

# 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**

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# D3.2.2 First Training Report *Final*

Version: 1.0 Author(s): Pekka Manninen, CSC Date: 20.6.2011

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Abstract:	A sustained, high-quality training and education programme is a prerequisite to ensure that the PRACE research infrastructure will remain productive. This document describes the training and education activities during the first 11 months of the project.

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## **References and Applicable Documents**

[1] Manninen, P.;& Robinson, T. (2010). *D3.2.1 Training Plan*. Partnership for Advanced Computing in Europe.

[2] Stitt, T.;& Robinson, T. (2008). A Survey on Training and Education Needs for Petascale. Partnership for Advanced Computing in Europe.

## List of Acronyms and Abbreviations

BSC	Barcelona Supercomputing Center (Spain)		
CaSToRC	Computation-based Science and Technology Research Center (Cyprus)		
CEA	Commissariat à l'Energie Atomique (represented in PRACE by GENCI, France)		
CINECA	Consorzio Interuniversitario, the largest Italian computing centre (Italy)		
CSC	Finnish IT Centre for Science (Finland)		
CSCS	The Swiss National Supercomputing Centre (represented in PRACE by ETHZ, Switzerland)		
CUDA	Compute Unified Device Architecture (NVIDIA)		
EPCC	Edinburgh Parallel Computing Centre (represented in PRACE by EPSRC, United Kingdom)		
EPSRC	The Engineering and Physical Sciences Research Council (United Kingdom)		
DEISA	Distributed European Infrastructure for Supercomputing Applications. EU project by leading national HPC centres.		
GENCI	Grand Equipement National de Calcul Intensif (France)		
GPU	Graphics Processing Unit		
GRNET	Greek Research and Technology Network (Greece)		
HPC	High Performance Computing; Computing at a high performance level at any given time; often used synonym with Supercomputing		
ICHEC	Irish Center for High-End Computing (Ireland)		
KTH	Kungliga Tekniska Högskolan (represented in PRACE by SNIC, Sweden)		
MPI	Message Passing Interface		
OpenCL	Open Computing Language		
Open MP	Open Multi-Processing		
PATC	PRACE Advanced Training Centre		
PGAS	Partitioned Global Address Space		
PRACE	Partnership for Advanced Computing in Europe; Project Acronym		
PSNC	Poznan Supercomputing and Networking Centre (Poland)		
SNIC	Swedish National Infrastructure for Computing (Sweden)		

Tier-0Denotes the apex of a conceptual pyramid of HPC systems. In this<br/>context the Supercomputing Research Infrastructure would host the<br/>Tier-0 systems; national or topical HPC centres would constitute Tier-1VSBTechnical University of Ostrava (Czech Republic)

WP Work Package

# **Executive Summary**

This deliverable summarises the activities of the PRACE-1IP training programme (task 3.2 in Work Package 3: 'Dissemination and Training') during the project months 1 to 11 (July 2010 to May 2011). These consisted of three "seasonal schools" in Spain, Cyprus and the UK; work for constructing an Internet hub in computational science education called as PRACE Training Portal; and groundwork for enabling remote learning methods within PRACE as well as for future education outreach activities.

The activities have been highly successful. All the seasonal schools gathered an international audience, featured high quality, high-expertise lectures on contemporary topics in high-performance computing, and excelled in the participant feedback. The Training Portal will be completed according to plans. During the remaining time of the PRACE-1IP project, there will be five seasonal schools more; and more emphasis will be put on the education outreach activities and further development of the Training Portal.

## 1 Introduction

The role of the training task in the PRACE first implementation phase (PRACE-1IP) project is to establish and promote a European-wide training network in high-performance computing. The task is a part of the PRACE-1IP Work Package (WP) 3: 'Dissemination and Training'. The plan for the training program was published as the deliverable D3.2.1 [1] during the first month of the PRACE-1IP project.

In this report, we review the activities and accomplishments of the training task during the first half (months 1 to 11 of the project, or July 2010 to May 2011). The activities undertaken range from traditional face-to-face training events, which we describe in Section 2, to more modern e-learning initiatives such as the establishment of an online training portal, which is discussed in Section 3. Section 3 also provides a description of an educational outreach programme, as well as detailing the progress made with the design of the "PRACE Advanced Training Centres", which will be implemented in the latter phases of PRACE. Section 4 provides some remarks on practical matters regarding the coordination of work across the partner sites. Finally, detailed reports of each of the face-to-face events, authored by the respective organizing sites, are provided as annexes.

## 2 Face-to-face training events

## 2.1 Overview

The backbone of the PRACE-1IP training programme is a series of seasonal schools addressing various topics and levels of HPC methodology, especially those closely related to the use of Tier-0 systems. In addition to them, two more discipline-specific seminars are organized, one in the first half and another on the second half of the project.

The target audience of the series is European researchers working with computational sciences. The series aims at increasing the awareness of the possibilities and challenges of Tier-0 high-performance computing together with general improvement the related skill set. Another target group is the employees of PRACE centres – the series provides them with a chance to keep up with the methodology progress and meet the researchers.

	•		
School	Time	Location	Organizer(s)
1st Autumn school	Oct 25-29, 2010	Barcelona, Spain	BSC
1st Winter school	Jan 24-27, 2011	Nicosia, Cyprus	CaSToRC & GRNET
1st Scientific seminar	Feb 20-22, 2011	Stockholm, Sweden	SNIC
1st Spring school	Mar 29-31, 2011	Edinburgh, UK	EPCC & ICHEC
1st Summer school	Aug 28-Sep 1,	Espoo, Finland	CSC & SNIC
	2011		
2nd Autumn school	Oct 25-27, 2011	Paris, France	GENCI
2nd Winter school	Feb 2012	Italy	CINECA
2nd Scientific seminar	Feb/Mar 2012	Ireland	ICHEC
2nd Spring school	Mar/Apr 2012	Krakow, Poland	PSNC & VSB
2nd Summer school	Jun/Jul 2012	Lugano, Switzerland	CSCS
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A full list of the planned and held events is presented in Table 1, including dates and locations where applicable. The planned times have been updated from those given in D3.2.1 [1] according to changes in local arrangements and convenience.

 Table 1: PRACE-1IP face-to-face training event series.

