



**SEVENTH FRAMEWORK PROGRAMME
Research Infrastructures**

**INFRA-2011-2.3.5 – Second Implementation Phase of the European High
Performance Computing (HPC) service PRACE**



PRACE-2IP

PRACE Second Implementation Phase Project

Grant Agreement Number: RI-283493

**D4.3
Final Training Report**

Final

Version: 1.0
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Date: 22.08.2013

Project and Deliverable Information Sheet

PRACE Project	Project Ref. №: RI-283493	
	Project Title: PRACE Second Implementation Phase Project	
	Project Web Site: http://www.prace-project.eu	
	Deliverable ID: < D4.3 >	
	Deliverable Nature: <DOC TYPE: Report >	
	Deliverable Level: PU	Contractual Date of Delivery: 31 / August / 2013
		Actual Date of Delivery: 31 / August / 2013
EC Project Officer: Leonardo Flores Añoover		

* - 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: Final Training Report	
	ID: D4.3	
	Version: <1.0>	Status: <i>Final</i>
	Available at: http://www.prace-project.eu	
	Software Tool: Microsoft Word 2007	
	File(s): D4.3.docx	
Authorship	Written by:	Simon Wong, ICHEC; Stelios Eritokritou, CaSToRC; Marianthi Polydourou, GRNET
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	Approved by:	MB/TB

Document Status Sheet

Version	Date	Status	Comments
0.1	22/06/2013	Draft	Skeleton
0.2	25/07/2013	Draft	Contributions from Stelios
0.5	06/08/2013	Draft	Contributions from Ioannis, added content to most other sections
0.8	08/08/2013	Draft	Almost complete
0.9	09/08/2013	Draft	Ready for internal review
1.0	22/08/2013	Final version	Revisions, corrections

Document Keywords

Keywords:	PRACE, HPC, Research Infrastructure, Training
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List of Acronyms and Abbreviations

AISBL	Association International Sans But Lucratif (legal form of the PRACE-RI)
AVS	Advanced Visualization Studio
BSC	Barcelona Supercomputing Center (Spain)
CAF	Co-Array Fortran
CaSToRC	Computation-based Science and Technology Research Center (Cyprus)
CEA	Commissariat à l’Energie Atomique (represented in PRACE by GENCI, France)
CFD	Computational Fluid Dynamics
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)
DECI	Distributed European Computing Initiative
DEISA	Distributed European Infrastructure for Supercomputing Applications. EU project by leading national HPC centres.
EC	European Commission
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)
ETSF	European Theoretical Spectroscopy Facility
FZJ	Forschungszentrum Jülich (Germany)

GCS	Gauss Centre for Supercomputing (Germany)
GENCI	Grand Equipement National de Calcul Intensif (France)
GPGPU	General Purpose GPU
GPU	Graphic Processing Unit
GRNET	Greek Research and Technology Network
GROMACS	GRoningen Machine for Chemical Simulations
HMPP	Hybrid Multi-core Parallel Programming (CAPS enterprise)
HPC	High Performance Computing; Computing at a high performance level at any given time; often used synonym with Supercomputing
HPC2N	High Performance Computing Center North, a national center for scientific and parallel computing in Sweden
IBM	Formerly known as International Business Machines
ICHEC	Irish Centre for High-End Computing (represented in PRACE by the National University of Ireland, Galway, Ireland)
I/O	Input/Output
IPB	Institute of Physics Belgrade (Serbia)
ISC	International Supercomputing Conference; European equivalent to the US based SC0x conference. Held annually in Germany.
JSC	Jülich Supercomputing Centre (FZJ, Germany)
KAUST	King Abdullah University of Science and Technology
KTH	Kungliga Tekniska Högsolan (represented in PRACE by SNIC, Sweden)
LiU	Linköping University (represented in PRACE by SNIC, Sweden)
LLNL	Laurence Livermore National Laboratory, Livermore, California (USA)
LRZ	Leibniz Supercomputing Centre (Garching, Germany)
MIC	Many Integrated Core (coprocessor architecture from Intel)
MPI	Message Passing Interface
NCSA	National Center for Supercomputing Applications (USA)
NCSA-BG	National Centre for Supercomputing Applications (Bulgaria)
NICS	National Institute for Computational Sciences (USA)
NIIFI	National Information Infrastructure Development Institute (Hungary)
NSC	National Supercomputer Centre in Linköping, Sweden
OpenMP	Open Multi-Processing
PATC	PRACE Advanced Training Centre
PATC OMB	Operational Management Board of the PRACE Advanced Training Centres
PETSc	Portable, Extensible Toolkit for Scientific Computation
PGAS	Partitioned Global Address Space
PRACE	Partnership for Advanced Computing in Europe
PRACE RI	PRACE Research Infrastructure
PSC	Pittsburgh Supercomputing Center (USA)
QCD	Quantum Chromodynamics
RIKEN AICS	RIKEN Advanced Institute for Computational Sciences
RZG	Rechenzentrum Garching (represented in PRACE by GCS, Germany)
SURFsara	Dutch national High Performance Computing & e-Science Support Center (Netherlands)
SNIC	Swedish National Infrastructure for Computing (Sweden)
STFC	Science and Technology Facilities Council (represented in PRACE by EPSRC, United Kingdom)

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
Tier-1	Denotes national or topical HPC centres in a conceptual pyramid of HPC systems (see Tier-0).
UC-LCA	Universidade de Coimbra, Laboratório de Computação Avançada
UmU	Umeå University (represented in PRACE by SNIC, Sweden)
UPC	Unified Parallel C
VŠB-TUO	Vysoká škola báňská - Technická univerzita Ostrava (Technical University of Ostrava, Czech Republic)
WP	Work Package
XSEDE	Extreme Science and Engineering Discovery Environment, USA

Executive Summary

This deliverable summarises the activities of the Training Work Package (WP4) of the PRACE Second Implementation Phase (PRACE-2IP) project, from 1 September 2011 to 31 August 2013. A key development has been the establishment and operation of six PRACE Advanced Training Centres (PATCs) hosted by PRACE partners in Finland, France, Germany, Italy, Spain and the UK. In total, WP4 oversaw the delivery of 98 face-to-face training events that included four seasonal schools, two workshops, two international HPC summer schools, and ninety PRACE Advanced Training Centre courses. Collectively these events were attended by over 2,500 participants, the majority of whom are based in European countries but there were also participants from the rest of the world. From the analyses of feedback responses there is a general perception that the PRACE-2IP training events have been extremely well organised, have consistently provided a high quality of training and are relevant to the needs of the audience. WP4 also carried out comprehensive training surveys to examine the needs of European HPC users, the professional opinions of HPC trainers and the supply of HPC training. The PRACE Training Portal, set up in PRACE-1IP, has been established as a hub for PRACE training information and it continues to act as a large repository of HPC training material, including videos of lectures and PRACE-generated tutorials.

1 Introduction

Contemporary HPC systems offer unprecedented computing power and their architectures are constantly evolving. The on-going challenge has always been to address the shortage of people with the relevant HPC skills to maximise efficiency and productivity, i.e. ensuring high returns on investment in HPC. There is a clear recognition that HPC education and training are greatly needed and should be expanded to develop a larger cohort of HPC experts (e.g. researchers, software developers) who are able to advance the computational sciences in keeping pace with the latest hardware.

The PRACE-2IP Training Work Package (WP4) consists of a two-year programme of HPC training-related activities that aim to enhance European competitiveness by providing researchers with relevant skills in harnessing the power of modern day HPC systems. While the programme initially set out to address the needs of industry users in many of the tasks, the focus on industry had been largely shifted to the PRACE-3IP project in order to enhance complementarity of the two partially overlapping PRACE Implementation Phase projects. The programme is composed of five tasks, each of which is described in subsequent sections of this deliverable.

Section 2 is a brief overview of an education and training survey (Task 4.1) carried out to gain an understanding of the HPC training landscape. Section 3 describes the establishment and operation of six PRACE Advanced Training Centres (Task 4.2) that serve as European hubs of high-quality training for researchers working in the computational sciences and key to the outcome of this Work Package. Section 4 reports on two International HPC Summer Schools (Task 4.3) that continue a very successful series of annual events organised in collaboration with international partners. Section 5 reports on four PRACE seasonal schools and two workshops (Task 4.4) that have been a mainstay of PRACE training in previous PRACE projects. Section 6 describes the work on developing the PRACE Training Portal (Task 4.5), set up during the PRACE-1IP project, to act as a key online resource for HPC training news and material.

Section 7 concludes the main text with a summary of the activities across the tasks and the key outcome. Supplementary text, tables and figures are provided in Annex 8.

2 Education and Training Survey (Task 4.1)

As PRACE-2IP provides extensive funding and support for HPC training in Europe, it was important to understand the needs of its target audience and the existing supply of training. Hence we have conducted a comprehensive survey to capture the training requirements of existing and candidate PRACE users, to obtain input from HPC trainers and assess the supply of HPC training in Europe. The results of the surveys carried out, along with analyses and recommendations (summarised below), have been fully described in the PRACE-2IP deliverable D4.1: “Education and Training Survey” [1].

In order to understand the training requirements of our target audience, we obtained 416 survey responses from HPC users distributed all around Europe. The results have led to a prioritised list of subjects where training is in demand or should be provided according to the professional opinions of trainers. Below is an excerpt from the list of recommendations that were made based on the survey:

1. Areas that can be considered as top priority for PRACE training:
 - a. Performance analysis and optimisation tools and techniques.
 - b. Debugging tools and techniques
 - c. Advanced MPI
2. Areas of high priority for PRACE training:
 - a. GPU computing (e.g. OpenCL, CUDA)
 - b. Mixed-mode (hybrid) OpenMP-MPI programming
 - c. Parallel algorithm design
 - d. Architecture-specific optimisation and tuning
 - e. General compiler usage and optimisation
 - f. Software engineering tools and techniques
 - g. Scientific visualisation tools (e.g. VisIt, Paraview)
 - h. OpenMP
 - i. Python
3. Areas where introductory courses should be provided as more “forward-looking” type of training:
 - a. Parallel I/O libraries (e.g. HDF5, parallel NetCDF)
 - b. High-level numerical libraries (e.g. PETSc, Trilinos)
 - c. PGAS languages (e.g. CAF, UPC)
 - d. Next-generation languages (e.g. Chapel, X10, Fortress)
4. Areas of lower priority but should be maintained to some level in the PRACE training programme:
 - a. Basic MPI
 - b. Advanced C/C++ and Fortran (90, 95...) programming
 - c. Third-party scientific applications or domain-specific training (e.g. tackling particular problems)

These recommendations have since been used for guiding PRACE training activities for the foreseeable future, e.g. when drawing up the joint curriculum of the PRACE Advanced Training Centres (see Section 3).

In addition, 205 HPC trainers from Europe and worldwide were surveyed to provide an overview of HPC training expertise currently available, along with professional opinions on such training (e.g. emerging topics that are apparently not in high demand but should be

taught). Notably, it has also established a large database of trainers with a diverse range of expertise that PRACE can utilise in the future to source the best available personnel for training events. Indeed, this database has been consulted in subsequent PRACE training events when searching for relevant trainers with specific expertise, e.g. when planning the PRACE seasonal schools (see Section 5.1).

3 PRACE Advanced Training Centres (Task 4.2)

The mission of the PRACE Advanced Training Centres (PATCs) is to serve as European hubs of advanced, high-quality training for researchers working in the computational sciences. The PATCs provide and coordinate training and education activities needed to achieve the best utilisation of the PRACE research infrastructure by the community. The PATCs promote a common PRACE brand, representing the whole PRACE community rather than only the hosting sites, and implement a jointly-conceived curriculum, designed and coordinated by PRACE with input from user communities.

The main concepts of the PATCs, including their mission and objectives, were outlined in PRACE-1IP D3.2.3: “PRACE Advanced Training Centres” [2]. PRACE-2IP was responsible for implementation, i.e. establishment of the PATCs and the commencement/ maintenance of their operation for the duration of the project.

3.1 Establishment of the PATCs

The establishment of the PATCs has been fully described in the deliverable PRACE-2IP D4.2: “Establishment of PRACE Advanced Training Centres” [3]. In summary, seven partner sites have submitted proposals to become PATCs. After a selection process, six PATCs were established in February 2012. The six PATCs are hosted by the following partners in six countries:

- BSC, Spain
- CINECA, Italy
- CSC, Finland
- EPCC, UK
- GCS, Germany
- Maison de la Simulation (including GENCI), France

3.2 Operation of the PATCs

The PATC operations are supervised and steered by a PATC Operational Management Board (OMB) shown in Figure 1, consisting of one representative from each of the PATCs, one member from the current PRACE project (the training WP leader), and one member appointed by the PRACE AISBL. The OMB is responsible for setting guidelines for curriculum planning, for allocating a budget to each centre, and for defining a set of best practices and processes that will be adopted by the PATCs. Overseeing of common functions for the whole PATC network, such as publicity, registration, reporting, surveys, etc., is the responsibility of an OMB coordinator appointed by the OMB.

