

# NEWSletter

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## Preparing a Comprehensive Legal and Administrative Framework for the PRACE Research Infrastructure

Damien Lecarpentier

The overall objective of the Partnership for Advanced Computing in Europe (PRACE) is to make preparations for the creation of a persistent pan-European High Performance Computing (HPC) service, consisting of 3–5 centres, similar to the US HPC infrastructure. The project began on January 1st 2008 and will last for two years.

The work of PRACE is structured into eight different parallel activities, referred to as Work Packages. Work Package 2 (WP2) has been charged with the preparation of a comprehensive legal and administrative framework that will lead to the establishment of the PRACE permanent Research Infrastructure as a legal entity. **Francesc Subirada**, from BSC (Barcelona Supercomputing Center), in Spain, is the leader of this pivotal activity. Here, he explains to us its main objectives.

### The main objectives of Work Package 2

“Work Package 2 is entitled ‘Organisational concept of Research Infrastructure’, and, in a nutshell, its aim is to prepare a comprehensive legal and administrative framework for the implementation phase of the Research Infrastructure. WP2, in terms of personnel resources at least, the second largest Work Package in the PRACE project, involving 253 ‘person-months’”, says Subirada.

WP2 is organised around seven main objectives, each of them important in its own right and giving rise to specific challenges.

The first of these is the definition of the legal form for the Research Infrastructure:

“This is one of the most important tasks in the PRACE project”, notes Subirada.

“We have to examine all of the legal forms available and select that which will be most appropriate for the PRACE entity, and also most acceptable to the project partners”, he continues.

Closely linked to the definition of the legal form of the Research Infrastructure is the definition of the governance structure (whose

shape will depend, to some extent, on the legal form that is eventually chosen). This second objective is, according to Subirada, also a crucial one:

“It is very important to have a strong governance structure to ensure the efficiency and independence of the infrastructure”, he points out.

This governance structure will have to provide sufficient freedom to carry out research and to innovate, but also sufficient structure and accountability to ensure that a useful service is provided. It requires a central authority strong enough to make binding decisions based on technical merit rather than political considerations, and, to ensure adequate coordination between the various elements of the project; yet this must operate within a framework that allows the project sponsors to hold both the institution and its members accountable.

The third main objective of the Work Package is to ensure that the PRACE legal entity re-

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Two New Countries Joined PRACE Initiative

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*Francesc Subirada, from BSC, is the leader of Work Package 2, which has been charged with the preparation of a comprehensive legal and administrative framework for the PRACE Research Infrastructure.*

ceives adequate funding, which is crucial for the project.

"Again, this is of crucial importance, without funding, there will be no PRACE", Subirada points out.

This objective is also a very challenging one: adequate funding of the PRACE Research Infrastructure must be secured for all stages of the project, from the initial investment, to the continued operation and the periodic renewal of leadership systems. It requires an evaluation of all available funding options, such as contributions from PRACE partners, from the European Union, industrial usage, and EIB loans.

One of the main challenges that will arise in seeking to achieve this objective is, according to Subirada, "to try to reconcile national interests with those of the European project". Terms of use of the Research Infrastructure, both for scientists who come from PRACE partner-countries who are funding the project, and those from other European user communities will have to be defined in such a manner as to maximise the scientific benefit to European research and, ultimately, to the European economy.

Because the European Union seeks to support and engage in research of the highest quality, the establishment of a peer-review process is also crucial to the success of the HPC service. This is the fourth objective that will have to be met under WP2.

"This process will decide who gets access to the Tier-0 computing power; the main challenge of establishing such a mechanism lies in ensuring that it is both balanced and impartial.

The success of the Tier-0 infrastructure also depends on the ways in which it interacts with, and builds upon, the healthy basis provided by HPC activities at the national level within partner countries, thus creating an overall European HPC ecosystem", he adds.

Establishing links with this ecosystem is the fifth objective of WP2.

"The main challenge here lies in the need to balance the ecosystem between local, national and European facilities", says Subirada.

Additionally, WP2 is tasked with defining a consistent operational model that will provide the research community with a single and permanent infrastructure, thus permitting and encouraging users to invest in the development of simulation codes based on computational sciences:

"PRACE will be a geographically distributed entity but should be able to operate as a single infrastructure" says Subirada.