## 2.2 Programmes

The purpose of the PRACE seasonal schools is to provide within a reasonably compact timeframe as a thorough and exhaustive treatment as possible of various topics in contemporary HPC programming, but from a particular angle in each case. To reach this goal, a length of 3-5 days was considered to be the optimum – any shorter workshops would necessarily result in the exclusion of important topics, any longer might be too much of a time commitment for certain participants (especially senior scientists). The Spring School was three days and the Winter School four days in duration, while the Autumn School spanned five days. There was strong support for these timeframes in the participant feedback from the schools, and we will therefore continue with this approach for subsequent schools.

The three seasonal schools held thus far focussed on slightly different themes. The Autumn School had three tracks: the first one aimed to cover the basic and standard concepts of HPC programming through realistic examples and hands-on sessions; the second focused on explaining alternative advanced programming models; and the third was oriented to advanced users and covered aspects of application debugging and performance analysis.

The goals of the Winter School were primarily to offer training in fundamental HPC topics ("must haves"), and to introduce selected advanced topics of importance and interest ("nice to have"). The school featured also industry collaboration initiated by WP5 ('Industrial User Relations') in the form of invited trainers. Based on the participant feedback, the school was extremely successful in providing a thorough grounding in basic skills as well as glimpses towards more advanced topics.

The topic for the Spring School was chosen to be "advanced techniques for extreme scalability" and the subject material included modern approaches to parallel programming for HPC, including PGAS languages (Unified Parallel C and Co-Array Fortran), GPU and hybrid programming and parallel performance analysis tools.

The first PRACE Scientific Seminar aimed at addressing questions essential to computational scientists from the end user's point of view rather than from that of HPC experts. Over the course of the seminar, prominent researchers from a wide range of scientific communities presented their research achievements and gave their opinions on current and future trends of HPC. In particular, they were encouraged to discuss their experiences adapting their codes to

different state-of-the-art HPC architectures, focusing on the difficulties encountered in obtaining scalability and performance, and how these difficulties were overcome.

## 2.3 Participants

The seasonal schools thus far have all been fully subscribed - a testament to the quality of teaching and material and the fact that the courses are offered free of charge. In some cases, it was necessary to employ a selection process to ensure that the most deserving participants were guaranteed places in the school.

The geographic distribution of the participants in the first three Schools is presented in Table 2.

Country	Autumn	Winter	Spring
	School	School	School
Albania	0	3	0
Croatia	0	1	0
Czech Rep.	3	0	6
Cyprus	0	18	2
Finland	0	0	3
France	0	1	0
Egypt	0	14	0
Greece	0	4	3
Germany	1	1	3
Ireland	0	0	7
Israel	0	3	0
Italy	1	0	3
Jordan	0	8	0
Lebanon	0	4	0
Netherlands	0	1	0
Norway	0	0	3
Poland	0	0	2
Saudi Arabia	0	1	0
Serbia	0	0	2
Spain	42	2	2
Sweden	1	0	0
Syria	0	1	0
Turkey	2	0	2
UK	1	1	33
USA	0	0	3
Total	51	63	74

 Table 2: Number of participants per country to the PRACE seasonal schools

The training events have attracted participants from nearly all PRACE member countries, and from countries even outside of PRACE. The participation of students from external countries is very positive, as the events serve to promote PRACE and foster international collaboration and networking. However, if the participation outside PRACE would be much more pronounced, some allocation preferences for PRACE member country affiliates could be imposed, as these events are a major PRACE investment. Presently this is not topical, however.

Only in the Autumn School, the fraction of the participants from the hosting country is undesirably high (82%). The Winter and Spring Schools managed to draw more international and widespread participation (29% and 44% of the attendees, respectively, were based on the hosting country). It is evident that most of the participants would be from the hosting country or its neighbouring countries – this premonition was one of the bases for the original distribution of the schools to maximise the geographical coverage and impact of the series – but the schools should be advertised and promoted in all PRACE countries in the future. A target of 50% at the maximum from the hosting country could be set for similar events in the future.

## 2.4 Feedback

The training schools have been well organised and have proceeded without incident. The high quality of practical arrangements and programme content was evident in the feedback gathered from the participants. The common feedback survey form for all T3.2 events is an appendix; see Subsection 5.5. After three schools, some need for collecting more information has arisen and the survey form will be expanded accordingly for the remaining events. The additional items will inquire the participant background in more detail as well as assess the usefulness of social events.

The three schools received more or less the same overall rating from the participants. In response to the question "Overall, how would you rate this school? [0 = waste of time, 10 = excellent]", the Autumn School received an average of 8.05, the Winter School 8.30, and the Spring School 8.08. The distribution of individual ratings is presented in Figure 1. The feedback from the Spring School was the most varied, with the largest fraction of "Excellent" ratings but also with some entries on the lower scale; this is perhaps not surprising considering that the school featured topics that demanded the highest prerequisites from the participants.



Figure 1: Distribution of overall ratings of the seasonal schools

# **3** Other activities

## 3.1 PRACE Training Portal development

One of the major subtasks of the PRACE training program is the development of a HPC Training Portal, which will be a central location on the Internet for the dissemination of highquality HPC training materials and information, catering for a range of competency levels. The initiative for such a portal arose first from the results of a survey of training requirements during the PRACE preparatory phase [2], which concluded that PRACE should immediately begin to investigate the introduction of a centralised European repository for training material and HPC knowledge dissemination.

According to the requirements of the user community, the HPC Training Portal encompasses the following elements: static training material, including video, audio and slides; interactive (or "self-learning") training material, where progress can be monitored via tests or quizzes; discussion forums for peer-to-peer discussion and problem solving; a blog, contributed to by multiple authors from PRACE sites; regular news items on the state of the art in HPC technology; and an up-to-date events calendar, which lists seminars, workshops and other events relating to HPC and computational science in Europe.

Users will have the ability to log in to the site to rate and/or comment on the training materials or news items. These features, in conjunction with the discussion forums, will provide a dynamic framework to increase the social interactions both amongst the PRACE users themselves and between PRACE staff and their users. Such interactions are not provided for in the current PRACE training website.

