SEVENTH FRAMEWORK PROGRAMME
Research Infrastructures

INFRA-2010-2.3.1 – First Implementation Phase of the European High Performance Computing (HPC) service PRACE

PRACE-1IP

PRACE First Implementation Project

Grant Agreement Number: RI-261557

D3.1.7
PRACE Magazine

Final

Version: 1.0
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Date: 23.04.2012

Project and Deliverable Information Sheet

PRACE Project	**Project Ref. №: RI-261557**	
	Project Title: PRACE First Implementation Project	
	Project Web Site: http://www.prace-project.eu	
	Deliverable ID: < D3.1.7>	
	Deliverable Nature: <DOC_TYPE: Report / Other>	
	Deliverable Level: PU	**Contractual Date of Delivery:** 30 / 04 / 2012
		Actual Date of Delivery: 30 / 04 / 2012
	EC Project Officer: Thomas Reibe	

* - The dissemination level are indicated as follows: **PU** – Public, **PP** – Restricted to other participants (including the Commission Services), **RE** – Restricted to a group specified by the consortium (including the Commission Services). **CO** – Confidential, only for members of the consortium (including the Commission Services).

Document Control Sheet

Document	**Title: PRACE Magazine >**	
	ID: <D3.1.7>	
	Version: <1.0 >	**Status:** Final
	Available at: http://www.prace-ri.eu	
	Software Tool: Microsoft Word 2007	
	File(s): D3.1.7.docx	
Authorship	**Written by:**	Ari Turunen, CSC
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	Reviewed by:	Nelly Stoyanova, NCSA; Tanja Weber, FZJ
	Approved by:	MB/TB

Document Status Sheet

Version	Date	Status	Comments
0.1	10/04/2012	Draft	
0.2	23/04/2012	Draft	Nelly Stoyanova, Tanja Weber
1.0	23/04/2012	Final version	

Document Keywords

Keywords:	PRACE, HPC, Research Infrastructure

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List of Acronyms and Abbreviations

BAdW	Bayerischen Akademie der Wissenschaften (Germany)
BSC	Barcelona Supercomputing Center (Spain)
CEA	Commissariat à l'Energie Atomique (represented in PRACE by GENCI, France)
CINECA	Consorzio Interuniversitario, the largest Italian computing centre (Italy)
CINES	Centre Informatique National de l'Enseignement Supérieur (represented in PRACE by GENCI, France)
CORIA	COmplexe de Recherche Interprofessionnel en Aérothermochimie
CSC	Finnish IT Centre for Science (Finland)
CSCS	The Swiss National Supercomputing Centre (represented in PRACE by ETHZ, Switzerland)
DECI	Distributed European Computing Initiative
DEISA	Distributed European Infrastructure for Supercomputing Applications. EU project by leading national HPC centres.
EC	European Community
EPCC	Edinburg Parallel Computing Centre (represented in PRACE by EPSRC, United Kingdom)
EPSRC	The Engineering and Physical Sciences Research Council (United Kingdom)
ETHZ	Eidgenössische Technische Hochschule Zuerich, ETH Zurich (Switzerland)
FZJ	Forschungszentrum Jülich (Germany)
GCS	Gauss Centre for Supercomputing (Germany)
GENCI	Grand Equipement National de Calcul Intensif (France)
HPC	High Performance Computing; Computing at a high performance level at any given time; often used synonym with Supercomputing
IDRIS	Institut du Développement et des Ressources en Informatique Scientifique (represented in PRACE by GENCI, France)
JSC	Jülich Supercomputing Centre (FZJ, Germany)
KTH	Kungliga Tekniska Högskolan (represented in PRACE by SNIC, Sweden)
LRZ	Leibniz Supercomputing Centre (Garching, Germany)
NCF	Netherlands Computing Facilities (Netherlands)
PRACE	Partnership for Advanced Computing in Europe; Project Acronym
PSNC	Poznan Supercomputing and Networking Centre (Poland)
SARA	Stichting Academisch Rekencentrum Amsterdam (Netherlands)
SNIC	Swedish National Infrastructure for Computing (Sweden)
Tier-0	Denotes the apex of a conceptual pyramid of HPC systems. In this context the Supercomputing Research Infrastructure would host the Tier-0 systems; national or topical HPC centres would constitute Tier-1

Executive Summary

Effectively organised dissemination, outreach and training activities are a prerequisite for the success of the PRACE First implementation project. This document describes the strategies to achieve these objectives and the resulting actions. One of the objectives of WP3 (Dissemination and training) in the PRACE 1IP project is to disseminate the achievements of the Research Infrastructure and the project results. One important media to fulfil this task is a magazine in which all the important scientific results are compiled in an understandable and popularized fashion. The first PRACE magazine was compiled in spring 2012. It presents 14 Tier-1 projects which have used PRACE resources. The Tier-0 results will be presented in the second and the third PRACE magazine during the 2IP-project.