Each PATC is managed by a director and a coordinator. The PATC director is in charge of the centre's operations and is responsible for reporting of the results. (S)he acts as a representative of the training centre at the OMB and is involved in the work of the OMB. The PATC coordinator is responsible for the practical operations of the training centre, including arrangement of lecturers, ensuring top-quality facilities, catering, etc. (S)he is also responsible

for monitoring the budget allocated to the centre. Both the PATC director and the PATC coordinator participate in curriculum planning for the centre according to the guidelines set by the OMB.

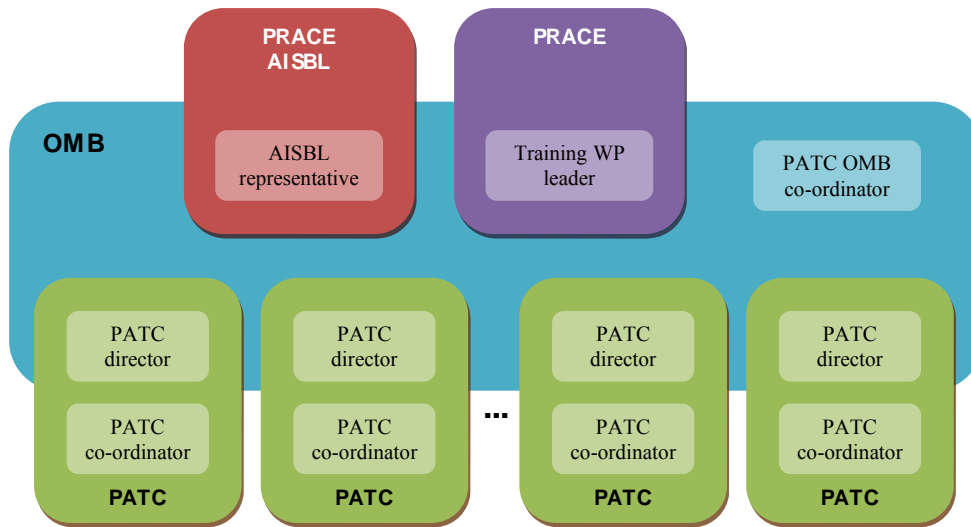


Figure 1: Members of the PATC Operational Management Board (OMB)

The PATC OMB is responsible for a range of activities during the course of the PRACE-2IP project. The following details reflect some of the main functions of the PATC and the relevant work carried out.

3.2.1 Curriculum planning

This is a key function of the PATC OMB. On an annual basis, the PATC OMB is responsible for establishing the joint PATC curriculum that includes a syllabus of PATC courses for implementation in the upcoming academic year.

For the period between March 2012 and August 2012, PATC courses had to be planned quickly, as the PATCs had just been announced in February 2012. A total of 19 courses were organised and delivered during this initial start-up phase for the PATCs (see Annex 8.1.1).

For the 2012-2013 academic year, the PATC OMB implemented the curriculum design process as outlined in Annex 8.1.2 that was conceived during PRACE-1IP [2]. An initial analysis of training requirements, taking into account input from other PRACE Work Packages and results from the Education and Training Survey (Section 2 and [1]), was carried out to draw up a list of guidelines for the PATCs to each propose a syllabus that collectively would form a joint curriculum, aimed to address a diverse range of HPC topics and users with varying levels of HPC experience. The resulting joint curriculum, including the syllabus of 72 courses to be delivered by the six PATC sites, is summarised in Annex 8.1.3.

Planning for the 2013-2014 joint curriculum took place in early 2013, although the implementation of the curriculum will be carried out as part of PRACE-3IP project where the PATCs also have been tasked to provide industry-oriented courses. The formation of the 2013-2014 joint curriculum followed a similar process as above, except that the PRACE Board of Directors (BoD) has since established an external panel of experts, who conducted a review and advised the BoD on the approval of this curriculum. Details of the 2013-2014 curriculum, including the syllabus of 79 courses, are provided in Annex 8.1.4.

3.2.2 Dissemination

With the PATCs delivering an unprecedented number of PRACE training courses, it requires a sound dissemination strategy to ensure that European researchers are informed of this important PRACE activity and upcoming courses. The following dissemination channels were used:

E-mail

E-mail remains the most popular channel through which researchers obtain information about HPC training courses [1]. The PRACE dissemination Work Package (WP3) maintains a contacts database that includes the e-mail addresses of participants who had attended past PRACE training events. A dedicated mailing list (prace-training-announce@fz-juelich.de), containing the e-mail addresses of these contacts, was subsequently set up.

Monthly e-mails with a list of upcoming courses (within the following three months) have been sent from PRACE as regular “training bulletins” to the mailing list. In spring 2013, PATC directors and coordinators were also given the ability to disseminate information about individual PATC courses to the same list. At the time of this report, the mailing list contains over 2,200 e-mail addresses.

The PRACE Training Portal

Modifications to the PRACE Training Portal were carried out to highlight the upcoming PATC courses on the landing page of the portal. The portal also hosted a PDF brochure containing the full list of courses in the joint PATC curriculum. The brochure for the 2013-2014 curriculum, for example, was also distributed as hard copies at ISC 2013.

3.2.3 Logistical harmonisation and PATC branding

In order to promote awareness of the PATC brand, a consistent look and feel to how course information is displayed and how registration is implemented was essential. In collaboration with the dissemination Work Package (WP3), work was carried out to ensure a tight integration between the PRACE Training Portal [4] and the PRACE events web site [5], powered by the Indico tool (see also Section 6.2). The result is that all PATC course information are entered, updated and displayed at one central point (the PRACE events web site); then as other pages (e.g. the PRACE Training Portal and the PRACE RI web site [6]) source their information from the PRACE events web site, any updates such as addition of new courses and date adjustments are automatically propagated to ensure provision of accurate and consistent information.

The PRACE events web site also provided functionalities such as event registration and evaluation. Hence, standard registration and course evaluation forms were established by the PATC OMB and used for most PATC events. Not only do these contribute to a PRACE branding of the courses, they have also greatly facilitated the collection of statistics from PATC courses and their subsequent analyses by ensuring data consistency.

Also in collaboration with WP3, PATC sites have been given and distributed a variety of PRACE promotional material (e.g. USB keys, pens, writing pads) at the PATC course events.

3.3 PATC courses from March 2012 to July 2013

The following provides some key statistics from the PATC courses delivered from March 2012 to July 2013 (i.e. for the duration of the PRACE-2IP project), followed by analyses of

the achievements and areas for improvement. Only one of the 72 planned PATC events had to be cancelled in the 2012-2013 curriculum.

3.3.1 *Key statistics on numbers of participants and courses*

In summary, the six PATCs have collectively delivered the following for the duration of the PRACE-2IP project:

- 90 training courses
- 260 days of training
- for 2,058 participants
- with a total of 6,417 participant-training-days
(one participant-training-day = one participant who completes one day of training)

On average, there are 22.9 participants for each PATC course. Further per-PATC statistics on the number of participants, number of courses, etc., can be found in Annex 8.1.5.

Additionally, the total number of 2,058 PATC course participants is comprised of:

- 14% female; 86% male
- 90% from academia; 10% from non-academic backgrounds

3.3.2 *Geographical distribution of the participants*

The affiliation of the participants (i.e. the institution where the participant works/studies) shows on average that:

- 78% of the participants are affiliated in the country where the PATC course is delivered.
- 7% of the participants are affiliated with institutions from other PATC hosting countries.
- 15% of the participants are affiliated with institutions from other (mainly European) countries.

While PATC course participants come from all over Europe (every PRACE partner country is represented), the proportion of participants from other (non-PATC hosting) countries does appear to be relatively low. As further examination entails comparison of participant numbers between different countries, one must take into account country-specific variations such as population or the size of the target audience, i.e. the expectation is that there would naturally be more participants from countries with larger populations (of scientists, for example). Hence the geographical distribution data was “normalised” in terms of participants per year for every 1,000 students studying mathematical, scientific and engineering disciplines (i.e. representative of the size of the PATCs’ target audience) in each country. The relevant student population data was sourced from the Eurostat database [7].

The comparison of the normalised number of PATC course participants (per year) who came from the different PRACE member states is shown in Figure 2. It can be seen that there is a notable imbalance where there is a large proportion of participants affiliated with PATC countries; even after normalisation, participants who came from PATC countries (0.419 participants / year per 1,000 students) outnumber those who came from other PRACE member states (0.054 participants / year per 1,000 students) by a factor of around eight.

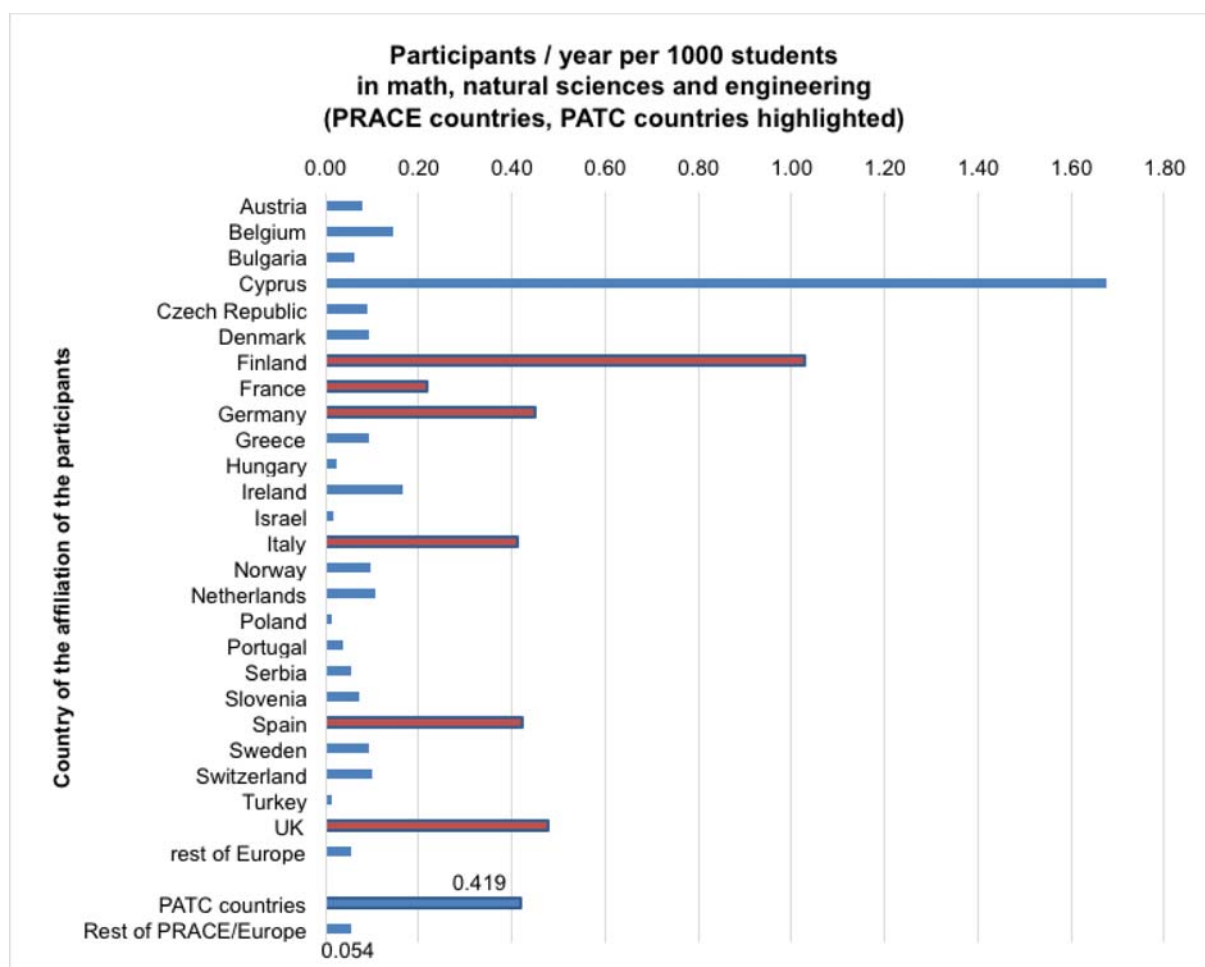


Figure 2: Participants per year per 1,000 students studying mathematics, natural sciences and engineering, individually listed for all PRACE countries. PATC hosting countries are highlighted by red bars. Data is based on all PATC courses from 03/2012 to 07/2013. The apparent high level of PATC course participation by Cyprus is due to 14 participants from a country with a significantly smaller student population (5,897 studying the relevant subjects) compared to other countries (whose corresponding populations range from ~29,000 to ~782,000).

