (Astrophysics, HEP & Plasma Physics);
- scientific-case-mcn@fz-juelich.de (Materials Science, Chemistry & Nanoscience);
- scientific-case-lm@fz-juelich.de (Life Sciences & Medicine);
- scientific-case-ei@fz-juelich.de (Engineering & Industry).

Furthermore, a WIKI support to facilitate the activity of the different Panels was prepared. The WIKI is reachable at <http://prace-wiki.ipb.ac.rs/>.

3.2 The Dublin Workshop

The workshop took place on March 14-15, 2012 at the Dublin Castle (Dublin) [6]. The workshop was combined with a meeting of the PRACE User Forum.

On the first day, there were presentations from the Management Group on the strategic nature of the Scientific Case and presentations from the five panel chairs. The second day consisted of parallel panel sessions. Due to space limitations, the number of participants was limited to 80 people. The Agenda of the Workshop is reported below:

March 14, 2012

12:00 Registration

12:30 Tea and Coffee

Session Chair: Richard Kenway

13:30 Welcome Address: Prof. **Alan Harvey**, Vice-President for Research & Innovation, Dublin City University

13:35 Update of the Science Case: **Thomas Lippert**

13:50 The Process: **Richard Kenway**

14:00 PRACE Strategy: **Maria Ramalho**

14:20 Weather, Climatology & Earth Sciences: **Giovanni Aloisio**

14:40 Astrophysics, HEP & Plasma Physics: **Andreas Schäfer**

15:00 Materials Science, Chemistry & Nanoscience: **Stefan Blügel**

15:20 Life Sciences & Medicine: **Modesto Orozco**

15:40 Engineering & Industry: **Philippe Ricoux**

16:00 Afternoon tea

Session Chair: Turlough Downes

16:30 [PRACE User Forum](#)

18:30 Close

March 15, 2012

09:00 Parallel Panel Sessions

12:00 Lunch

Session Chair: **Martyn Guest**

13:00 Reports from panel chairs

14:00 Next steps: **Martyn Guest**

14:30 Close

During the workshop, the following timetable for the preparation of the panel contributions was agreed:

- 2 April 2012: first drafts of Panel Reports sent to M .F. Guest;
- 16 April 2012: first draft of Scientific Case publicly available;
- 30 April 2012: complete Panel input sent to M. F. Guest;
- 18 May 2012: full draft of Scientific Case publicly available;
- 25 May 2012: final comments to M.F. Guest;
- 10 June 2012: version ready for comments by other scientists;
- 30 June 2012: final version of Scientific Case approved.

3.3 The Document Updated

After the workshop in Dublin, the scientific panels and the main editor continued their work on the individual scientific domain areas and the overall document, scheduled by the timetable agreed. In this work, they stayed close to the recommendations from the meeting on November 30 2011, concerning the purpose, objectives and contents of the updated Scientific Case.

A draft Scientific Case was made available for comments to the scientific community on June 10 2012, before to release the official release. The Table of Contents of this document is reported in **Annex C**, while the whole document is available at <http://prace-wiki.ipb.ac.rs/>.

The deadline for submitting comments is June 30. The final version of the Scientific Case will be published shortly after this deadline.

4 Concluding Remarks

In this Deliverable, the process adopted to update the Scientific Case has been described. The resulting update document is not part of the Deliverable and it is published separately to reach a wider audience. The document presents research programmes which, in many cases, go beyond the purely computational aspect and make a strong case that HPC is integral to achieving their broader objectives. The document is of high strategic importance to PRACE and the European HPC communities so an extensive endorsement of the Scientific Case by the associated research organisations is recommended. This endorsement, guided by PRACE AISBL, can be reached through the involvement of the panel members that were active in the updating process, the PRACE SSC and the PRACE member states themselves.

In the future, a regular update of the Scientific Case will be beneficial for PRACE. Regular updates are needed to identify for example new scientific areas for which PRACE is an important Research Infrastructure and to identify the key challenges within existing and new areas. In addition, the Scientific Case can in such a way continue to highlight the crucial role of large-scale computer simulation and identify the potential outcomes in science and engineering, and the impact of computer simulation on economy and society in general.

A period of 3-5 years is suggested as a suitable time frame for the update of the Scientific Case.

Since the Scientific Case is of strategic importance for the PRACE RI, it will be useful that the PRACE AISBL and associated Scientific Steering Committee and User Forum take further ownership of the Scientific Case and future updates.

5 Annex

5.1 Annex A Membership of International Scientific Panel

AREA	COUNTRY	TITLE	FIRST NAME	LAST NAME	INSTITUTION	E-MAIL ADDRESS
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