1 Introduction

This document describes the first PRACE magazine and its contents. Chapter 2 describes the objectives of the magazine and the intended audience. Chapter 3 describes the methods to compile the magazine. Chapter 4 describes the contents of the magazine.

2 Objectives and the intended audience

The principal objectives for dissemination, outreach, and training in PRACE are to disseminate the achievements of the Research Infrastructure and the PRACE-1IP project results to the major HPC stakeholders, the European scientific and research communities, Research Infrastructure organizations, universities and centres for higher education, and the general public. The magazine offers detailed information about key scientific results, and available training material. Magazine will be disseminated at various events and via each PRACE site. PRACE partners are encouraged to disseminate it to various stakeholders. The number of copies is 2000. The PDF-version can be downloaded from the PRACE web site.

3 Methods

Initially the first PRACE magazine was aimed to cover the results achieved by using the Tier-0 systems. During the 1IP-project it was decided by the management board (MB) that the first magazine presents the results of the DECI-projects. DECI (Distributed European Computing Initiative) became part of the PRACE infrastructure and concentrates on Tier-1 projects. It was decided that the Tier-0 -projects will be presented on the following magazines which will be produced during the 2IP-project.

In order to select suitable projects to the magazine Dr. Hermann Lederer was asked to take care of this. This was suggested by the PRACE director Maria Ramalho and approved by Dr. Richard Kenway from the PRACE Scientific Steering Committee. Initially 15 projects were chosen. Due the lack of the availability of the researchers only one project (one from Netherlands could not be included to the magazine. In total 14 projects were presented and one article on training activities of PRACE. The selection criteria in addition to the scientific results were based on the variety of disciplines and countries. The countries represented are: Belgium, Italy, Sweden, UK, Switzerland, Germany, Spain, France, and Finland. Disciplines

vary from engineering to astrophysics, geophysics, fusion research, molecular biology and drug design.

In order to serve the general audience better the researchers were interviewed by the professional journalists. Journalists were given the DECI-reports and brief description of the chosen project. After that the researchers were interviewed. The idea was to make a normal newspaper interview, not a scientific monograph in order to avoid jargon. The drafts of the articles were sent to researchers and Hermann Lederer for the proof reading. After that the language was checked and suitable visualizations were chosen.

Figure 1: The Cover of PRACE DIGEST

PRACE PRACE

CONTENTS EDITORIAL

PRACE DIGEST
www.prace-ri.eu

ISBN 978-952-5520-45-3

Editor-in-Chief
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Pirjo Rötkönen
Samppa Haapio
Graphic Design and layout
Up to Point Ltd / Paula Winter
Cover picture
DGDROG project
Printed by
777 Ltd

The PRACE Research Infrastructure is established as an international non-profit association with seat in Brussels and is named 'Partnership for Advanced Computing in Europe AISBL'. It has 24 member countries whose representative organizations are creating a pan-European supercomputing infrastructure, providing access to computing and data management resources and services for large-scale scientific and engineering applications at the highest performance level.

DECI: pooling national high performance computing resources to enable world-class computational science

Computational science is thriving in Europe. Important scientific breakthroughs increasingly depend on our scientists being able to undertake complex modelling and simulation. This is made possible by the availability of a European ecosystem of world-leading HPC facilities, by a network of national and regional HPC centres of expertise and by an eInfrastructure that promotes and supports collaborative research.

DECI (Distributed European Computing Initiative, formerly DEISA) is a scheme through which collaborative projects, headed by European scientists, can apply for access to world-leading national (Tier-1) computational resources in the European HPC infrastructure for a period of up to 12 months per project. EC reviewers described DECI as "among the best outcomes of EC research infrastructure projects".