3.3.3 Feedback from PATC course participants

A total of 1,037 feedback responses have been collected from 77 PATC courses (from 03/2012 to 07/2013). Since the common feedback form only came online during the start-up phase of the PATCs, it was not possible to integrate feedback from (mostly) the early PATC courses; hence from here onwards our feedback analyses will be based only on the 77 PATC courses with feedback. On average, the feedback response rate (i.e. the percentage of respondents or participants who provided feedback at or after the course) per course is approximately 63%.

One key question in the feedback form is the overall rating for the course on a scale of 0 (waste of time) to 10 (excellent). From 1,037 respondents, the average rating for a PATC course is 8.45. Other indicators of participant satisfaction include questions on the logistical aspects of the course, >90% of respondents have consistently rated the quality of course information, registration, venue, and organisation as being either good or excellent. There is general agreement that the topics of the courses were relevant to the respondents' research, that the hands-on exercises were useful and that the pace of teaching was right.

3.3.4 *Analyses of the statistics*

From the key statistics, it can be concluded that the PATCs have been very successful so far. Every PATC has fulfilled its role to plan and implement the joint curriculum and as a result a large number of people (2,058) had been trained through 90 PATC courses that covered a diverse range of topics catering for users with varying levels of HPC experience.

There is also substantial evidence from 1,037 participants that the PATCs are providing high-quality, well-organised courses as reflected by a high (8.45 out of 10) average overall rating. Responses to other course evaluation criteria have also been overwhelmingly positive.

Perhaps one area where improvements can be made is access to PATC courses for those who do not work/study in PATC hosting countries. The normalised geographical distribution of the participants (Section 3.3.2) show that participants predominantly came from PATC countries and that they greatly outnumber those from other PRACE member states in a disproportionate manner. This issue has already been identified recently in the PRACE-3IP project, and D4.1: “Continuity Plan for the PRACE Advanced Training Centres” [8] has outlined some remedial actions. These include the delivery of a subset of PATC courses in non-PATC hosting countries (to enhance trainer mobility) and/or the offering of travel subsidies for non-PATC participants (to enhance trainee mobility).

It is notable that other PRACE training events (e.g. seasonal schools; see Sections 4 and 5) in PRACE-2IP have typically been organised in non-PATC countries in order for them to complement PATC activities. Should one carry out the same normalised geographical distribution analysis of the participants of these other PRACE training events, participants from non-PATC hosting PRACE member states (0.063 participants / year per 1,000 students) outnumber those from PATC hosting countries (0.018 participants / year per 1,000 students) by a factor of about 3.5; although the total number of participants involved here is relatively small. Annex 8.1.6 provides a combined picture of the geographical distribution of all PRACE-2IP training event participants. It shows that delivery of training events outside of PATC countries does alleviate some of the imbalance seen above; hence the scaling up of such efforts should improve the current situation.

4 International HPC Summer Schools (Task 4.3)

The PRACE projects have continually supported a series of annual international HPC summer schools in collaboration with the Extreme Science and Engineering Discovery Environment (XSEDE) project (formerly Teragrid) in the US. The original collaboration, between the European DEISA project and Teragrid in the US, hosted the first event in Catania, Italy in 2010. The PRACE-1IP project, in collaboration with Teragrid, supported the second event, which took place in Lake Tahoe, USA in 2011 (see PRACE-1IP D3.2.5: “Final Training Report” [9]). PRACE-2IP was set to continue this collaboration by supporting the following two events:

- The 2012 EU-US Summer School on HPC Challenges in Computational Sciences, 24-28 June, Dublin, Ireland.
- The 2013 International Summer School on HPC Challenges in Computational Sciences, 23-28 June, New York City, USA.

The name of the event has been adjusted in 2013 as the collaboration had grown to include Japanese participation. For the sake of brevity, the short title “International HPC Summer School” will be used here to refer to the series of schools.

4.1 Overview of the schools

The objectives of the International HPC Summer School series are to:

- Expand the knowledge of the attendees about HPC and its application in multiple fields of science and engineering.
- Foster new collegial friendships and partnerships, nationally and internationally, among presenters and attendees.

The format of the school has remained similar over the years, but it has also been constantly fine-tuned to take into account user feedback. Typically, the full programme of the school includes:

- About 50% of the “day-time” programme allocated to presentations by leading scientists and technologists. The topics of these presentations focuses on:
 - Challenges and solutions for conducting leading-edge research across multiple fields of study (using HPC and related technologies)
 - Algorithmic approaches and numerical libraries
 - Data-intensive computing
- About 50% of the “day-time” programme allocated to short talks and hands-on tutorials on different HPC usage topics, including:
 - Parallel programming paradigms
 - Performance analysis and profiling
 - Scientific visualisation
- Apart from the “day-time” programme mentioned above, there are also extensive social and mentoring programmes (mostly during evenings) to promote interaction among participants and presenters. These include the following activities:
 - Electronic poster sessions for participants to showcase and to discuss their research
 - Mentoring sessions where presenters provides guidance and discusses research with small groups of participants
 - Organised group dinners and social activities during the evenings of the school

4.2 Implementation

Each year, the schools are organised by a single programme/organising committee that includes representatives from PRACE and XSEDE. RIKEN Advanced Institute for Computational Science (RIKEN AICS) joined the collaboration, and hence also the committee, in 2013. The number of places for European, US and Japanese participants are limited and agreed upon every year and the respective organisation at each locale is locally responsible for the selection of students. All schools so far have been heavily over-subscribed.

The 2012 International HPC Summer School was held in Dublin, Ireland on 24-28 June 2012. From about 236 applications, 60 participants (35 European participants from 15 countries; 25 US participants), were selected to attend. Details of the school can be found in Annex 8.2.

The 2013 International HPC Summer School was held in New York City, USA on 23-28 June 2013. From over 390 applications, 73 participants (30 European participants from 11 countries; 32 US participants; 11 Japanese participants) were selected to attend. Details of the school can be found in Annex 8.3.

4.3 Feedback and evaluation

At the end of every school, participants were asked to provide feedback via an online survey. The response rates were 98% in 2012 and 88% in 2013. The overwhelming consensus from the feedback of both schools was that the majority of respondents (>95%) have deemed their experience of the school to be a success. A similar proportion of respondents found both schools to have been very well organised.

There is also evidence from the feedback that the unique format of the International HPC Summer School series (i.e. a multi-disciplinary conference with hands-on tutorials on HPC tools and techniques) and the abundant opportunities to interact with a diverse international audience have both contributed to the successful experience of the participants.

When participants were asked about their goals for attending the event, the most common goals were the opportunity to meet other students and experts in the field they could talk with and exchange ideas with, and the opportunity to meet people in different disciplines and from different cultures to learn about the methods, techniques and trends these people are using to advance research in their field. Learning about HPC tools and software, including state-of-art technologies and future trends, were the next most common goals. More than 85% of respondents from both schools have stated that the events have met, or even exceeded, their goals for attending. Participants were extremely positive about the networking opportunities and had meaningful engagements with others at the schools. Many have stated that the international audience have contributed to their learning and a number have indicated that new collaborations have resulted or were likely to result from the events.

5 Training Events (Task 4.4)

PRACE-2IP had been responsible for hosting four seasonal schools over a one year period, continuing a very successful series of such schools organised by PRACE-1IP, and two workshops that are targeted at specific groups or communities. The details for these events are summarised in Table 1.

With the establishment and operation of the PATCs (see Section 3), the seasonal schools and workshops were organised to complement PATC activities. Most importantly, these events were held in non-PATC hosting countries, in order to maintain a wide geographic distribution

of PRACE training, i.e. PATCs act as hubs of PRACE training activities with seasonal schools and workshops hosted in other European countries around them. Furthermore, as these schools and workshops attract a significant local audience, they also serve an outreach purpose, raising PRACE awareness among researchers who may not have other opportunities to engage in PRACE events. Care was also taken when organising the seasonal schools and workshops that there was no significant overlap in the theme/content of events occurring within a similar timeframe in proximal locations.

Event name	Theme/topic	Date	Location	Organising site
PRACE Tier-1 Workshop	Practical knowledge of PRACE Tier-1 resources	29-30 Nov 2011	Amsterdam, The Netherlands	SARA
PRACE Autumn School 2012	Massively parallel architectures and molecular simulations	24-28 Sep 2012	Sofia, Bulgaria	NCSA-BG
PRACE@COIMBRA 2012	UPC, ab-initio condensed matter physics	4-5 Oct 2012	Coimbra, Portugal	UC-LCA
PRACE Winter School 2013	Scientific visualisation	19-22 Mar 2013	Dublin, Ireland	ICHEC
PRACE Spring School 2013	New and emerging technologies - programming for accelerators	23-26 Apr 2013	Umeå, Sweden	SNIC (UmU and LiU)
PRACE Summer School 2013	Frameworks for scientific computing on supercomputers	17-21 Jun 2013	Ostrava, Czech Rep.	VŠB-TUO

Table 1: List of seasonal schools and workshops in PRACE-2IP

5.1 Seasonal Schools

Four seasonal schools were organised in PRACE-2IP, from the PRACE Autumn School 2012 thru to the PRACE Summer School 2013. They cover a wide variety of themes and topics from massively parallel architectures and molecular dynamics (Autumn School 2012), scientific visualisation (Winter School 2013), emerging many-core technologies (Spring School 2013) and frameworks for HPC simulations (Summer School 2013). Full details of all four schools can be found in the Annex (8.4 to 8.7).

All seasonal schools were very well attended with approximately 40-50 participants at each event. There were a total of 184 seasonal school participants and the geographic distribution of participants at the four schools are summarised in Table 2. As seen for the PATCs, the level of participation from local researchers remain to be high, but here only 16 participants (9%) came from PATC countries, i.e. it appears that the seasonal schools do complement PATC activities by capturing a more geographically diverse audience around Europe, although on a relatively smaller scale.

Country	Autumn School 2012	Winter School 2013	Spring School 2013	Summer School 2013	Total
Bulgaria	33		2	2	37
Czech Republic	2		1	31	34
Denmark				5	5
Egypt	2				2
Finland			1		1
France		1	2	2	5
Germany	1	1		2	4
Greece	1				1
Ireland	1	38		3	42
Italy		2		1	3
Norway			1		1
Poland	2			1	3
Romania		1			1
Slovakia				1	1
Slovenia	2				2
Sweden			34		34
Turkey	3				3
UK	1		2		3
USA				2	2
Total	48	43	43	50	184

Table 2: All seasonal school participants and their geographic distribution

All seasonal school participants were requested to provide feedback using a standard PRACE training feedback online form (established in PRACE-1IP, see [9]). A total of 103 feedback responses were collected, representing 56% of the participants (Table 3). All feedback received from each of the seasonal schools have been extremely positive. Perhaps one of the key metric is the response to the question: “Overall, how would you rate this school? [0 = waste of time, 10 = excellent]”; the average score attained by each seasonal school to this question, as shown in Table 3, have all been consistently high (8.4 - 8.5). There is a general perception that the PRACE seasonal schools are well organised and that the participants are satisfied with the delivery of the training and the content covered.

Event	Number of participants	Number & percentage of feedback responses	Average overall rating
Autumn School 2012	48	27 (56%)	8.4
Winter School 2013	43	26 (60%)	8.5
Spring School 2013	43	28 (65%)	8.4
Summer School 2013	50	22 (44%)	8.5
Total	186	103 (55%)	8.5

Table 3: Key feedback statistics from seasonal schools

5.2 Workshops

Two workshops were organised in PRACE-2IP, each of which had been designed to be smaller/shorter in nature compared to seasonal schools and targeted at specific groups or communities. In particular, they are aimed to be flexible in nature, organised in response to specific needs from the community and/or to coincide with scientific events relevant to PRACE.

The first of such workshops was the PRACE Tier-1 Workshop, 29-30 November 2011, Amsterdam, the Netherlands (see Annex 8.8 for the full report). The idea for the workshop arose from an internal PRACE request to host an event to address the needs of PRACE Tier-1 users, especially those who were awarded compute resources through the DECI-7 call. The objective of the workshop was to provide practical guidelines and experience on utilising various European Tier-1 systems, highlighting the hardware, software, services and support that are available. There was a heavy emphasis on the hands-on sessions where participants had the opportunity to implement codes, including their own, on target architectures with the assistance of PRACE staff.