The portal framework is implemented using open source web technologies (TYPO3 and WordPress) and is extensible such that that additional functionality can be added as and when required. All partner sites with person months in WP3 are expected to contribute to the development and maintenance of the material made available through the portal, as well as contribute to forum discussions, add news items and blog postings, and so on. Content will be contributed by all relevant WPs, especially WP7.

The development and implementation of the training portal is documented in detail in PRACE-1IP deliverable D3.1.5, and the portal is expected to go live in late June 2011.

## 3.2 Developing the concept of PRACE Advanced Training Centres

The PRACE Advanced Training Centres (PATCs) will provide top-class training events in many fields of scientific computing and serve as European hubs of advanced training for computational scientists working in PRACE countries. They will also develop and lead outreach efforts relating to education.

Guidelines for the establishment of the PATCs, covering issues such as their management, business models and processes for hosting the centres and their locations, will be defined during the PRACE-1IP project and reported in deliverable D3.2.3. This deliverable, originally due in M18, was brought forward to M12 as its conclusions are required input for the early stages of the PRACE 2<sup>nd</sup> implementation phase project (PRACE-2IP). We have held two face-to-face meetings – one in Edinburgh and the other in Helsinki – to discuss in detail the establishment of the PATCs, and the associated deliverable.

## 3.3 Remote learning initiatives

Initiatives regarding remote learning, both in terms of virtual learning environments and also the ability to attend courses remotely (via "webinars"), have been postponed to the second half of the project due in part to the lack of a subtask manager.

## 3.4 Education outreach initiatives

The importance of reaching out to the secondary and tertiary education sectors was identified during the PRACE preparatory phase and stressed in the training plan for PRACE-1IP. The task has realised an "education outreach plan of actions" (annexed to this document, see Subsection 5.6), and the activities presented within will be realized during the first part of the project.

## 4 Coordination of the work

During the first half of the PRACE-1IP training task the work has been coordinated based on milestones and action points and their regular review in teleconferences. Every two weeks a training task teleconference has been held, alternating between training portal-specific issues and general topics. The general teleconferences have been chaired by the training task leader and the training portal meetings by the subtask manager. The minutes of the teleconferences have been archived in the BSCW document repository. The teleconferences have, in general, been well attended and have generated lively and useful discussion.

Training topics have also been discussed in the monthly WP3 all-hands teleconferences as well as in WP3 face-to-face meetings (in Krakow and Belgrade).

One of the very few shortcomings encountered so far was the failure to find subtask managers for the two planned subtasks ("education outreach" & "remote learning").

# 5 Annex

## 5.1 Report on the first Autumn School

By Renata Giménez, BSC

Basic information about the event

Name: PRACE Autumn School 2010

**Dates:** 25- 29<sup>th</sup> October, 2010

Location: UPC Campus North, Barcelona (Spain)

Organizing sites: BSC

Organizational details

## Local organizing committee

- Carlos Merida (BSC)
- Renata Giménez (BSC)
- Sara Ibáñez (BSC)

**Venue:** UPC North Campus. This venue was chosen for the computer rooms and its close location to BSC. The facilities required were three computer rooms for the training as well as good access to the supercomputer MareNostrum.

**Budgeting:** The prices indicated below are exclusive of VAT and are based on a total of 50 participants. All participants had coffee breaks and lunches included as well as a dinner on Wednesday.

Concept	Cost
Computer Rooms PUE (3 in total)	3,823 €
Aula Master + Polivalent	803 €
Coffee breaks (3,6 euros)	900 €
Lunch (11 euros)	2,200 €
Dinner Monday teachers	390 €
Dinner Wednesday	1,000 €
Dinner Thursday (40 euros/person)	2,000 €
Welcome pack	100 €
Documentation	100 €
Video recording	6,650 €
TOTAL	17,966 €

## Program & content

## **Program committee**

- Jesús Labarta (BSC)
- Eduard Ayguadé (BSC)
- Rosa M. Badia (BSC)
- Carlos Mérida (BSC)
- Toni Cortés (BSC)

Final program: http://www.bsc.es/media/3899.pdf

Teacher	Торіс
Rajeev Thakur	MPI
Xavier Martorell	Basic Programming Models
Alex Durán	OpenMP Programming
Brad Chamberlain	Chapel
Nacho Navarro & Manuel Ujaldón	Accelerator programming
Rosa Maria Badia	StarSs
David Henty	Co-Array Fortran
John Donners	Debugging tools
Jesus Labarta, Judit Gimenez	Performance Analysis

## List of trainers

**Designing the program** The Autumn School aimed to expand and intensify the existing ecosystem of scientists who use HPC technologies. Researchers and students from Europe and beyond received lectures on topics ranging from basic concepts on programming frameworks to specialized tools and techniques for advanced users. This five day PRACE Autumn School focused on the in-depth presentation of HPC topics during morning lectures followed by hands-on training in the afternoon. To enable students to solve problems in scalable scientific computing, access was provided to the supercomputer MareNostrum at BSC as well as other HPC facilities.

**Description of the contents:** The school ran three tracks in parallel. The first aimed to cover the basic concepts of HPC programming through realistic examples and hands-on sessions. The second track focused on explaining alternative advanced programming models. Aside from the standard programming models (MPI and OpenMP), novel solutions such as StarSs (developed at BSC), CUDA and OpenCL – targetting GPUs – and Chapel and CAF – addressing programmability and productivity – were also presented. The third track was oriented to advanced users and covered aspects of application debugging and performance analysis.

Computer resources: the supercomputer MareNostrum as well as other HPC facilities.

## Participants & feedback

**Number of participants by country:** It gathered almost 50 attendees from many European countries (mostly from Spain).

**Process for selecting the participants:** the organizing committee had a meeting and decided the topics of the training course. They decided to target an audience of varied abilities, and defined a program accordingly (three tracks depending on the experience level of the participants).

Analysis of the feedback: The feedback from the school supports the impression of a successful and well-organized school. Video presentations can be found at <u>www.prace-ri.eu/hpc-training/prace-code-porting-videos/prace-autumn-school-bsc-2010</u>

**Conclusions & lessons learned:** in order to get good trainers and teachers from abroad, some fees for their teaching classes should be budgeted.