DECI was introduced in 2005, by DEISA as an instrument to enable European computational scientists to obtain access to the most powerful national computing resources in Europe regardless of their country of origin or work, and to enhance the impact of European science. Through a regular call, capability computing projects are selected by peer-review on the basis of innovation and scientific excellence.

To date, eight DECI calls have been held and the scheme is now running under the umbrella of PRACE.

Successful projects are given access to the national HPC resources in the European infrastructure (on HPC architecture selected for its suitability to run the project's codes efficiently) and are offered applications support to enable them to use it productively. DECI has been of key importance in building a European HPC user community, supported in their use of top-level HPC facilities by applications experts from leading European HPC centres. More than 350 different researchers from 40 countries have participated in the scheme, including collaborators from four other continents. DECI enhances Europe's international standing in science, by providing access to world-class resources which are complementary to resources available locally (i.e. at the researchers' national facility). DECI is a very successful instrument for the European Union research policy of enabling smaller countries to take part in research at the cutting-edge and enables all European researchers to participate in internationally competitive computational science.

This booklet offers a fascinating insight into the range, quality, breadth and depth of computational science being undertaken in Europe today and illustrates not only the key role of HPC in solving many of the societal, industrial and scientific challenges facing us today, but also the extent to which synergy between scientists and HPC experts is key in delivering these results.

Alison Kennedy
Executive Director
EPCC

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Figure 2: Table of contents and editorial

Advanced tools to design future jet engines

Koen Hillewaert

Increasingly stringent requirements for energy efficiency and noise reduction in jet engines are tightening the screw in their development and design. The computational methods available now will not be sufficient in the future. Cenaero, an applied research centre for modelling and numerical simulation, is developing new methods that will help in designing high-performance jet engines.

For a long time one of the main problems in applied fluid mechanics – especially in industrial flows – has been the estimation of the impact of turbulence.

"Up to now aircraft and engine manufacturers have been using mostly time-averaged computational methods, in combination with lower accuracy discretisation techniques, for their design purposes. These algorithms will continue to be used, at least for a while, but they need to be complemented with more advanced computational tools. First of all, these methods are simply not applicable for some types of flows. An important application is the prediction of noise, for example generated by a flow from propellers or flow instabilities in compressors and fans. By applying larger computing resources we can directly simulate part of the turbulence," explains **Koen Hillewaert**, Argo Team Leader at the Cenaero research centre in Belgium.

"For low speeds or small geometries the size of the turbulence is such that we cannot even get an accurate value of the time-averaged forces and performance if we do not compute part of the turbulent structures directly. These conditions are prevalent for instance on part of wind turbine blades and in some parts of a jet engine," he adds.

Industrial applications in mind

Cenaero's aim is to provide a numerical algorithm based on the Discontinuous Galerkin Method (DGM), to be used for computations with full (DNS or Direct Numerical Simulation) and partial (LES or Large Eddy Simulation) resolution of turbulence in wall-bounded flows, especially in turbomachines.

"We are convinced that DGM combines the high order of accuracy that is currently offered by academic codes to the geometric flexibility characteristic of industrial codes, and at the same time provides computational efficiency and parallelizability. This high order of accuracy is indispensable to represent turbulent structures adequately, but is not provided by state-of-the-art industrial codes. At Cenaero, we are primarily interested in the industrial application. The academic aspect – although also very important as some of the numerical technology still needs to be developed – is a secondary goal."

"We will be able to use our method in the context where the turbulence occurs very close to walls, where there is more complexity to take into account – you simply have larger demands for resolution there. The turbulence is influenced by the walls in the flows that interest us, because we focus on turbomachinery: jet engines and propellers."

Huge computational resources

For the turbulence computations performed by the research team at Cenaero, huge computational resources are needed.

"That is why we turned to the world-class supercomputers of DECI. With these resources we could provide a proof-of-concept of the method focused on full resolution of the turbulence, by performing the direct simulation of the transitional flow around a low-speed airfoil. DECI also gave us access to machines that have different architecture from

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what we usually have at computational centres. It was a unique opportunity to test if the code would work satisfactorily in this kind of architecture. Furthermore we were attracted by the support from specialists in porting and optimizing the code," Koen Hillewaert says.

"To show that the method is viable, we compared it to experimental results and DNS computations with a conventional low-order discretisation. It was clear that the computations really correspond to what was measured, and that the method really offers a huge advantage with respect to the standard discretisation method, as it allowed us to capture the real physics rather than a result that only looks acceptable. DGM moreover offers us a visual means to assess mesh resolution."