Country	PRACE Tier-1 Workshop, 2011	PRACE@COIMBRA, 2012	Total
Austria		1	1
Belgium		24	24
Finland	2		2
France	3	24	27
Germany	3	16	19
Greece	1		1
Hungary	1		1
Italy	1	14	15
Japan		1	1
Luxembourg		1	1
Portugal	2	24	26
Serbia	2		2
Spain	2	9	11
Sweden	1	3	4
Switzerland	1		1
United Kingdom		2	2
USA		1	1
Total	19	120	139

Table 4: All PRACE-2IP workshop participants and their geographical distribution

The PRACE Tier-1 Workshop was attended by 19 participants from 11 European countries (Table 4). It was quite successful in attracting the target audience, assisted by the provision of a small travel subsidy; 14 (74%) of the participants were researchers associated with awarded DECI projects. After the workshop, 16 feedback responses were collected and the average overall rating for the event was 7.3 out of 10 (0: worst, 10: best). While most participants

have found the workshop useful, there was a perception that more time could be allowed for participants to work on and learn about their target system architectures. Hence rather than a single event that tries to cover all Tier-1 architectures, it may be more sensible in future to hold different courses for participants to have time to focus on specific architectures, e.g. the systems workshops hosted by the PATCs.

The second workshop was organised to coincide with the 17th European Theoretical Spectroscopy Facility (ETSF) conference at Coimbra, Portugal (October 2012). The so-called PRACE@COIMBRA 2012 event (see full report in Annex 8.9) consisted of two parts: a one-day UPC course and a half-day PRACE session, which is aimed to introduce a large number of conference attendees to PRACE services and activities relevant to that specific community. Hence the scope of the workshop was to address the audience interests by providing insights into condensed matter and material science codes, including porting, tuning and performance issues in HPC systems and using accelerators like GPGPUs with those codes.

The PRACE@COIMBRA UPC course was attended by 17 participants from Portugal, while the half-day PRACE session was attended by most of the 103 ETSF conference attendees from all around Europe and further afield (Table 4). The overall participants' experience from the UPC course and the PRACE session "High Performance Computing for ab-initio Condensed Matter Physics" at the ETSF meeting, was very positive with regards to the material presented, the interest of the topics and the usefulness of the interaction between PRACE collaborators and members of the scientific community.

6 The PRACE Training Portal (Task 4.5)

The PRACE training portal [4] was set up during PRACE-1IP and acts as an online repository for PRACE training resources. It is hosted at CSCS (Switzerland), maintained by CaSToRC (Cyprus) and during PRACE-2IP has received contribution from NCSA-BG (Bulgaria), VŠB-TUO (Czech Republic), CSC (Finland), GRNET (Greece) and ICHEC (Ireland).

6.1 Training material

Some training material was made available on the training portal during PRACE-1IP. The majority of the currently available material though was collected, uploaded and made available on the training portal during PRACE-2IP.

The portal now hosts training material from 45 PRACE training events, including PATC courses, and these can be found under the "Material" tab [10] of the portal. The whole collection amounts to over 250 different training material. By training material we refer to lectures presented at a training event, which either include video material or which are different (in subject) to other lectures presented at a training event.

Training material include copies (PDF documents) of the lectures that were presented at a training event. For training events that included hands-on sessions, the exercises given to trainees as well as their coded solutions have also been made available. Furthermore, close to 90 training material include the video recording of the lecture itself where the lecturer and the slides both appear. This was done whenever the training budget allowed for such expenditure. Such videos can allow people to follow a lecture online if they were not able to attend a training event.

Training material has also been appropriately categorised based on the categories presented in Table 5. These categories were agreed upon by a panel established in this Work Package. Further to the above categories, training material are also tagged appropriately based on the

content of the material. This was done to allow for better Google search results as well as easier ways for visitors of the portal to find and browse material they are looking for. Training material available on the training portal are also grouped together based on the event in which they were presented. By selecting the link of an event, one will thus be able to follow the full set of lectures delivered in a specific PRACE training event.

Categories					
Programming languages	Parallel programming paradigms	Scientific visualisation tools	Programming tools and libraries	Debugging, profiling and optimisation tools	Parallel I/O and fault tolerance
C/C++	MPI	Paraview	Numerical libraries	Compiler suites	Checkpoint/restart implementation
Fortran	OpenMP	VisIt	Source code documentation tools	Debugging techniques	Parallel I/O implementation
Java	Mixed-mode (hybrid) OpenMP-MPI	AVS	Version control systems	Debugging tools	
Scripting languages	GPU computing	OpenDX	Batch job systems	Optimisation tools	
Matlab / R	HPC architectures	EnSight	Grid middleware	Parallel debugging	
PGAS languages	HPC principles			Testing methodologies	
Next-gen languages (Chapel, X10, Fortress)					

Table 5: Training material categories

6.2 Training Portal & PRACE events web site integration

The PRACE events web site was set up using the Indico software to provide a service where PRACE and PATC training events could be advertised. The events web site can be found in the following link: <http://www.events.prace-ri.eu>

The necessity for a separate PRACE events web site came about after the establishment of the six PATCs and the large number of training events they aim to operate on an annual basis. Because of this, a platform was needed where the full details of a training event could be made available to the public. Such details include a training event's date and location, details of the intended training programme and registration/feedback forms.

Before the PRACE events web site was setup, description of training events could be found on the PRACE web site. Registration to events was carried out in an ad-hoc manner by different event organisers - either through email registration or online surveys.

Through the use of the Indico tool to implement the PRACE events web site (which is hosted at IPB, Serbia) a more structured and consistent way of advertising PRACE and PATC events was in place – allowing for a more professional and correct way to advertise PRACE training events.

Thus two separate PRACE training event services exist. The PRACE training portal contains training material and the PRACE events web-site provides details about training events. The two are connected to each other in the following manner:

- Training Portal to Events web site
 - The homepage of the training portal advertises forthcoming PRACE and PATC training events. These appear as direct links to the event description page found on the PRACE events web site.
 - The grouping of training material on the training portal based on events also provides a direct link to the event description page found on the PRACE events web site.
- Events web site to Training Portal
 - The description of a training event also includes a “Training Material” link which directs users to the training material page (for the particular event) which can be found on the PRACE portal.

The way the PRACE portal and PRACE events web site are integrated between them can be described in Figure 3.

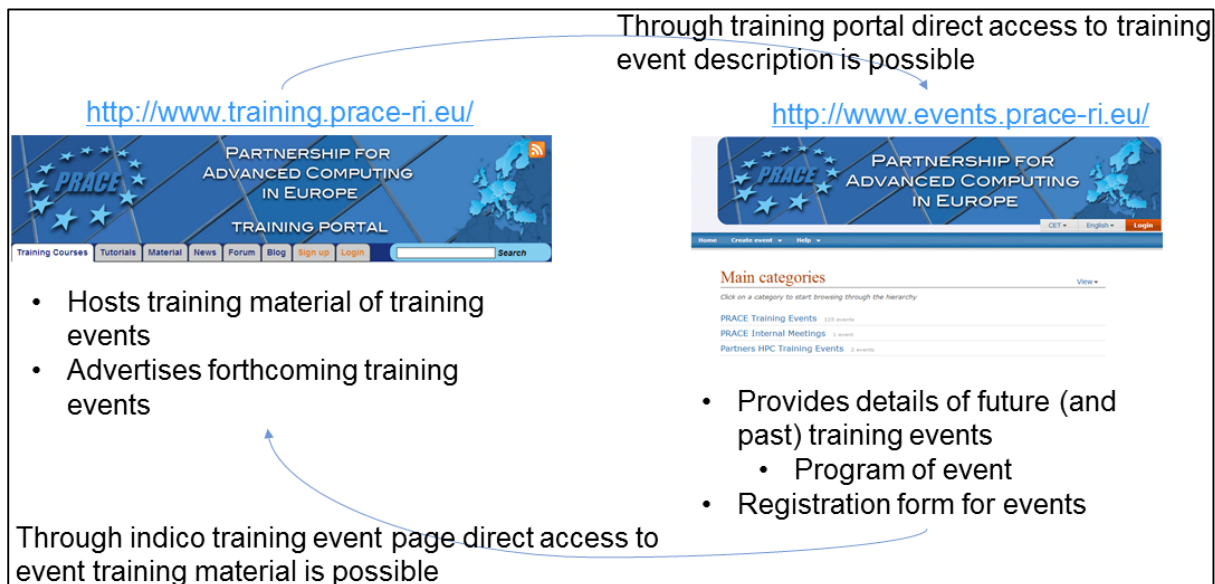


Figure 3: PRACE Training Portal and PRACE events web site integration

6.3 Video tutorials

The original description of this Work Package included a plan to extend the functionality of the PRACE Training Portal via the deployment of technologies and or teachware to offer interactive learning opportunities. However, this was dependent upon some analysis of the requirements and an investigation into the most appropriate software solutions from PRACE-1IP.

In June 2011, PRACE-1IP published a report (D3.1.5: “HPC Training Portal”, [11]) on the PRACE Training Portal including a survey of HPC users on their requirements. Only ~50% of the respondents have indicated a willingness to take advantage of remote, interactive learning technologies and there was a strong concern about technical issues. Subsequent discussion in the Work Package has also identified further issues with pre-existing, widely used

technologies that enable interactive learning (e.g. Moodle), which are typically aimed at academic, semester-length course modules; the nature of this type of training delivery is quite different to that typically provided by PRACE (e.g. relatively short, multi-day events). In conclusion, the proper deployment of an interactive learning infrastructure would have carried a high risk of failure while demanding a significant investment of human resources and time.

Therefore, it was deemed that the effort originally devoted towards this sub-task could be put to an alternative use: creation of several sets of short training videos on specific topics of various parallel programming paradigms. Unlike individual lectures, these training videos are coordinated and structured, giving consumers the flexibility to either follow through the entire “course” of material, or simply to watch a specific video of interest in order to resolve a problem. Such videos would be uploaded to the training portal and other online video hosting sites (see Section 6.3.1 below).

Based on the expertise of partners, it was decided to create videos on MPI, OpenMP and PETSc (see Table 6 for the list of topics, sub-topics and the distribution of work). These would extend the work from PRACE-IIP when CSC created three short videos on “A short introduction to MPI”. Most of these videos were uploaded to the training portal in May 2013 with the rest of the videos made available by the end of July 2013.

MPI videos		OpenMP videos	
NCSA-BG, Bulgaria	Design and Implementation of Parallel Programs with MPI. Case study TSP.	NCSA-BG, Bulgaria	Design and Implementation of Parallel Programs with OpenMP. Case study NQueens (Sam Loyd's puzzle).
CSC, Finland	Defining your own communicators	GRNET, Greece	OpenMP Synchronisation Constructs
CSC, Finland	Process Topologies in MPI	ICHEC, Ireland	Introduction to OpenMP
CSC, Finland	User Defined Datatypes	ICHEC, Ireland	OpenMP Loop Level Parallelism
GRNET, Greece	MPI I/O	ICHEC, Ireland	New Features after OpenMP 2.5
PETSc video tutorials (Parts I - V): VŠB-TUO, Czech Republic			

Table 6: PRACE training video tutorials - topics, sub-topics and distribution of work

6.3.1 Availability on public video-hosting sites

The PRACE training videos, either the video tutorials created by partners or video lectures from training events, were also uploaded to a number of public video-hosting sites. This was done for outreach purposes since by making the videos available on other sites, PRACE videos are easier to find (through better search engine results) and would be viewed more often. This in turn could attract more visits to the PRACE Training Portal (e.g. to download the PDF slides of the video lectures) and the PRACE RI web site (for other PRACE details).

In May 2013, the completed series of video tutorials, consisting of 13 clips, were uploaded to the “praceCourses” YouTube channel, in addition to their availability through the PRACE Training Portal. A complete list of video lectures recorded during PRACE Training events was compiled. The speakers for each of these videos, were contacted asking them for their consent to upload the video(s) in which they appear onto public video hosting sites. Such sites include YouTube, iTunesU (although geographic restrictions on using iTunesU exist) and

VideoLectures.net (for which official consent from PRACE is required before any videos could be uploaded to the site). The videos for which positive consent was received from the speakers will be uploaded to these sites in the near future.