## 5.2 Report on the first Winter School

By Christos Nicolaou, CaSToRC

Basic information about the event

Name: PRACE/LinkSCEEM Winter 2011 School

Dates: January 24-27, 2011

Location: The Cyprus Institute Athalassa Campus, Nicosia, Cyprus

**Organizing sites**: Computation-based Science and Technology Research Center (CaSToRC) and Greek Research and Technology Network (GRNET)

Organizational details

## Local organizing committee

- Constantia Alexandrou, CaSToRC
- Christos Nicolaou, CaSToRC (Chair)
- Fotis Georgatos, CaSToRC

The local organizing committee was strengthened by Ioannis Liabotis from GRNET, who assisted in the organization of the school, bringing with him a wealth of prior experience.

**Venue:** The school was organized at the Athalassa campus of the former Higher Technical Institute at the entrance of Nicosia, which is gradually being transferred to the Cyprus Institute. The Athalassa campus has a lecture room with a capacity of about 100 persons. The lecture room has all necessary facilities including projectors, projector panels, microphones, etc., and in addition, standard classrooms and other facilities could be used used to support the school on an as needed basis. While part of the Athalassa campus has been given to CyI and has been refurbished appropriately, the possession of the part of the campus including the lecture room has not yet been transferred to the Institute. The necessary permissions were secured from the current owner, the Ministry of Labor of the Republic of Cyprus and the room was provided free of charge (provided that the necessary maintenance would take place). CyI staff gained access to the lecture room one month before the event for maintenance, testing and planning purposes in order to ensure that the room was fully prepared for the school. Network connectivity with the main CyI building – and through it to the Internet – was put in place by CaSToRC staff.

The selection of the Athalassa campus venue proved crucial to the success of the school since the local organizers were supported by the administration of the Cyprus Institute and made use of its facilities. Among the CyI facilities used by the school were the cluster where the trainees were given access for hands-on exercises, network connection, meeting rooms for small groups, etc. The location of the campus, at the entrance of the city, enabled easy access for all school participants including local trainees.

**Budgeting**: The budget for the organization of the school was supported by two FP7 projects, PRACE and LinkSCEEM-2, and the organizing partners, the Cyprus Institute and GRNET. The costs allocated to PRACE amounted to  $13,504 \in$  including  $2,300 \in$  for the video recording and  $11,204 \in$  for general school organization expenses. The general school expenses include expenses for three trainers, catering for school participants, two social events, transportation of the participants to the site of the school, maintenance and operation expenses for the lecture hall used as well as smaller amounts for other expenses such as

stationary supplies and preparation of leaflets. LinkSCEEM-2 contributed to the budget by supporting three additional trainers and by covering the expenses of over 30 students from the region to attend the event. In addition, the event was supported by staff from CaSToRC, GRNET and general CyI support staff, who invested numerous person hours to ensure the success of the school.

**Synergetic events:** The event was co-organized with the LinkSCEEM-2 FP7 project 2011 Advanced Training Workshop. No other PRACE activity took place concurrently with the school.

## Program & content

#### **Program committee**

Name	Affiliation	Country
Constantia Alexandrou	CYI	Cyprus
Norbert Attig	JSC	Germany
Paschalis Korosoglou	AUTH/GRNET	Greece
Ioannis Liabotis	GRNET	Greece
SalwaNassar	NARSS	Egypt
Christos Nicolaou	CaSToRC	Cyprus
Tim Robinson	CSCS	Switzerland
Stephane Requena	GENCI	France

## Final program: The final program can be found at

http://www.linksceem.eu/joomla/index.php?option=com\_content&view=article&id=116&Ite mid=127.

## List of trainers:

- Dr. N. Sinanis
- Eng. F. Georgatos
- Mr. P. Korosoglou
- Dr. G. Koutsou
- Mr. Heiko J. Schick
- Dr. R. Bader
- Dr. N. Eicker
- Mr. J. C. Vasnier
- Dr. A. Strelchenko
- Dr. M. Geimer
- Dr. J. M. Favre
- Mr. Lindon Locks

**Designing the program**: The program committee (PC) consisted of experts from HPC centers as well as computational scientists with experience in organizing training schools in the EU and the Eastern Mediterranean region. Due to the dual nature of the school, serving the needs of both the PRACE and LinkSCEEM communities, the PC expected applicants to come from different countries and have substantial differences in expertise level. Consequently, the program has been designed so as to accommodate trainees with varying expertise levels and professional backgrounds. The goals of the school were primarily to offer training in fundamental HPC topics (must have), and, to introduce selected topics of great importance and interest (nice to have) to the computational science community targeted. As a first step, the committee compiled the list of

topics that needed to be addressed including both the 'must have' and the 'nice to have'. All fundamental topics were included in the program. Specifically, these topics covered an introduction to parallel programming techniques, MPI (lecture and hands-on), OpenMP (lecture and hands-on) as well as a programming refresh and a session on core skills. In a second step, the PC selected additional topics from the list of the 'nice to have' based on the expected interests of the participants to the school and the availability of trainers. These latter topics included advanced MPI programming, HPC system architectures and supercomputer design, introduction to PGAS, introduction and hands-on to OpenCL, application performance analysis, visualization techniques and advanced debugging tools. Moreover, it was decided that an applications workshop would be organized where special interest groups representing the scientific fields more strongly represented by the school participants would have the opportunity to get together and exchange ideas and experiences lead by a domain expert.

**Description of the contents:** Please see the blog of the school at: <u>http://gridtalk-project.blogspot.com/search/label/PRACE%2FLinkSCEEM%202011</u> which contains info on the lectures given including photos.

**Computer resources:** The school made use of the CaSToRC infrastructure facilities for training purposes. Specifically, the school participants were given accounts to Euclid, a small hybrid cluster combining both traditional nodes with GPU accelerators located on a different building of the same campus. Euclid proved sufficient for the purposes of the school.

## Participants & feedback

Country	Number of Participants
Albania	3
Croatia	1
Cyprus	18
France	1
Egypt	14
Greece	4
Germany	1
Israel	3
Jordan	8
Lebanon	4
Netherlands	1
Saudi Arabia	1
Spain	2
Syria	1
UK	1
Total	63

## Number of participants by country

**Process for selecting the participants**: The school was originally planned to host 50-60 students from Europe and the Eastern Mediterranean. Initially there were selection criteria only for Eastern Mediterranean participants that applied for funding support available through the LinkSCEEM-2 project. Following the large number of applications received, of the order of 80, and to avoid having to reject some of the candidates, the organizing committee made the necessary arrangements to accept all applicants not requesting funding.