The promising results of this project lay the ground for further development using the supercomputing resources of PRACE. A first project "stuDGE" has just been finished, and concerns the transitional flow on a section of low-pressure jet engine turbine blade.

"We are moving towards the resolution of more complex flows and flow conditions that are rather ambitious, leveraging both on the availability of ever more powerful computational resources and the further development of the numerical algorithms."

Convincing the industrial partners

The results achieved in these computations are part of a roadmap towards industrial use of DNS and LES.

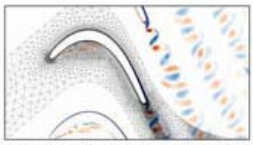
"We are showing that with the discontinuous Galerkin method well-resolved computations are feasible, and will give more accurate results, not only for the prediction of noise generation or flow instabilities, but for some cases also in terms of global time-average performance."

"The computations have helped us to convince our industrial partners that we will be able to provide the technology for the computations they would like to do within a few years. These cover essentially broadband and tonal noise generation by fans and open rotors, as well as flow instabilities in turboreactors, such as rotating stall."

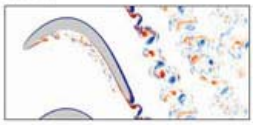
These types of computation will be needed if jet engine industry is to meet the more stringent requirements and regulations in terms of energy efficiency and noise. To keep their competitive edge, manufacturers need to invest in new computational technology now.

"If manufacturers do not provide high efficiency and low noise engines, they will be unable to sell them in the future," Koen Hillewaert points out.

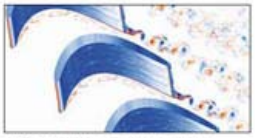
"Clearly the evolution of computation techniques goes hand in hand with the availability of computers. On the one hand as more and more powerful computers are available, we can do more complex computations. On the other hand computational technology has to evolve as more direct resolution of the turbulence becomes feasible and large scale resources need to be used efficiently."



DNS computations of the transitional flow around the Eppler E387 airfoil during the DECI project "CoBaltF" – computed isocontours of vorticity on the spanwise periodic plane and skin friction on the airfoil surface.



Weak scaling of the code obtained on the BlueGene/P architecture. The time integration strategy is implicit, to allow for the large disparities in cell size, and based on Newton-GMRES iterations.



DNS of the transitional flow around a LP turbine blade at Re=30000 computed during the PRACE project "stuDGE" – vorticity isocontours on the spanwise periodic plane and skin friction on the blade surface.

FURTHER INFORMATION
http://www.deisa.eu/science/deci/projects2009-2010/COBALTF
CPU hours used: 83,000 CPU-h IDRIS GB/P

- Cenaero, CFD and multiphysics group, Gosselies, Belgium
- Katholieke Universiteit Leuven, Belgium
- University of Liege, LTAS, Liège, Belgium
- Clarkson University, Dept of Mechanical and Aeronautical Engineering, Potsdam, USA

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Figure 3. An example of the article

4 Contents

The magazine has one editorial and 14 articles. All chapters are briefly introduced below.

4.1 Editorial

Editorial was written by Alison Kennedy from EPCC. In the editorial the PRACE Tier-1 projects and the call process is briefly explained.

4.2 Advanced tools to design future jet engines

Increasingly stringent requirements for energy efficiency and noise reduction in jet engines are tightening the screw in their development and design. The computational methods available now will not be sufficient in the future. Cenaero, an applied research centre for modelling and numerical simulation, is developing new methods that will help in designing high-performance jet engines. Researcher Koen Hillewaert (Cenaero) was interviewed.

4.3 Secrets of boiling

An everyday routine in the kitchen can be a complicated problem when studied theoretically. Numerical simulations of boiling convection are especially interesting because of the great range of applications. Professor Luca Biferale (University of Rome) was interviewed.

4.4 Understanding the brain, with the aid of large-scale simulations

Brain science and neuroinformatics are some of the newest fields for supercomputer simulations. High-performance computing can be used for biophysically detailed brain-scale simulations and for analyzing data obtained in measurements of the brain. Professor Anders Lansner (Stocholm's Royal Institute of Technology) was interviewed.

4.5 Numerical tools to aid the design of engines and burners

High-fidelity databases of turbulent reactive flow simulations can be used to devise novel turbulent combustion models that ultimately assist in designing engines and burners with lower emissions. Dr. Vincent Moureau (CORIA) was interviewed.