6.4 Google Analytics integration

Google Analytics was integrated into the PRACE Training Portal in May 2013. During the period of 15th May - 15th June 2013, the visitor statistics for the portal are summarised in Figure 4. It is interesting to note the number of non-European visitors to the PRACE training portal. It includes visitors from Africa, South America, North America and Asia - which suggests the global presence, outreach and impact that the PRACE training program has achieved.

It is hoped that outreach activities, such as the advertisement of the PRACE Training Portal at ISC 2013 and through the PRACE newsletter (typically sent to a large audience, i.e. all PRACE contacts) will increase the interest, traffic and visits to the portal.

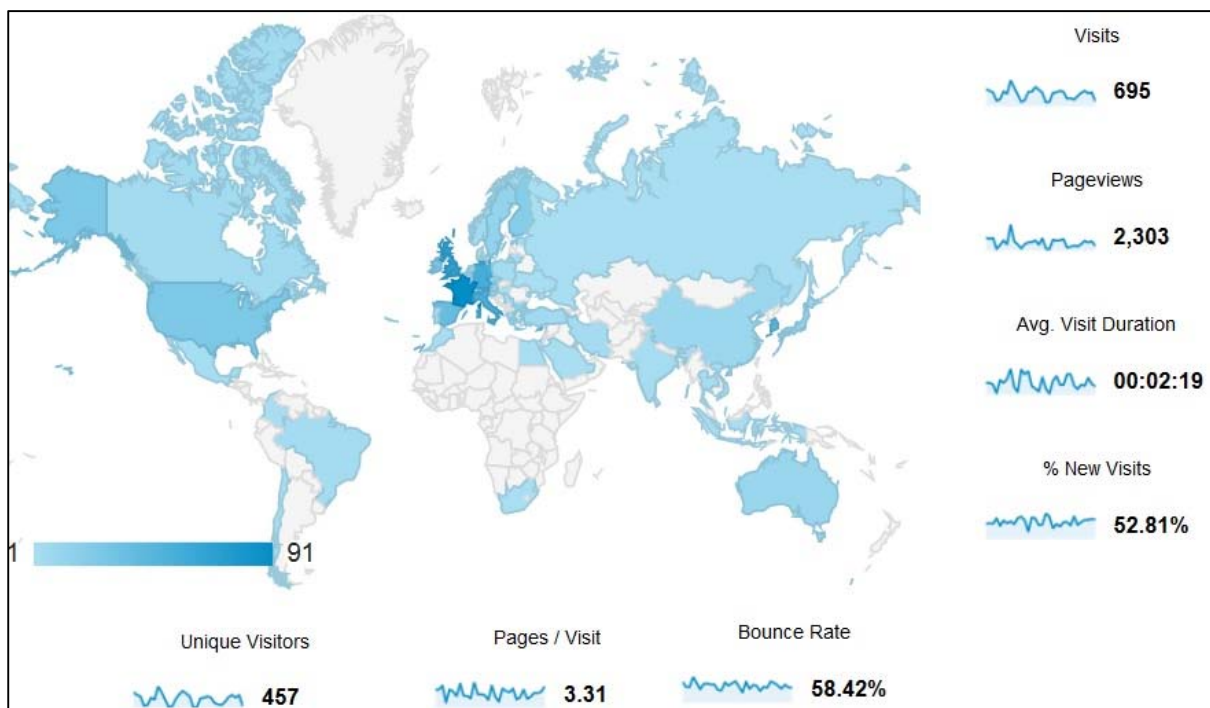


Figure 4. Google Analytics output describing visitors to the PRACE Training Portal

7 Conclusions

In summary, the outcome of PRACE-2IP WP4 has been a resounding success. Six PRACE Advanced Training Centres have been established to serve as hubs for providing world class HPC training in Europe (Section 3). They have since been responsible for an unprecedented level of training delivery under PRACE and should become central to future PRACE training strategy. The key activities of the PATCs have also been effectively complemented with training events organised by other PRACE partners. The seasonal schools and workshops (Section 5) have widened the geographical distribution of PRACE training and played an important role in PRACE outreach. The International HPC Summer Schools (Section 4) continued a rewarding collaboration with international partners in running a prestigious series of events that are unique from typical HPC courses. The key output statistics from all face-to-face training events in this Work Package are summarised in Table 7.

Key statistics	PATCs	Seasonal schools	International HPC Summer Schools	Workshops	Total
# courses/events	90	4	2	2	98
# days of training	260	18	9	4	291
# participants	2,058	184	133	139	2,514

Table 7: Key output statistics of all face-to-face training events in PRACE-2IP WP4

Not only has this Work Package been successful in delivering a large quantity of training (in terms of numbers of events and participants), the quality of the events has consistently been highly rated by participants. There is a sense that PRACE is commonly associated with training events that confer successful experiences on the participants; courses are relevant (to the needs of the audience), well organised and taught by proficient trainers.

Apart from face-to-face events this Work Package has also carried out other important activities related to training. The outcome of the comprehensive Education and Training Survey (Section 2) has been used to gauge training demand and for sourcing trainers in the planning of PRACE training events. The PRACE Training Portal (Section 6) has established itself as a valuable, central access point for PRACE training news and HPC training material, including videos, exercises and tutorials for distance learning.

8 Annex

This section includes supplementary information, figures and tables to support the main text above. Annex 8.1 contains supplementary material for reporting on the PRACE Advanced Training Centres (Task 4.2). Annex 8.2 and 8.3 contain individual reports on two International HPC Summer Schools (Task 4.3). Annex 8.4 thru 8.7 contain four seasonal school reports; Annex 8.8 and 8.9 contain the reports on two workshops (Task 4.4).

8.1 Supplementary material: the PRACE Advanced Training Centres

8.1.1 PATC courses from March 2012 to August 2012

Course name	PATC	Start date	Duration (days)
Advanced Topics in HPC	GCS	19/03/2012	4
Training-for-trainers: Activating Training Skills in a Practical Way	CSC	26/03/2012	3
Cray XE6 Optimization Workshop	GCS	02/04/2012	4
Python in High-Performance Computing	CSC	11/04/2012	3
Message-Passing Programming with MPI	EPCC	24/04/2012	3
Next generation sequencing data analysis with Chipster	CSC	26/04/2012	2
OpenACC programming for parallel accelerated supercomputers	GCS	14/05/2012	2
OpenMP for the QCD community	EPCC	21/05/2012	2
Programming and usage of the supercomputing resources in Jülich	GCS	21/05/2012	2
Performance analysis and tools	BSC	21/05/2012	2
Heterogeneous programming on GPUs with MPI+OmpSs	BSC	23/05/2012	2
Programming PRACE and MontBlanc prototypes: Tibidabo machine	BSC	25/05/2012	1
Introduction to CUDA programming	BSC	05/06/2012	4
Summer school on Scientific visualization	CINECA	11/06/2012	5
OpenMP, OpenACC and HMPP	MdS	19/06/2012	3
PUMPS school offered jointly with CUDA excellence centre	BSC	02/07/2012	5
Introduction to the usage of the superMUC petaflop system at LRZ	GCS	02/07/2012	5
Unified parallel C (UPC) and co-array fortran (CAF)	GCS	05/07/2012	2
Cray XE6 Systems Workshop	EPCC	11/07/2012	2

8.1.2 PATC joint curriculum planning and execution process

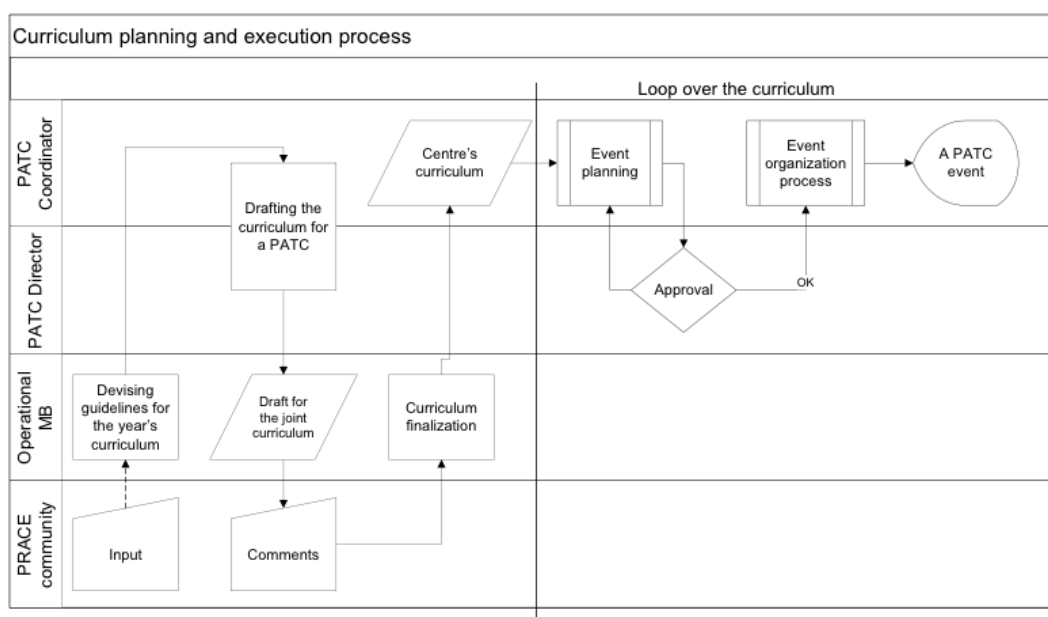


Figure 5: PATC curriculum planning and execution process

8.1.3 PATC joint curriculum for the 2012-2013 academic year

For the 2012-2013 academic year, the following details the joint PATC curriculum, including the syllabus of 72 courses and the topics/level these courses address.

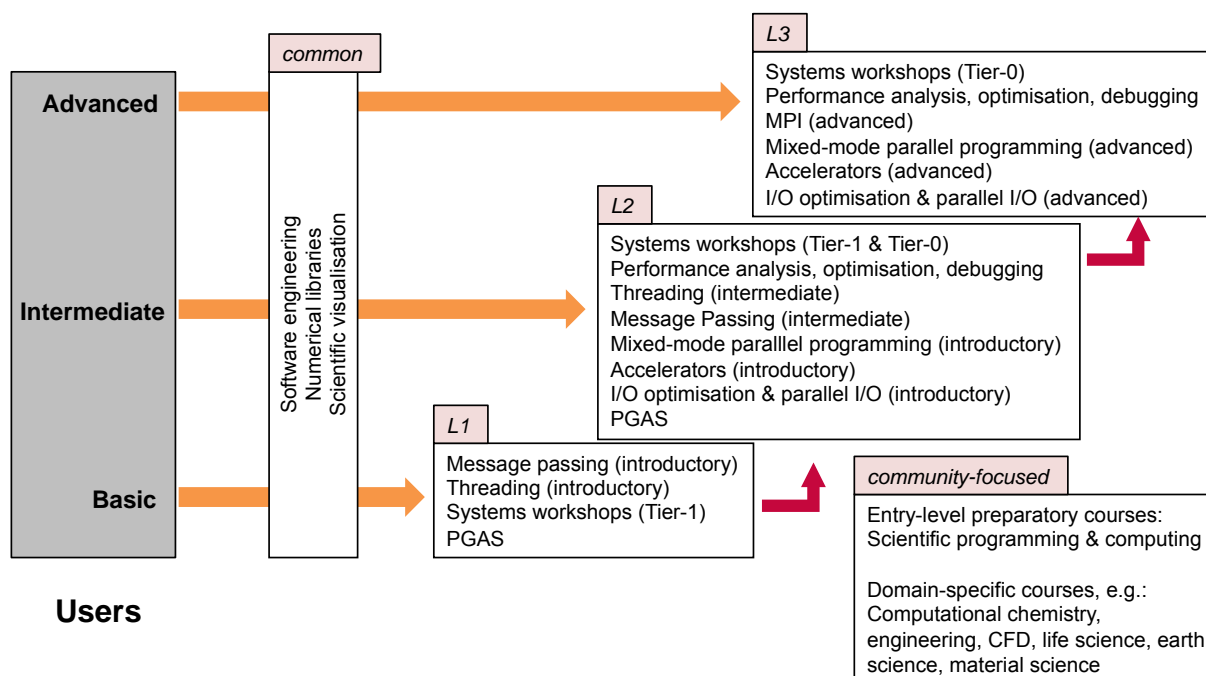


Figure 6: Outline of the 2012-2013 PATC HPC curriculum with optional study paths that form a “ladder” of training that can be followed to build up HPC competencies in a structured manner. L1, L2, and L3 topics are aimed at basic, intermediate and advanced users, respectively. “Common” topics refers to those topics that are aimed at all levels of users. “Community-focused” topics are targeted at specific domain users.