Statistics of the feedback survey: The feedback survey was completed by 37 participants.

Analysis of the feedback: School participants' responses indicate that they had at least some skills on the fundamental topics targeted by the school. Specifically participants were experienced with programming languages (only 4 responded that they were uncomfortable with the languages used during the school), had been exposed to MPI previously (~80% had fair or better knowledge) and, in general, had adequate knowledge of OpenMP (~60% had fair or better knowledge). Knowledge on the other topics covered by the school can be characterized as intermediate; 45% were unfamiliar with performance analysis tools and techniques, 20% with code optimization, nearly 50% with parallel program debugging, 84% with PGAS and 75% with OpenCL.

Feedback on the organization of the school was in general very good and positive. Specifically, 97% were happy with the level of information provided for the school, 97% with the registration system, 85% with the venue, 94% with catering and 97% with the overall organization.

With respect to the training offered over 90% of the participants found the topics of the school to be relevant to their research and a sizeable 75% stated that the school inspired them to new ways of thinking. An overwhelming majority gave positive marks to the training activities with over 85% stating that the lectures were clearly presented and comprehensible, about 75% agreeing that the pace of teaching was appropriate, 85% finding the teaching aids well prepared and 81% finding the hands-on and demonstrations to be a valuable contribution. The responses were in general extremely positive with the exception of two individuals who felt that either the trainer was not sufficiently experienced or the lecture was too lengthy and lacked a hands-on component. Ratings of these two lectures caused the limited negative ratings of the school training activities. Some lectures, including the advanced MPI and visualization lecture and hands-on, received many favorable comments - some actually thanking the trainers. A small number of general comments (~10%) expressed a desire for more intense lectures and hands-on on the fundamental topics covered by the school. The overall impression for the school was rated quite positively with the respondents rating it with an average of 8.3 out of 10. There were several general comments thanking the organizers, positively commenting on the catering service and asking for more schools of the same type. Positive comments were also received for the applications workshop where participants from the same research community had the opportunity to present their research, discuss problems and ideas and receive feedback from other scientists.

Responses to questions about the necessity for future schools covering the topics of the school indicated that the school provided training on topics of great interest and usefulness to the scientific community targeted. Responses to general comments also suggested more training on fundamental topics and the preparation of training material to be made available to trainees before a given school. These comments will be taken into account for future training activities undertaken by CaSToRC and GRNET.

**Conclusions & lessons learned:** The organization of such a major HPC school has been a major undertaking for CaSToRC. Although members of the center had previously been involved in the organization of conferences, summer schools and other similar events, the center had not assumed the responsibility of a HPC school of this size and reach. Fortunately, the local organizing committee was supplemented with a member from GRNET with past experience in such events. This facilitated the timely preparation of the school plan covering all organizational aspects including – but not limited to – the announcement(s) for the school, the selection and preparation of the venue, the selection and invitation of the trainers, the accommodation arrangements for hosting the school participants, the social program of the school, etc. The early formation of the program committee, consisting mainly of members from PRACE partners with significant expertise in the organization of HPC training events proved to be instrumental for the preparation of an interesting program that met the

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expectations of the participants. Additionally, support from PRACE also proved very useful through the provision of the online registration form and the school evaluation survey. The tool, provided by PRACE partner IPB, allowed the preparation of the necessary online forms that applicants used to register for the school, elaborate on their profile and, following the completion of the school, evaluate the event.

Securing trainers is a crucial part of the organization process; particular attention should be paid to avoid the situation where the committee is firmly proposing a subject but nobody is able/available deliver it; therefore, recommended practice in future events may be to rather suggest/nominate expertise fields along with candidates, rather than just merely a training slot. That would also promote the reuse/enhancement of training material. Overall, it was clear that the success of the school was a direct consequence of careful and thorough planning and preparation. Among the keys to success, we found that the execution of a survey in parallel to the registration process allowed us to better identify the needs of the participants and judge correctly about the topics to be covered and the expertise level to expect. An additional key factor that contributed to the success of the school has been the early preparation of a thorough organizational plan, which was strictly followed. Among the difficulties found was securing high quality trainers, a task that took considerably longer than initially expected, and coordinating the preparations for the school, which was made easier by the ample support provided by the Cyprus Institute.

## 5.3 Report on the first Spring School

By Nicola Mc Donnell, ICHEC

## Basic information about the event

The 'DEISA/PRACE Spring School 2011' was a combined event between DEISA and PRACE, with DEISA providing funding for travel and accommodation for some of the attendees and PRACE providing the funding for the event itself. It was held at EPCC, University of Edinburgh, UK from 29<sup>th</sup> until 31<sup>st</sup> of March 2011 and was jointly organized by EPCC and ICHEC.

## Organizational details

#### Local organizing committee: The event organization team comprised of

Team member (Centre)	Role
David Henty (EPCC)	Lead organizer
Irina Nazarova (EPCC)	System and registrants
Linda Tait (EPCC)	Administration
Nix Mc Donnell (ICHEC)	Assistant organizer

**Venue**: The Spring School was held at EPCC, which is located in the Kings Building Campus of the University of Edinburgh. Three rooms were used for the event, a large lecture theatre for the introductory morning, and two smaller rooms accommodating up to 35 and 72 students respectively for the parallel sessions. Registration was set up in front of the large lecture theatre and the break-out area for tea/coffee/lunch breaks was reserved. All of these locations were on the 3<sup>rd</sup> floor of the James Clerk Maxwell Building (JCMB) building.

These venues were chosen as they are close to each other and free to book for University events. All provided good wireless connectivity, and were ideal for hands-on training. In the smaller venue, all students can see the main projection screen from their desks; in the larger venue, there are also individual screens at each cluster of six desks that mirror the main screen. It was important to have everyone in the same room for the first session, so for this we used a more standard lecture theatre.