"Realising this in the context of different architectures supplied by different vendors hosted at different sites and, moreover, in the context of rapidly evolving technologies and architectures is the biggest challenge posed by this sixth objective", he notes.

Finally, WP2 is charged with the task of documenting the process and rationale behind the decision of the Management Board on the selection of prototypes and production systems (based on the technical assessment carried out by WP7 as to the availability and capability of Petaflop/s systems for the potential vendors).

## A Work Package Fully Connected to the Others

Given this set of objectives, WP2 is of crucial importance for the establishment of the PRACE Research Infrastructure. It plays a pivotal role in the project and is also fully interconnected with the other Work Packages:

"As the project progresses, we are realizing just how closely our activity is connected to the other Work Packages. There are very clear interdependencies in relation to WP7, in that the process for selecting the most appropriate set of prototypes for the project, which is carried out by WP7 and decided by the PRACE Management Board, must be documented by us. There are also procurement issues that both WP7 and WP2 must deal with – WP2 on a fairly general level and WP7 on a more technical level. WP2 is also responsible for establishing links with the HPC ecosystem and so has links to WP4 on distributed system management", says Subirada.

"However, given that it will be responsible for producing the signature ready contract for the PRACE entity, which will involve defining the legal and governance structure, developing funding strategies and usage rules, setting out procurement principles, establishing the peer review process and developing links with the HPC Ecosystem, it is fair to say that WP2 has links to all of the other Work Packages", he concludes.



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## And the PRACE Award Went to...

**PRACE, Partnership for Advanced Computing in Europe, awarded a prize for the best scientific paper submitted to ISC'08 by a European student or young scientist.**

The authors of the award winning paper are **Stefan Turek, Dominik Göddeke, Christian Becker, Sven H.M. Buijssen** and **Hilmar Wobker** from the department of Applied Mathematics, Dortmund University of Technology, Germany.

Their work, UCHPC – UnConventional High Performance Computing for Finite Element Simulations, was selected by the ISC'08 Award Committee, headed by **Michael Resch**, HLRS, The High Performance Computing Center Stuttgart. **Achim Bachem**, Chairman of the Board Forschungszentrum Jülich and

PRACE coordinator will present the PRACE Award at the ISC' 08 opening ceremony in Dresden on Wednesday, 18 June.

Dominik Göddeke, Ph. D. student in the team of Professor Stefan Turek will receive a sponsorship for the participation in a conference relevant to Petascale computing.

This was the first time the prize was awarded. The PRACE Award will be continued in the years to come to encourage young European scientists to work on innovative solutions for Petascale computing.

PRACE congratulates the winners!

The winning paper can be read on:  
[http://www.mathematik.uni-dortmund.de/lsiii/static/showpdffile\\_TurekGoeddekeBeckerBuijssenWobker2008.pdf](http://www.mathematik.uni-dortmund.de/lsiii/static/showpdffile_TurekGoeddekeBeckerBuijssenWobker2008.pdf)

# Students to Learn High Performance Computing Skills at PRACE Petascale Summer School

PRACE, Partnership for Advanced Computing in Europe, hosts Petascale Summer School 26–29 August, 2008 at the Royal Institute of Technology (KTH) in Stockholm, Sweden.

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*Stockholm's picturesque Old Town is a lovely place to visit in the summertime.*

This four day PRACE Petascale Summer School will be held at the Paralleldatorcentrum (PDC) on the KTH campus in Stockholm, Sweden. It will have lectures in the morning and hands-on exercises in the afternoon.

"The first two days are focused on the challenges in porting an application to massively parallel computers. In order for students to get experience on this important and interesting subject, the Summer School provides access to Europe's fastest computer, the Blue Gene/L in Jülich, Germany", says **Ulf Andersson**, the chair of the PRACE Petascale Summer School Program Committee and application expert at PDC.

Students are encouraged to bring their own applications to the Summer School and test how they perform.

"The students should bring applications they are using now and desire to use in the fu-

ture on Petascale systems in Europe", Andersson continues.

"The final two days will cover advanced parallel programming and the use of performance tools and techniques to improve scalability of an application. During these exercises the students will have access to the Cray XT4 at the Finnish IT Center for Science (CSC) in Espoo, Finland", he adds.

## Targetting experienced users

The PRACE Petascale Summer School targets students from research groups that have the ambition of becoming users of future Petascale systems in Europe.