Code	Course name	PATC	Start date	Duration (days)
CSC01	FEM Workshop	CSC	27/08/2012	3
EPCC01	GPU Programming with CUDA and OpenACC	EPCC	28/08/2012	3
GCS01	Parallel Programming with MPI and OpenMP and Advanced Parallel Programming	GCS	03/09/2012	5
CSC02	Fortran 2003/2008	CSC	11/09/2012	3
MdS01	Parallel Programming with MPI and MPI-IO	MdS	11/09/2012	4
GCS02	Advanced Fortran Topics	GCS	17/09/2012	5
CSC03	Introduction to Parallel Programming with MPI & OpenMP	CSC	24/09/2012	3
MdS02	C-C++ Multicore Application Programming	MdS	01/10/2012	4
CINECA02	Introduction to Parallel Programming and Message Passing Paradigm (MPI)	CINECA	08/10/2012	3
CINECA03	Introduction to OpenMP Programming	CINECA	11/10/2012	1
CINECA04	Introduction to Hybrid Programming MPI+OpenMP	CINECA	12/10/2012	1
GCS03	10th VI-HPS Tuning Workshop	GCS	16/10/2012	4
CINECA05	Hybrid Programming for Material Science	CINECA	19/10/2012	1
MdS03	Usage of CURIE@CEA-TGCC Tier-0 Supercomputer and Related Best Practices	MdS	24/10/2012	3
CSC04	Advanced Parallel Programming	CSC	29/10/2012	3
(GCS05)	Cray XE6 Optimization Workshop	GCS	05/11/2012	4
CINECA01	HPC Surgery: debugging, profiling and optimization of a scientific code	CINECA	12/11/2012 (cancelled)	
EPCC02	Cray Systems Workshop	EPCC	20/11/2012	3
MdS05	Large Scale Data Visualization with Visit	MdS	26/11/2012	2
CINECA06	HPC Enabling of OpenFOAM for CFD Applications	CINECA	26/11/2012	3
BSC10	Parallel Programming Workshop	BSC	26/11/2012	5
CINECA07	Tools and techniques for scientific programming on BG/Q (Fermi)	CINECA	03/12/2012	2
EPCC03	Software Carpentry Boot Camp	EPCC	04/12/2012	2
(GCS05)	Node-level Performance Engineering	GCS	06/12/2012	2
MdS06	Software Development Tools	MdS	10/12/2012	2
MdS04	Programming on GPUs	MdS	12/12/2012	3
BSC09	Introduction to simulation environment for earth sciences	BSC	13/12/2012	2
EPCC04	PGAS Programming with UPC and Fortran Coarrays	EPCC	09/01/2013	2
MdS07	OpenMP / OpenACC programming	MdS	22/01/2013	3
GCS06	JUQUEEN Porting and Tuning Workshop	GCS	04/02/2013	3

Code	Course name	PATC	Start date	Duration (days)
BSC07	Engineering simulation tools: ALYA, FALL3D & PANDORA	BSC	06/02/2013	3
CINECA08	Advanced School on Parallel Programming	CINECA	11/02/2013	5
CSC07	Introduction to GPU programming	CSC	12/02/2013	2
MdS08	Jade Tier-1 System Workshop	MdS	18/02/2013	1
GCS07	Fortran for Scientific Computing	GCS	04/03/2013	5
CINECA10	HPC numerical libraries	CINECA	11/03/2013	3
BSC08	Simulation Environment for Life Sciences	BSC	14/03/2013	2
CINECA09	Introduction to the FERMI Blue Gene/Q, for users and developers	CINECA	18/03/2013	1
GCS10	Parallel I/O and Portable Data Formats	GCS	18/03/2013	3
GCS08	Advanced Topics in HPC (includes parallel I/O and PGAS)	GCS	18/03/2013	4
CSC08	Spring School in Computational Chemistry	CSC	19/03/2013	4
MdS09	Parallel Linear Algebra	MdS	27/03/2013	3
EPCC06	Large-Scale Parallel Profiling with VAMPIR	EPCC	08/04/2013	1
EPCC06	Large-Scale Parallel Debugging with DDT	EPCC	12/04/2013	1
EPCC05	Performance optimisation	EPCC	15/04/2013	2
GCS09	GPU Programming	GCS	15/04/2013	3
MdS10	Advanced Usage on CURIE tier-0 supercomputer: Best practices and code optimization	MdS	15/04/2013	3
CSC09	Python in High-Performance Computing	CSC	16/04/2013	3
GCS04	Cray XE6 Optimization Workshop	GCS	16/04/2013	4
BSC06	Systems Workshop - MareNostrum III	BSC	17/04/2013	2
MdS11	VI HPS Tuning Workshop	MdS	22/04/2013	4
CSC06	Scientific visualization	CSC	2013-04-23	3
GCS11	OpenACC Programming for Parallel Accelerated Supercomputers -- an alternative to CUDA from Cray perspective	GCS	29/04/2013	2
GCS13	Introduction to Unified Parallel C (UPC) and Co-Array Fortran (CAF)	GCS	02/05/2013	2
CINECA11	Introduction to GPGPU and CUDA programming	CINECA	09/05/2013	2
BSC01	Performance analysis and tools	BSC	13/05/2013	2
CSC10	Porting and optimizing applications on Cray XC30	CSC	14/05/2013	4
MdS12	Initiation to Parallelization with MPI	MdS	14/05/2013	4
BSC02	Heterogeneous programming on GPUs with MPI+OmpSs	BSC	15/05/2013	2
CINECA12	Parallel I/O and management of large scientific data	CINECA	16/05/2013	2

Code	Course name	PATC	Start date	Duration (days)
BSC03	Systems Workshop: Programming ARM based prototypes	BSC	17/05/2013	1
MdS13	Code Coupling using OpenPalm	MdS	29/05/2013	3
EPCC09	Statistical Analysis for Post-Genomic Data: Parallel Computing with R	EPCC	29/05/2013	2
BSC04	Introduction to CUDA programming	BSC	03/06/2013	5
CINECA13	Summer School on Scientific Visualisation	CINECA	10/06/2013	5
MdS14	Hybrid MPI/OpenMP Programming	MdS	18/06/2013	4
EPCC07	Shared-Memory Programming with OpenMP	EPCC	01/07/2013	2
EPCC08	Message-Passing Programming with MPI	EPCC	03/07/2013	3
BSC05	PUMPS Summer School	BSC	08/07/2013	5
GCS12	Introduction to the Usage of the SuperMUC Petaflop System at LRZ	GCS	08/07/2013	4
EPCC11	Advanced Cray Tools	EPCC	10/07/2013	2
EPCC10	Advanced OpenMP	EPCC	17/07/2013	2

Table 8: Syllabus of the 2012-2013 PATC joint curriculum

Level	Subject	Relevant PATC course codes
L1	Message passing	BSC10, CINECA02, CSC03, EPCC08, GCS01, MDS01, MDS12
	Threading	BSC10, CINECA03, CSC03, EPCC07, EPCC10, GCS01, MDS02, MDS07
	Systems workshops	CINECA09, MDS08
	PGAS	CSC02, EPCC04, GCS12
L2	Systems workshops	BSC03, BSC06, CINECA07, CINECA09, CSC05, CSC10, EPCC02, GCS04, GCS10, MDS03, MDS08, MDS10
	Performance analysis, optimisation, debugging	BSC01, CINECA01, EPCC05, EPCC06, EPCC11, GCS01, GCS03, GCS07, MDS11
	Mixed-mode parallel programming (introductory)	BSC02, CINECA04, CINECA05, CINECA08, CSC04, EPCC11, GCS01, MDS14
	Accelerators (introductory)	BSC04, CINECA11, CSC07, EPCC01, GCS08, GCS10, MDS04, MDS07
	I/O optimisation and parallel I/O (introductory)	CINECA12, CSC04, GCS01, GCS07, GCS09, MDS01
	PGAS	EPCC04, GCS07, GCS12
L3	Systes workshops	BSC03, BSC06, CINECA07, CINECA09, CSC05, CSC10, EPCC02, EPCC11, GCS04, GCS05, GCS10, GCS11, MDS03, MDS10
	Performance analysis, optimisation, debugging	EPCC06, EPCC11, GCS03, GCS05, GCS07, GCS10, MDS03, MDS10, MDS11
	Mixed-mode parallel programming (advanced)	BSC02, CINECA08

Level	Subject	Relevant PATC course codes
	Accelerators (advanced)	BSC05
Common	Software engineering	EPCC03, MDS06
	Numerical libraries	CINECA10, CSC04, GCS01, MDS09, MDS13
	Scientific visualisation	CINECA13, CSC06, GCS07, MDS05
Community-focused	Scientific programming and computing	CSC02, CSC09, GCS02, GCS06
	Domain-specific courses/workshops	BSC07, BSC08, BSC09, CINECA05, CINECA06, CSC01, CSC08, EPCC09

Table 9: Mapping between courses in the 2012-2013 syllabus and the HPC curriculum as shown above

8.1.4 PATC joint curriculum for the 2013-2014 academic year

For the 2013-2014 academic year, the following details the joint PATC curriculum, including the syllabus of 79 courses and the topics/level these courses address.

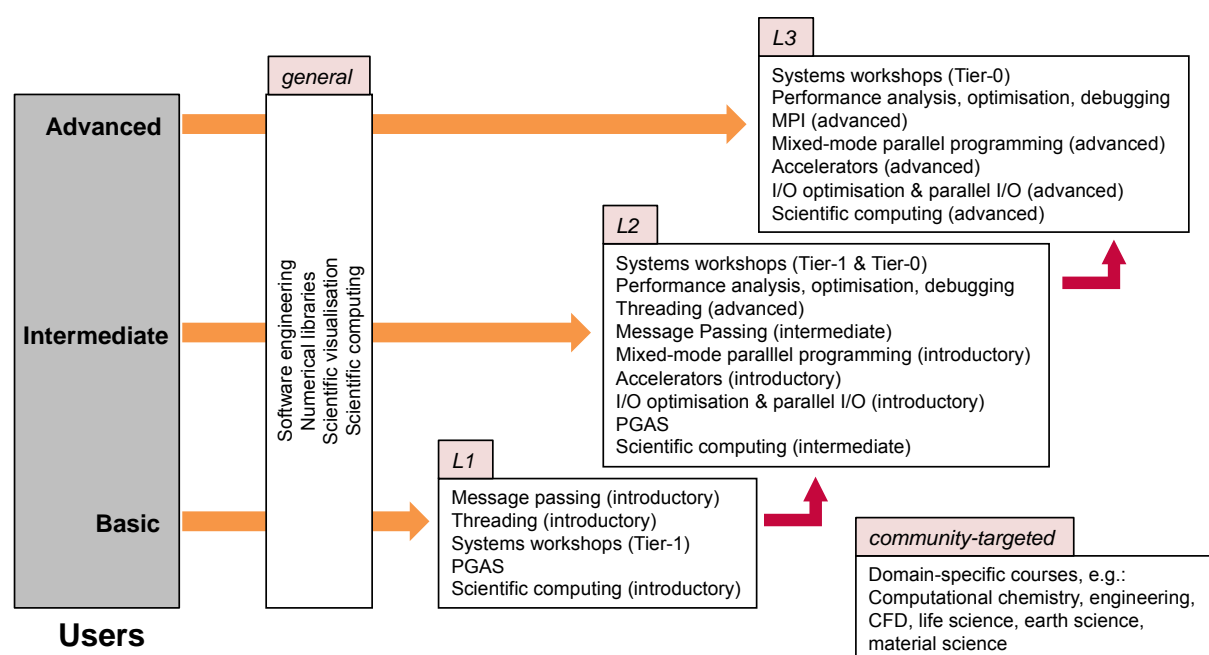


Figure 7: Outline of the 2013-2014 PATC HPC curriculum with optional study paths that form a “ladder” of training that can be followed to build up HPC competencies in a structured manner. L1, L2, and L3 topics are aimed at basic, intermediate and advanced users, respectively. “General” topics refers to those topics that are aimed at all levels of users. “Community-targeted” topics are targeted at specific domain users.