All the venues worked very well for the mixture of hands-on and lecture-based training delivered at the school. There were some intermittent issues regarding 'eduroam' access for visitors, but the attendees were always able to use the special wireless accounts supplied to them at registration so this did not cause any significant problems.

**Budgeting**: The budget comprised expenses for the remote speakers, food at the event and the School meal, as the venue was free.

Expense	Budgeted (EUR)	Actual (EUR) <sup>1</sup>
Speaker expenses	6,000	4,287
Tea/coffee/lunches	3,534	4,293
School Meal	5,200	4,735
Pack	380	0
Total	15,114	13,315

<sup>&</sup>lt;sup>1</sup> The expense budget can only be approximate. The exchange rate of 0.8 was used to convert from USD to EUR and 1.23 to convert from GBP to EUR.

There were four remote speakers, three coming from the USA (Tarek El-Ghazawi and Oliver Serres from the George Washington University and Gabriele Jost from the Texas Advanced Computing Center) and one from the EU (Brian Wylie, Forschungszentrum Jülich); their expenses were budgeted to be 6,000 €in total. The actual cost of the travel was 4,287 €

The school was planned to have a maximum of 65 students and there were 11 organizers/trainers making a total 76 participants. The tea, coffee and lunches were budgeted at 15.50  $\notin$  per participant per day, so for the 3-day school this came to 3,534  $\notin$  The actual cost of the tea/coffee and lunches is estimated to be 4,293  $\notin$  arising from £1,163 per day. The main reason for the difference in the budget and actual cost arise from exchange rate differences at both costings.

The venue selected for the school meal could only accommodate 65 attendees and was budgeted at  $80 \notin per$  attendee, thus totalling  $5,200 \notin The$  actual cost of the meal is estimated to be  $4,735 \notin arising$  from £3,850. Lastly,  $5 \notin per$  participant was allocated for the production of the school pack, totalling  $380 \notin for the end$  the packs cost nothing to provide as, rather than photocopying material, we provided it in electronic form on a USB stick.

The combined budget for the school came to  $15,114 \in$  with the actual cost estimated to be  $13,315 \in$ 

**DEISA** Within DEISA there was  $20,000 \in$  that was allocated to pay for the travel and accommodation for students who wished to attend the DEISA/PRACE Spring School. A maximum of 750  $\in$  could be claimed per student to cover four nights accommodation and flights; other meals were not included. Up to twenty-seven students could have been funded. The PRACE partners' sites nominated twenty-six students and all were awarded funding.

## Program & content

David Henty designed the program; he selected a dual track series of invited lectures and associated hands-on practical sessions, covering new PGAS languages, UPC and Co-Array Fortran, programming paradigms and tools for extreme scalability, specifically the parallel debugger from Scalasca. The final agenda can be found at <u>http://www.epcc.ed.ac.uk/news/pracedeisa-spring-school-29-31-march-2011-edinburgh-tools-and-techniques-for-extreme-scalability</u>

## List of trainers:

- Dr. Tom Edwards, Cray Centre of Excellence, Edinburgh
- Dr. Alan Gray, EPCC Edinburgh
- Mr. James Perry, EPCC Edinburgh
- Dr. David Henty, EPCC Edinburgh
- Dr. Harvey Richardson, Cray Centre of Excellence, Edinburgh
- Dr. Brian Wylie, Jülich Supercomputing Centre (JSC), Germany
- Prof. Tarek El-Ghazawi, The George Washington University, USA
- Mr. Olivier Serres, The George Washington University, USA
- Dr. Gabriele Jost, Texas Advanced Computing Centre, USA

**Designing the program:** The program was designed with a target audience of people already familiar with standard parallel programming (e.g. MPI with C or Fortran) in mind, such that they could expand their knowledge with new tools and techniques relevant to very large-scale parallelism. The timing of the School also coincided with the upgrade of EPCC's Cray system to the new Gemini interconnect. This enables very low-latency communications and so is therefore ideal for PGAS languages, making an ideal training platform.

We decided that there should to be a short introductory session to describe the general Cray architecture to all attendees because it would be used for all practical sessions, except for those using GPUs. We thought that some people might be further interested in the details of the Cray XE6 itself, so an in-depth training session was provided by local Cray staff. As an alternative, we felt that many attendees would be interested in learning about GPU programming, as it is such a hot topic at present.

We decided to cover both of the mainstream PGAS languages, UPC and Co-Array Fortran, and scheduled them on different days so attendees would have a chance to attend both sessions. PGAS is seen as a possible alternative to MPI for exascale machines, so was an obvious topic for the School.

As the other alternative to pure MPI is to extend codes to use OpenMP on a node, we decided that a session on Hybrid programming was essential.

Finally, analysing performance becomes a real problem on large systems so we considered that a session on tools was also essential. We selected SCALASCA as it is high quality, European and freely available; the SCALASCA team also maintain very good training materials.

**Computer resources:** Two machines were used for the School: the UK National Supercomputing Service, HECTOR XE6, and EPCC's GPU Service, Ness. The current HECTOR system (Phase 2b, XE6) is contained in 20 cabinets and comprises a total of 464 compute blades. Each blade contains four compute nodes, each with two 12-core AMD Opteron 2.1 GHz Magny Cours processors. This amounts to a total of 44,544 cores. Each 12-core socket is coupled with a Cray Gemini interconnect. Each 12-core processor shares 16 GB of memory, giving a system total of 59.4 TB. The theoretical peak performance of the phase 2b system is over 360 Tflops. Forty-four thousand allocation units were reserved on HECTOR for the school. A dedicated queue was created for the School that provided the students with almost instant turnaround for the hands-on exercises.

Each student brought their own laptop and accessed the machine through University of Edinburgh visitor Wi-Fi accounts. Although this placed a very heavy load on the wireless infrastructure, it was sufficient for the number of attendees and there were no issues.

## Participants & feedback

Country	Number of Participants
Cyprus	2
Czech Rep	6
Finland	3
Germany	3
Greece	3
Ireland	7
Italy	3
Norway	3
Poland	2
Serbia	2
Spain	2
Turkey	2
UK	33
USA	3

#### Number of participants by country

**Process for selecting the participants:** The School was oversubscribed and the students were selected on a first come first served basis. In practice, only a few students were rejected as those on the waiting list were accepted whenever a registered person dropped out.