"Our main target group is experienced users from European research groups that aspire to become users of future Petascale systems in Europe. We expect the students to be familiar with the basics of High Performance Computing (HPC) such as MPI and be active users of HPC systems. We welcome anyone with HPC experience to apply for our summer school", Andersson says.

Registration is open until 23 June, 2008, at the Summer School web page.

"The number of participants is limited to 30, so students are advised to apply as early as possible", Andersson notes.

A PRACE Admission Committee will be responsible for selecting the students, but the timely registration is important, so students

are encouraged to apply at their earliest convenience.

Why was the Royal Institute of Technology, KTH, in Stockholm selected to host this summer school?

"Paralleldatorcentrum at KTH has organized an annual Introduction to High Performance Computing Summer School since 1996 and also hosted the International Summer School in Grid Computing (ISSGC07) last year. We thus have a proven record of successfully organizing summer schools. Another important reason is that Stockholm is a lovely place to visit in the summer", Andersson summarises.

The Summer School is part of the PRACE project's education and training task and its aim is to implement a European High Performance Computing education and training programme for scalable scientific computing.

The Summer School will be followed by a Winter School in Greece in February 2009.

To register, and find out more about the school, visit the PRACE Petascale Summer School web page at:

[http://www.pdc.kth.se/systems\\_support/training/2008/PRACE-P2S2/](http://www.pdc.kth.se/systems_support/training/2008/PRACE-P2S2/)

Contact: [prace-p2s2-info@pdc.kth.se](mailto:prace-p2s2-info@pdc.kth.se)

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*PRACE Petascale Summer School will be arranged in the Royal Institute of Technology (KTH), in Stockholm, Sweden.*

# PRACE Arranges a Seminar on Industrial Use of World-Class HPC Services

PRACE, Partnership for Advanced Computing in Europe, arranges a seminar for industrial HPC (High Performance Computing) users in Amsterdam, The Netherlands on 3–4 September, 2008.

The seminar “Industrial competitiveness: Europe goes HPC” is exclusively designed for CIOs (Chief Information Officers), CTOs (Chief Technical Officers) and R&D (Research and Development) managers, responsible for research and development infrastructures in business sectors that are likely to benefit from the use of Europe’s fastest ever computing. The seminar is based on invitation only.

Applications in aerospace, car manufacturing, energy, chemicals, drug design and medical industry, metal industry, bioinformatics, telecommunication companies, finance and insurance and many other industrial areas can benefit from the European wide new high-end research infrastructure.

## Industry runs seven years behind

In many domains industry is too conservative in its use of High Performance Computing. When compared to academic HPC installations in Europe, industry is several years behind.

In the United States, huge efforts are under-

taken to reduce this time gap and thereby strengthen the competitiveness of US industry. PRACE will help European industry to shorten their time-to-solutions and gain or regain competitiveness with the Americas and the Asian Region, including India, China and Japan.

## Nobel Laureate to speak

Participants will receive first hand information about the planned PRACE research infrastructure, services and usage models.

Scientist **Peter Grünberg**, who won the 2007 Nobel Prize in Physics for his discovery of giant magnetoresistance which is utilised in modern hard disk drives, will give an interactive interview about advances in simulation sciences. Representatives from industry will demonstrate their competitive advantage through the use of HPC.

For example, computer simulations on the highest level played a decisive role in the development of the Airbus A380, as they do in the automotive industry (Audi), in the mobile phone industry (Nokia) and in drug design (Organon). Scientific simulations in catalysis help reduce energy consumption in every day chemical processes.

The seminar presents a unique opportunity for industry to voice their specific requirements and potential obstacles in using the PRACE



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The seminar: “Industrial competitiveness: Europe goes HPC”, will be arranged in The Netherlands, which is famous for its windmills.

services in an early stage of its conception. The input from industry counts as the infrastructure is being designed now and will prove adaptive to industry’s needs. The first installations are already at the planning stage.

Representatives from industries that conduct research and development in Europe, from IT industries, developers of commercial software, service companies, and the European Commission are invited to share their views and explore the potential.

More info: [www.prace-project.eu](http://www.prace-project.eu)  
e-mail: [prace-industry@fz-juelich.de](mailto:prace-industry@fz-juelich.de)

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Countless canals cross the city of Amsterdam, where the PRACE seminar takes place in September.