Code	Course name	PATC	Date
UK-06	GPU programming with CUDA and OpenACC	EPCC	Aug-13
UK-13	Parallel systems: getting the benefits	EPCC	Aug-13
FI-04	Data staging and data movement with EUDAT	CSC	Sep-13
FI-02	Fortran 95/2003	CSC	Sep-13
UK-14	Parallel CFD packages	EPCC	Sep-13

Code	Course name	PATC	Date
DE-04	Advanced parallel programming	GCS	Sep-13
DE-01	Advanced Fortran topics	GCS	Sep-13
FR-13	HPC simulation in CFD with Trio_U	MdS	Sep-13
FR-04	Visualization	MdS	Sep-13
ES-01	Parallel programming workshop	BSC	Oct-13
FI-03	Advanced Fortran topics & Coarray Fortran	CSC	Oct-13
FI-05	Introduction to parallel programming	CSC	Oct-13
UK-07	PGAS programming with UPC and Fortran Coarrays	EPCC	Oct-13
DE-12	Cray XE6/XC30 optimization workshop	GCS	Oct-13
DE-08	VI-HPS tuning workshop	GCS	Oct-13
FR-07	Multi-core application programming	MdS	Oct-13
FI-06	Advanced parallel programming	CSC	Nov-13
FR-01	Software development tools	MdS	Nov-13
ES-10	Introduction to simulation environment for Earth Sciences	BSC	Dec-13
FI-07	Introduction to programming the Xeon Phi	CSC	Dec-13
FI-11	Parallel workflows for computational science and engineering	CSC	Dec-13
UK-01	Software carpentry	EPCC	Dec-13
DE-09	Node-level performance engineering	GCS	Dec-13
FR-10	GPU programming	MdS	Dec-13
ES-11	System administration on a petaflop system, MareNostrum III	BSC	Jan-14
IT-12	HPC enabling of OpenFOAM for CFD applications	CINECA	Jan-14
IT-01	Introduction to Fortran90	CINECA	Jan-14
FI-08	Advanced OpenACC & CUDA	CSC	Jan-14
UK-02	Data staging and data movement with EUDAT	EPCC	Jan-14
UK-09	Systems workshop	EPCC	Jan-14
FR-06	Programming with OpenACC	MdS	Jan-14
ES-03	Engineering simulation tools: ALYA, FALL3D & PANDORA	BSC	Feb-14
IT-07	Advanced school on parallel computing	CINECA	Feb-14
IT-02	Introduction to scientific and technical computing in C++	CINECA	Feb-14
DE-10	JUQUEEN porting and scaling workshop	GCS	Feb-14
FR-14	HPC, Cloud: which solution for which business?	MdS	Feb-14
FR-05	Parallel filesystems and parallel IO libraries	MdS	Feb-14
ES-09	Simulation environment for Life Sciences	BSC	Mar-14
IT-04	HPC numerical libraries	CINECA	Mar-14
IT-11	Introduction to the FERMI Blue Gene/Q, for users and developers	CINECA	Mar-14
FI-10	Spring school in computational chemistry	CSC	Mar-14
DE-02	Advanced Fortran programming for scientific computing	GCS	Mar-14
DE-07	Parallel I/O and portable data formats	GCS	Mar-14

Code	Course name	PATC	Date
DE-03	Advanced topics in HPC (includes parallel I/O and PGAS)	GCS	Mar-14
FR-03	Parallel linear algebra	MdS	Mar-14
FR-12	Advanced usage on CURIE Tier-0 supercomputer: best practices and code optimization	MdS	Mar-14
ES-07	Systems workshop: programming MareNostrum III	BSC	Apr-14
IT-03	Introduction to C programming language for scientific applications	CINECA	Apr-14
IT-08	Programming paradigm for new hybrid architecture	CINECA	Apr-14
FI-01	Python in high-performance computing	CSC	Apr-14
UK-12	Parallel materials modeling packages	EPCC	Apr-14
UK-08	Tools for large-scale parallel debugging and profiling	EPCC	Apr-14
DE-13	Cray XE6/XC30 optimization workshop	GCS	Apr-14
DE-14	OpenACC programming for parallel accelerated supercomputers – an alternative to CUDA from Cray perspective	GCS	Apr-14
DE-05	GPU Programming	GCS	Apr-14
FR-11	VI-HPS tuning workshop	MdS	Apr-14
ES-04	Heterogeneous programming on GPUs with MPI + OmpSs	BSC	May-14
ES-05	Introduction to CUDA programming (with CCOE)	BSC	May-14
ES-06	Performance analysis and tools	BSC	May-14
ES-08	Programming ARM based prototypes	BSC	May-14
IT-09	Introduction to GPGPU and CUDA programming	CINECA	May-14
IT-06	Introduction to parallel computing with MPI and OpenMP	CINECA	May-14
IT-10	Parallel I/O and management of large scientific data	CINECA	May-14
FI-09	Cray XC Workshop	CSC	May-14
UK-03	Message-passing programming with MPI	EPCC	May-14
UK-11	Statistical analysis for post-genomic data: parallel computing with R	EPCC	May-14
DE-06	Unified Parallel C (UPC) and Co-Array Fortran (CAF)	GCS	May-14
FR-02	Code coupling using OpenPalm	MdS	May-14
FR-08	Runtime systems for heterogeneous platform programming	MdS	May-14
FR-15	Uncertainty quantification	MdS	May-14
ES-12	Alya system as a computational mechanics environment	BSC	Jun-14
IT-13	HPC computer aided engineering	CINECA	Jun-14
IT-05	Summer school on scientific visualization	CINECA	Jun-14
UK-04	Advanced OpenMP	EPCC	Jun-14
DE-11	Introduction to the usage of the SuperMUC petaflop system at LRZ	GCS	Jun-14
FR-09	Hybrid MPI/OpenMP programming	MdS	Jun-14
ES-02	PUMPS summer school (with CCOE)	BSC	Jul-14
UK-05	Programming the Xeon Phi	EPCC	Jul-14
UK-10	Systems workshop	EPCC	Jul-14

Table 10: Syllabus of the 2013-2014 PATC joint curriculum

Level	Subject	Relevant PATC course codes
General	Scientific programming and computing (introductory)	IT-01, IT-02, IT-03, FI-01
	Software engineering	UK-01, FR-01, FI-04, UK-02, FR-02, ES-01, ES-02, ES-03
	Numerical libraries	IT-04, FR-03
	Scientific visualisation	FR-04, IT-05, DE-03
L1	Message passing (basic)	FI-05, IT-06, UK-03, FR-05, ES-01
	Threading Basic	FI-05, IT-06, FR-06
	Systems workshop (Tier-1)	IT-11, DE-11, FI-09
	PGAS (basic)	DE-06, DE-01
	Scientific programming and computing (basic)	FI-01, FI-02, DE-01, DE-02
L2	Message passing (intermediate)	IT-06, UK-03, FR-05, ES-01, FI-06, DE-04, ES-02
	Threading (advanced)	IT-06, FR-06, FR-07, UK-04, FI-06, DE-04, ES-02, FR-08
	Systems workshops	DE-11, DE-10, FR-12, ES-07, UK-09, UK-10
	Performance analysis, optimisation and debugging (basic)	UK-08, ES-06, DE-08, FR-11, FI-09, DE-10, DE-11, UK-04, DE-04, DE-01, DE-03, DE-02
	Mixed-mode parallel programming (basic)	FR-09, ES-04, FI-06, DE-04, UK-04
	Accelerators (basic)	IT-09, ES-05, FI-07, UK-05, DE-05, FR-10, FR-06, UK-06, FI-08, ES-02, FR-07, FR-08
	I/O optimisation and parallel I/O.	FI-04, UK-02, FR-05, IT-10, DE-07, DE-03, FI-06, DE-04
	PGAS (advanced)	DE-06, DE-01, UK-07, FI-03, DE-03
	Scientific programming and computing (intermediate)	DE-01, DE-02, FI-03
L3	Message passing (advanced)	FI-06, DE-04, ES-02, IT-07
	Systems workshops	DE-11, FR-12, FI-09, UK-09, UK-10, ES-08
	Performance analysis, optimisation and debugging (advanced)	UK-08, ES-06, DE-08, FR-11, DE-09, FI-09, DE-11, UK-04, DE-04, DE-01, DE-03, DE-02, IT-07
	Mixed-mode parallel programming (advanced)	FR-09, ES-04, FI-06, DE-04, UK-04, IT-08, IT-07
	Accelerators (advanced)	UK-05, DE-05, FR-10, UK-06, FI-08, ES-02, FR-07, FR-08
	I/O optimisation and parallel I/O (advanced)	DE-07, DE-03, FI-06, DE-04
	Scientific programming and computing (advanced)	DE-01, DE-02, FI-03
Community-specific	Domain-specific courses/workshops	ES-09, UK-11, FI-10, UK-12, ES-03, ES-10, FR-02, DE-10

Level	Subject	Relevant PATC course codes
Industry-oriented	Industry and HPC	UK-13, UK-14, DE-12, DE-13, DE-14, IT-12, IT-13, FI-11, FR-13, FR-14, FR-15, ES-11, ES-12

Table 11: Mapping between courses in the 2013-2014 syllabus and the HPC curriculum as shown above

8.1.5 Per-PATC breakdown of numbers of participants and courses

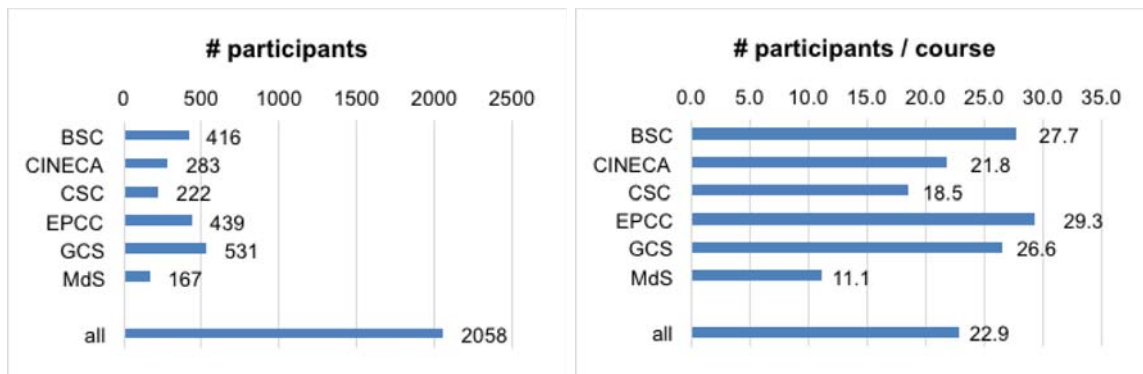


Figure 8: Total and average numbers of course participants at each PATC (03/2012 to 07/2013)

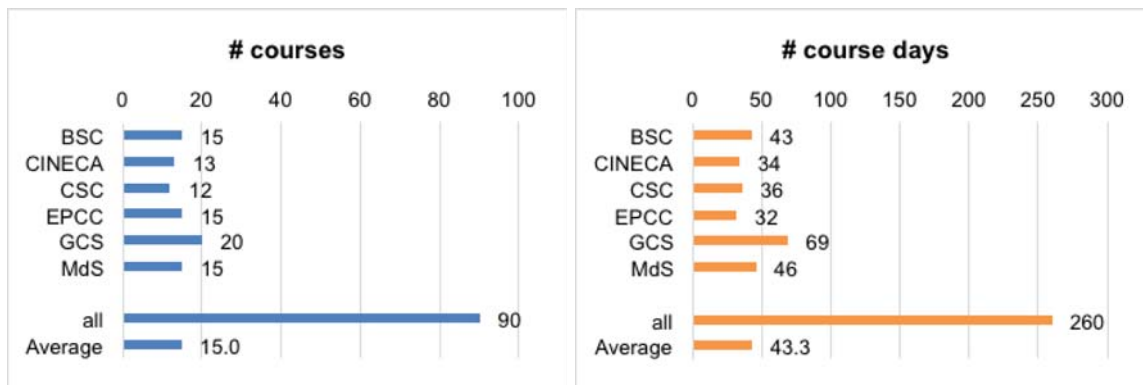


Figure 9: Number of courses and course days delivered by each PATC (03/2012 to 07/2013)