## Feedback

**Overall Score:** Overall, the feedback from the course was very good. We had 48 responses to the survey, and the School scored an overall 8.1/10. The venue and overall organisation were rated very highly with a mark between Good and Excellent; the catering was the lowest score in this section, but still rated Good. The feedback on the lectures was also very good. The lowest score was for the pace of the lectures, although the overall rating was still that people generally agreed that the pace was about right.



**Students skill set:** When assessing their skills levels prior to the course, attendees rated their HPC Programming skills as good, followed by MPI as good/fair. All of shared-memory programming, performance analysis, code optimization and debugging were rated as fair. The lowest skills rating, fair/unskilled, were given to new HPC languages and accelerator programming.



When commenting on what areas they would like to see addressed in future schools, there was a strong preference for training in the areas that students felt themselves weak in, namely Hybrid MPI/OpenMP, PGAS and CUDA. Although all these areas were actually covered by the Spring School, and generally very well regarded, it is clear that there is scope for further training in these areas.

Additional comments feedback: The additional comments feedback was very positive in the areas of the hands-on exercises. The only negative comments were that in some courses there was a little too much lecturing, which squeezed out the practical sessions. This aspect is hard to control when using invited lectures, although we could emphasise the need to leave sufficient time for hands-on exercises in future.

Another comment was that access to the HPC resources in advance of the course would be useful to enable porting to take place before arrival. This is an interesting suggestion, but might be hard to achieve in practice as we typically use special accounts for courses that can only be enabled for a limited time.

**Conclusions & lessons learned:** The only significant lesson learned was related to visa application times for non-EU nationals. Although we sent invitation letters immediately on request, there were unexpected delays. Unfortunately, this meant that the British Foreign Office did not issue visas in time for some Turkish students travelling from Germany to be able to attend the School. This was only an issue for those applying for funding from DEISA and was due to the time was required to collect and process all the nominations. For events that do not offer funding for travel we should simply encourage non-EU nationals to apply as early as possible. If funding were available on a competitive basis, we would set an earlier closing date perhaps two months in advance of the event.

## 5.4 Report on the first Scientific Seminar

By Lilit Axner, SNIC-KTH

Basic information about the event

Name: PRACE Scientific Seminar - HPC Boosts Science

**Dates:** 21-23 February 2011

Location: Stockholm, Sweden

Organizing sites: SNIC-KTH (Sweden) and CSC (Finland)

Organizational details

## Local organizing committee:

- Dr. Lilit Axner (SNIC-KTH)
- Dr. Pekka Manninen (CSC)

**Venue:** Auditorium at Royal Institute of Technology, Osquldas Väg 6B, KTH, 114 28 Stockholm, Sweden. The venue was comfortably located close to the center and in the university area which makes it attractive for students and researchers to attend. The place was chosen also considering the limited budget given for this event and prioritizing the possibly larger number of participants.

**Budgeting** In total about 4600 € has been spent on the Scientific Seminar 2011. The costs include the location, lunches, drinks for poster session and dinner as well as reimbursement of speakers from abroad and Sweden (outside of Stockholm).

Expense	Amount (EUR)*
Location	700
Travel coverage of speakers	1,300
Badges and folders	200
Dinner	900
Drinks for the poster session	300
Lunches and coffee breaks	1,200
Total	4,600

(\*) Note the expenses have been carried out in SEK.

**Synergetic events:** The 3<sup>rd</sup> PRACE Industry Seminar took part of the efforts from SNIC-KTH as it was being organized the same time.

## Program & content

## **Program committee**

- Dr. Pekka Manninen (CSC)
- Dr. Lilit Axner (SNIC-KTH)
- Prof. Lennart Johnsson (KTH)
- Prof. Dan Henningson (KTH)
- Prof. Lisa Björling (KTH)

**Designing the program:** The PRACE Scientific Seminar aimed to address questions essential to scientists from the user's point of view rather than that of the HPC experts. Prominent researchers from a wide range of scientific communities were invited to present

their achievements and give their opinions on current and future trends of HPC. They outlined their results and discussed the appropriateness of HPC architectures for different disciplines, while focusing on difficulties encountered and possible solutions. The seminar was concluded by a panel discussion where PRACE HPC experts, together with researchers, discussed possible improvements to the services that the current HPC ecosystem provides.

**Description of the contents:** The culmination of the seminar was the panel discussion where PRACE HPC experts, together with researchers, discussed possible improvements to the services that the current HPC ecosystem provides. The members of the panel were Prof. Lennart Johnsson (The University of Houston and PDC - Center for High Performance Computing, KTH), Prof. Igor Abrikosov (University of Linköping), Dr. Berk Hess (KTH) and Prof. Kari Laasonen (Aalto University).

One of the points of the discussion was that in order for scientific community codes to scale well on petascale, and in the future, exascale machines, hardware-tuned codes and low-level libraries are needed. Developers need to know more details about topology as well as hardware components of systems, which is currently one of the aims that PRACE is pursuing. Easy access to systems is important for scientists to have easy access to systems; a common submission environment is an absolute necessity. It was pointed out that such an environment has already been in use by DEISA and is being carried forward in PRACE. In order to foster the enthusiasm of researchers for applying for compute time, the current waiting periods between application submission and acceptance should be shortened. Current procedures from a scientists' perspective require too much paperwork, and appears bureaucratic. It would be ideal if the grant applications for funding scientists also included both requests for Ph.D. students as well as compute time, it was clear that for some disciplines the codes can scale to several thousands of cores while for the others, several hundred will do, but more compute time is needed to conduct several simulations.

For the later type of disciplines, queuing and prioritizing systems can become a bottleneck and thus new approaches are needed. It was also discussed how to motivate communities to work with application experts. Currently, most of the community codes are 10 to 20 years old. Codes are huge and researchers tend to not touch the old parts of it. In this situation, the assistance of application experts is essential. However, more methodological code development is needed rather than hardware specific tuning. For a researcher to hire a programmer is three times more expensive than to hire a Ph.D. student. Thus initiatives such as PRACE are helping to fill the gap of knowledge in the area of computer science that research communities have. Moreover, there is an urgent need for a greater number of committed work hours by application experts on community codes.