4.6 Shedding light of supernovae

The mechanism behind the explosion has not been fully untangled. Scientists are looking to three-dimensional computer modelling for help. Dr. Hans-Thomas Janka (Max Planck Institute for Astrophysics) was interviewed.

4.7 High-performance biomolecular simulations to improve drug development

Sophisticated, high-performance simulation methods help researchers reduce time and cost when developing new drugs. Dr. Julien Michel (Edinburg University) was interviewed.

4.8 New configurations for film cooling of turbine blades

Gas turbines are the heart of gas-fired power plants, as well as of aircraft jet engines and transport vessels. Their combustion temperatures are now so high that turbine blades need additional cooling for efficient performance. Simulations for the appropriate coolant flows require high-performance computing resources. Professor Leonhard Kleiser (ETH) was interviewed.

4.9 Problems of fusion energy simulated with Elmfire-software

Nuclear fusion is the process that powers the sun, and all the stars in the universe. If nuclear fusion could be mastered on earth, it would be a reasonably clean, almost limitless supply of energy. Dr. Jukka Heikkinen (VTT Research Centre of Finland) was interviewed.

4.10 Photo-switching the conformation of azobenzene

The first large-scale study of photo-isomerization of azobenzene in a liquid crystal host has been conducted in Italy and Germany with the aid of atomistic computer simulation. The majority of previous studies were carried out in vacuums. The knowledge gained in the study has invaluable practical applications in photo-switchable devices and nano-actuators, such as artificial muscles. For future extensions of the molecular dynamics technique (MD), the study suggests investigating the behaviour of molecules in excited states. Dr. Antonio Pizzirusso (University of Bologna) was interviewed.

4.11 Getting prepared for earthquakes and their consequences

The interior structure of the earth and its geophysical properties are generally studied by seismology but high-performance computing simulations of the propagation of seismic waves are a new and invaluable tool for understanding wave phenomena, how they are generated and what their consequences are. Ph.D Christian Pelties (Ludwig Maximillian University of Munich) was interviewed.

4.12 Saving time with two parallel simulation models for particle flows

Some mathematical models for the movement of microscale particles in fluid flow pose time challenges even for supercomputers. In an attempt to find solutions to this problem, researchers on the DiParTS- project combined two simulation models; one fast and computationally cheap, the other computationally expensive and much longer lasting. They ran the models in parallel, constantly comparing the results. When the codes agreed, i.e. when only running the cheap variant was sufficient, they continued for a while exclusively with the fast code. Dr. Tobias Weinzierl (Technische Universität München) was interviewed.

4.13 Solving secrets of influenza

Influenza is one of the most common infectious diseases. It spreads around the world in seasonal epidemics, resulting in the deaths of between 250,000 and 500,000 people every year. Researchers all over the world are investigating mechanisms of influenza and developing tools to reduce the injurious effects of epidemics. The focus is on new antiviral drugs and drug delivery systems. Dr. Peter Kasson (University of Stockholm) was interviewed.

4.14 PRACE trains users to take the most out of supercomputers

PRACE provides Europe with state-of-the art Research Infrastructure and supercomputing systems. To use these leadership class systems, European scientists and engineers must have the technical knowledge and abilities to use them effectively. That is why PRACE is putting a lot of effort into training, and has allocated 120 person months of work to this activity in the PRACE 1IP (First Implementation Phase) project. PRACE Training coordinator Pekka Manninen was interviewed.

4.15 High-throughput single-particle analysis in 3D electron microscopy

The research group of Carlos Oscar Sánchez Sorzano from the National Center of Biotechnology in Madrid aims at optimizing the steps in the 3D analysis of single-particles, This will increase the productivity of structural biologists and optimize the use of available.

5 Conclusions

HPC-related research is a challenging subject to popularise. To complete one popularised article is a very time consuming process. It takes a minimum of 6 months to produce the magazine with 36 pages or more. One must take account the availability of the researchers and the access to the background material (reports, reviewed articles). After that the interviews can take place. The interviews bring usually more important insights of the research and increase substantially readability. In order to avoid disturbing mistakes by the editor, the interviews had to be checked both by a researcher and a copy editor who is usually familiar with the substance. Otherwise the magazine with this level of comprehensibility lacks credibility.