# European HPC Training and Education Needs Revealed In PRACE Study

To remain at the cutting edge of simulation science, Europe's High Performance Computing (HPC) users will be required to harness the huge parallelism embodied in Petascale computing architectures containing potentially hundreds of thousands of cores. Unfortunately, improving existing training materials alone will not be enough to keep researchers competitive – a concerted effort is needed to develop new material that exploits tried-and-tested education methodologies as well as new modes of training delivery.

Recently, a comprehensive study was undertaken to evaluate the training and education needs of top-tier HPC users across all PRACE partner sites. Users were invited to participate in an online survey that examined a broad range of HPC topic areas including novel architectures and programming paradigms, tools and techniques for code development, I/O and visualisation.

"The purpose of the study was to evaluate the educational needs of PRACE users by assessing existing proficiency and satisfaction in traditional HPC techniques as well as soliciting their training requirements for forthcoming software and hardware technologies that are shaping the future HPC landscape," said **Timothy Stitt** from the Swiss National Supercomputing Centre (CSCS), who was responsible for conducting the survey.

The results of this survey, which is arguably the most comprehensive evaluation of user

training requirements undertaken by top European HPC users, will steer future training and education programmes within the PRACE HPC Research Infrastructure.

## Need for HPC training programmes

The results of the survey highlighted both the strengths and weaknesses of current HPC training amongst European users, and revealed the need for a high-quality centralised training repository and an improvement in HPC knowledge dissemination channels. Other significant findings included:

1. There is a deficiency amongst a significant proportion of the user community (including those with many years of experience in the HPC field) in understanding the fundamental principles of HPC programming and practice on both existing and novel architectures.

2. Ninety-three percent (93%) of users were unfamiliar with Partitioned Global Address Space (PGAS) languages (a programming paradigm that is gaining widespread attention as an alternative model for developing HPC codes).

3. There is a significant shortcoming in expertise with mixed-mode (MPI-OpenMP) programming. More than two-thirds of respondents indicated they had no competency in this technique. Furthermore, a third of respondents rated the quality of training they had received in mixed-mode programming as 'poor'. Subsequent PRACE training programmes and events will need to remedy this imbalance so that users are fully prepared to

exploit Tier-0 systems when they become available.

4. Only one-fifth of respondents have received training in multi-core programming techniques, the majority of which regarded their proficiency as basic or non-existent.

5. Over 90% of respondents believed they would benefit from formal training in each of the following areas: performance optimization, debugging tools and techniques, code testing and compiler optimisations.

6. Ninety percent (90%) of users considered that there is a need for improved HPC training programmes.

While many areas of HPC training were highlighted as currently deficient in content and/or quality, encouragingly the vast majority of respondents were enthusiastic about the opportunity to benefit from training delivered through a PRACE HPC Training and Education Infrastructure. Furthermore, 95% of all respondents agreed that they would profit from a pan-European centralised repository of regularly updated, high-quality training material.

"Over the coming months, members of the PRACE Training and Education team will begin to implement the recommendations presented by this survey," Stitt added.

Activities planned include a series of European summer schools, winter schools and workshops, as well initiatives to introduce new and improved channels for HPC knowledge transfer.

Contact: Ph. D. Timothy Stitt, CSCS  
e-mail: [stitt@cscs.ch](mailto:stitt@cscs.ch)

## Two New Countries Joined PRACE

Ireland and Turkey joined the PRACE initiative on 29 May 2008. Sixteen countries now support the Partnership for Advanced Computing in Europe.

At the PRACE Management Board meeting in Schiphol, The Netherlands, **Patrick Aerts**, chairman of the PRACE Initiative Management Board, Prof. **James Slevin**, Director of the Irish Centre for High End Computing (ICHEC) and Prof. **M. Serdar Çelebi**, Project Director of the

National Center for High Performance Computing (UYBHM) signed the Memorandum of Understanding. Several additional countries have also expressed their interest in the initiative.

The following countries collaborate in PRACE: Germany (project coordinator), Austria, Finland, France, Greece, Ireland, Italy, The Netherlands, Norway, Poland, Portugal, Spain, Sweden, Switzerland, Turkey and UK.



**Coordinator/Contact:**  
Prof. Dr. Achim Bachem:  
[prace-coordinator@fz-juelich.de](mailto:prace-coordinator@fz-juelich.de)

[www.prace-project.eu](http://www.prace-project.eu)



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