## Participants & feedback

## Number of participants by country

- Sweden 40
- Finland -4
- Norway 1

Statistics of the feedback survey– From all the participants only six have filled in the feedback survey.

Criteria	Excellent	Good	Average	Bad
Information quality	3	2	1	0
Registration quality	2	3	1	0
Venue quality	2	3	1	0
Catering	0	4	2	0
Overall quality	1	5	0	0
Relevance of the topics	0	6	0	0
I was inspired to new ways of thinking	0	4	2	0
The lectures were clearly presented and comprehensible	1	4	1	0
The pace of the seminar was about right	1	5	0	0

Analysis of the feedback: the overall evaluation showed pleasing results, however the number of survey participants was low. We consider that these types of surveys are more appropriate for training events or seasonal schools rather than general seminars.

**Conclusions & lessons learned:** The seminar went well and had good and interesting addresses; however, the audience could have been more international.

If such events are organized in the future, the budget should be larger than the 8  $k \in to$  allow for a larger audience, and the event should be advertised more widely.

## 5.5 Seasonal School feedback survey form

The participant feedback survey of each PRACE-1IP training event is carried out with an electronic survey tool (LimeSurvey) using the question set as follows. The data from the surveys is available upon request from the task leader.

## Your Background

- Name, institution, and email (optional)
- Where did you hear about the school?
- Your area of work/research?
- Please rate your level of expertise in the following (prior to attending the school).

	Unskilled	Fair	Good	Excellent
HPC programming languages (Fortran, C/C++)				
Message-passing interface				
Shared-memory parallel programming (e.g.				
OpenMP)				
Performance analysis (incl. use of tools)				
Code optimisation techniques				
Parallel program debugging				
Next-generation HPC languages (e.g. PGAS)				
Accelerator programming				

## Organisation & Facilities

Please rate the following in terms of quality.

	Very bad	Bad	Not	Good	Excellent	Don't
			good			know
			nor			
			bad			
Information about the school						
Registration						
Venue						
Catering						
Overall organisation						

## About the School

Please rate the following statements.

	Disagree	Disagree	No	Agree	Agree	Don't
	completely		strong		completely	know
			feelings			
The topics are relevant to my						
work/research interests						
I was inspired to new ways of						
thinking						
The lectures were clearly						
presented and						
comprehensible						

The pace of teaching was			
about right			
Teaching aids used (e.g.			
slides) were well prepared			
The hands-on exercises and			
demonstrations were a			
valuable contribution to the			
school			

- Additional comments on the content, specific lectures, etc.
- Please give any other general comments about this school or any other issues arising from it.
- Overall, how would you rate this school? (10 = excellent, 0 = waste of time)

## Future activities

Please let us know if you see the need for future schools to cover the following areas.

	No need	Some	Important	Urgent	Don't
		need	need	need	know
General HPC programming					
(MPI, OpenMP)					
Advanced HPC programming					
(Hybrid MPI-OpenMP;					
next-gen HPC languages e.g.					
PGAS;					
GPU computing e.g. CUDA)					
Code optimisation & performance					
analysis					
Porting of existing codes to HPC					
architectures					
Specific HPC application(s)					
Parallel program debugging					
HPC programming and					
applications specific to my					
research community					
Visualisation techniques					

• Are there some other fields of training you feel PRACE should provide training events in?

• Please give any other general comments about PRACE training activities.

## 5.6 Education Outreach Plan of Actions

## Introduction

Computing has become the third pillar of scientific research, together with theory and experimentation. While scientific computing, in principle, can be performed with almost any device featuring a sufficient central processing unit, it is the high-performance computing (HPC) systems that provide the most important opportunity to improve our understanding of nature and reality by developing and testing complex models and comparing them against measured data. Not only does basic research benefit from high-performance computing, but applied industrial research and development is increasingly reliant on computer simulations: to verify, complement and replace studies with prototype systems, and to bring insight in building them. It is hard to imagine an area of industrial production where computing would not bring any added value. Therefore it is of utmost importance that themes of scientific computing are brought into science education from as early stage as possible.

## Education outreach themes

The activities include three subtopics: education and dissemination events aimed at science teachers as well as pupils; classroom visits; and contribution to educational material. The visits to science classes are carried out by both experts working in the field of scientific computing, as well as undergraduate university students trained to carry out these visits.

## Popular science events for teachers and pupils

In these regular seminars organized around Europe the science teachers working in secondary education will meet people working in computational sciences as well as with e-infrastructure. They consist of popular science presentations, in which researchers in computational sciences present the current topics in their field together with HPC centre and vendor representatives present the state of the art of the HPC systems.

The goal is to get the teachers and pupils enthusiastic about computational science and to teach them the importance of computing and data analysis in modern science; in the hope this would then get channelled to the science classes.

## Visits to science classes

We plan to prepare a ready-to-run presentation kit for making a one-hour lesson on computational science in science classes of secondary education. Interested scientists, HPC experts and undergraduate students of some relevant field of science would carry out these visits.

The undergraduate students are mentored to these visits in special training events by staff of HPC centres involved with PRACE.

## Preparing educational material

Having ready-to-run teaching material – presentation slides, video clips, problems with answers, computer demos and assignments and so forth – might lower the barrier of incorporating HPC themes in existing classes. These could include, for example, simple electronic-structure calculations and visualizations and molecular dynamics simulations within chemistry classes; simulations of everyday phenomena in physics classes; gene sequencing techniques in biology and simple climate and weather models in geography

classes. As these are not part of the school curricula in most European countries, PRACE research infrastructure could take a driver role here.

The material would be planned and completed together with science teachers and other experts in pedagogy. The teachers involved in preparing the material could be found from the teachers' events described above.

## Realisation

These themes could be piloted in a couple of partner countries. As the school systems differ from each other quite a lot between European countries, the educational material is not translatable as such, i.e. completely centralized preparation of material is not a desirable solution. However, materials produced in different countries can most likely be utilized to a large extent in another; and therefore PRACE could maintain a common working area for the educational material preparation. PRACE WP3 pm's can be used for all of the activities described above. The findings of these piloting efforts are documented in D3.2.5 and put to use in later stages of PRACE.