8.1.6 Geographical distribution of participants at PATC and other PRACE-2IP training events

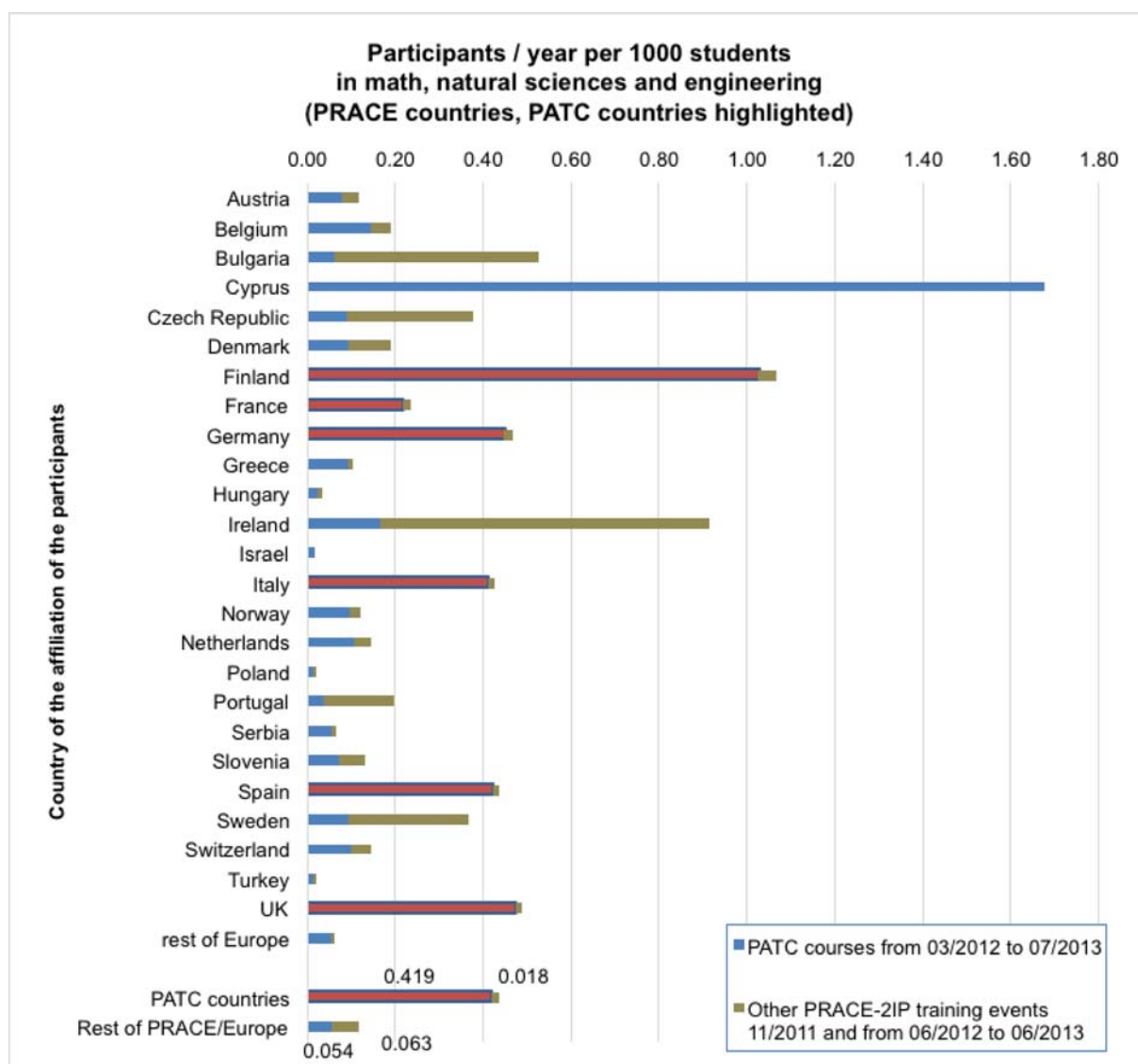


Figure 10: Participants / year per 1,000 students in mathematics, natural sciences and engineering, individually listed for all PRACE countries. Data is based on PATC courses from 03/2012 to 07/2013 together with other PRACE-2IP training events

8.2 2012 EU-US Summer School on HPC Challenges in Computational Sciences, Dublin, Ireland

8.2.1 Basic information about the event

Name: 2012 EU-US Summer School on HPC Challenges in Computational Sciences

Dates: 24-28 June 2012

Location: Dublin, Ireland

Organising sites: PRACE (ICHEC, Ireland; RZG, Germany), XSEDE (NCSA, USA)

8.2.2 Organisational details

Local organising committee

See programme committee below.

Venue

The location was selected to provide convenient access to US and European attendees as well as providing a scenic location with ready access to tourist attractions, restaurants and stores, as well as the advantages of a large city including mass transit. The Royal Marine Hotel in Dublin provided suitable classrooms and accommodation for almost all participants and presenters.

8.2.3 Programme & content

Programme/Organisation committee

Name	Affiliation, Country
Galen Arnold	NCSA, USA
Philip Blood	PSC, USA
Shawn Brown	PSC, USA
Pekka Manninen	CSC, Finland
Jim Ferguson	NICS, USA
David Henty	EPCC, UK
Scott Lathrop	Shodor Education Foundation Inc./NCSA, USA
Hermann Lederer	RZG, Germany
Simon Wong	ICHEC, Ireland

Table 12: Programme committee of the 2012 EU-US Summer School on HPC Challenges in Computational Sciences

Final programme

Sunday, June 24		
18:00 - 21:00	Welcome reception with finger food	
Monday, June 25		
08:30 - 10:00	Introduction of participants	
10:00 - 10:30	HPC challenges and opportunities: PRACE and XSEDE Simon Wong, Irish Centre for High-End Computing Scott Lathrop, Shodor Education Foundation Inc.	
10:30 - 11:00	BREAK	
11:00 - 12:00	Keynote: "The exascale, why and how" David Keyes, KAUST/Columbia University	
12:00 - 13:30	LUNCH	
13:30 - 14:30	Introduction to accelerators Rob Farber, ICHEC and BlackDog Endeavours, LLC	
14:30 - 17:00	Parallel hands-on session (continued on Tuesday)	
	Parallel programming I (OpenMP & MPI) David Henty, EPCC Xavier Teruel, Barcelona Supercomputing Center	GPU programming I (CUDA) Rob Farber, ICHEC and BlackDog Endeavors, LLC
18:00 - 19:30	Dinner at the Royal Marine Hotel [Dun restaurant]	
19:30 - 20:15	Electronic poster session I	
20:15 - 21:00	Electronic poster session II	
Tuesday, June 26		
08:30 - 09:30	Material science Joost VandeVondele, University of Zurich	Plasma physics Frank Jenko, Max Planck Institute of Plasma Physics
09:30 - 10:30	Life science Erik Lindahl, Stockholm University	Computational fluid dynamics James Hetherington, University College London
10:30 - 11:00	BREAK	
11:00 - 12:00	Extreme scaling Shawn Brown, University of Pittsburgh	
12:00 - 13:00	LUNCH	
13:00 - 16:00	Parallel hands-on session (continued from Monday)	
	Parallel programming II (OpenMP & MPI) David Henty, EPCC Xavier Teruel, Barcelona Supercomputing Center	GPU programming II (CUDA) Rob Farber, ICHEC and BlackDog Endeavors, LLC
18:00 - 23:00	Jameson shindig evening	
Wednesday, June 27		
08:30 - 09:30	Life science Thomas Cheatham, University of Utah	Large-scale agent-based modeling for public health decision making: a guide on how to save lives with supercomputers Shawn Brown, University of Pittsburgh
09:30 - 10:30	Astrophysics Bronson Messer, Oak Ridge National Laboratory	Nanoscience Umberto Ravaioli, University of Illinois
10:30 - 11:00	BREAK	
11:00 - 12:00	HPC software engineering Erik Lindahl, Stockholm University	Workflow tools Scott Callaghan, Southern California Earthquake Center
12:00 - 13:00	LUNCH	
13:00 - 13:15	Group Photo	
13:15 - 13:45	Ministerial address by Richard Bruton TD, Irish Minister for Jobs, Enterprise and Innovation	

13:45 - 17:15	Hands-on session	
	Performance analysis and optimization Philip Blood, Pittsburgh Supercomputing Center Christian Rössel, Juelich Supercomputing Center	
18:15 - 19:30	Dinner in Bray	
19:30 - 21:30	Bray to Greystones Cliff Walk	
Thursday, June 28		
08:30 - 09:30	Data-intensive computing: introduction Robert Sinkovits, San Diego Supercomputer Center	
09:30 - 10:30	Numerical libraries Tony Drummond, Lawrence Berkeley National Laboratory	Parallel filesystems, I/O, data transfer Lars Koesterke, Texas Advanced Computing Center
10:30 - 11:00	<i>BREAK</i>	
11:00 - 12:00	Numerical algorithms Piotr Luszczek, University of Tennessee Knoxville	Data-intensive case study: climate Luis Kornblueh, Max Planck Institute for Meteorology
12:00 - 13:30	<i>LUNCH</i>	
13:30 - 17:00	Hands-on session	
	Scientific visualization Amy Szczepanski, University of Tennessee/National Institute for Computational Sciences Galen Arnold, National Center for Supercomputing Applications, University of Illinois	
18:30 - 20:00	Dinner at city centre restaurant	
20:00 - 21:00	Guided city walk in Dublin city centre	

Table 13: Final programme of the 2012 EU-US Summer School on HPC Challenges in Computational Sciences

List of presenters and staff

Name	Affiliation, Country
Galen Arnold	NCSA, USA
Philip Blood	PSC, USA
Shawn Brown	PSC, USA
Scott Callaghan	University of Southern California, USA
Tom Cheatham	University of Utah, USA
Leroy Drummond	Lawrence Berkeley National Laboratory, USA
Robert Farber	ICHEC and BlackDog Endeavors, LLC, Ireland and USA
Jim Ferguson	NICS, USA
David Henty	EPCC, UK
James Hetherington	University College London, UK
Frank Jenko	Institute for Plasma Physics, Germany
David Keyes	King Abdullah University of Science and Technology, Saudi Arabia
Lars Koesterke	Texas Advanced Computing Center, USA
Luis Kornblueh	Max Planck Institute for Meteorology, Germany
Scott Lathrop	Shodor Education Foundation Inc./NCSA, USA
Hermann Lederer	RZG, Germany

Name	Affiliation, Country
Erik Lindahl	KTH, Sweden
Piotr Luszczek	The University of Tennessee, Knoxville, USA
Bronson Messer	Oak Ridge National Laboratory, USA
Umberto Ravaioli	University of Illinois, USA
Christian Roessel	JSC, Germany
Robert Sinkovits	San Diego Supercomputer Center, USA
Amy Szczepanski	NICS, USA
Xavier Teruel	BSC, Spain
Joost VandeVondele	University of Zurich, Switzerland

Table 14: List of presenters and staff at the 2012 EU-US Summer School on HPC Challenges in Computational Sciences

Designing the programme

Presenters were selected from the US and Europe to address a broader range of science topics, to cover the hands-on topics, and to engage experts in the field. They were also selected to mentor the attendees during the summer school. Support staff were selected from the US and Europe to provide assistance during the hands-on sessions, to provide mentoring to the attendees, and to coordinate logistics.

Description of the content

The 2012 participants were engaged in learning about:

- Long-term trends and strategies for advancing scientific discovery
- Availability of PRACE and XSEDE cyberinfrastructure in Europe and the United States to support computational science research and education
- Challenges and solutions for conducting leading-edge research across multiple fields of study
- Scientific programming and software development strategies
- Performance analysis and profiling
- Algorithmic approaches and numerical libraries
- Data-intensive computing
- Scientific visualization

Computer resources

All participants were asked to bring laptops for the hands-on tutorials. Course account access to both PRACE and XSEDE compute resources, as well as a local system hosted by ICHEC, were provided to participants.

8.2.4 Participants & feedback

Number of participants by country

Country	Number of participants
Austria	2
Belgium	4
Czech Republic	1

Country	Number of participants
Finland	1
France	2
Germany	8
Ireland	3
Italy	2
Netherlands	3
Poland	1
Portugal	1
Russia	1
Spain	2
Sweden	1
UK	3
USA	25
Total	60

Table 15: Number of participants by country at the 2012 EU-US Summer School on HPC Challenges in Computational Sciences

Process for selecting the participants

Applicants from Europe and the US were selected by PRACE and XSEDE, respectively. The European selection committee consisted of six scientists and HPC experts from Finland (CSC), France (CEA), Italy (CINECA), Germany (RZG), Spain (BSC) and the UK (EPCC). The selection criteria used include:

- Description of current research project and how it will benefit from the applicant learning about HPC
- Support of their faculty or research advisor to participate
- A basic understanding of computational science and high performance computing and experience with at least one of MPI, OpenMP, multi-core, or GPU programming
- Compelling statement of the applicant's reason for attending the Summer School
- A broad cross-section among the science and engineering communities from among the applicants
- A broad cross-section from institutions across the US and Europe
- Diversity among the participants

Statistics and analysis of the feedback survey

Through a survey conducted at the end of the Summer School, 90% of the attendees, and 100% of the presenters and support staff, indicated that they found the summer school to be excellent or very good. Through the surveys, the respondents provided a number of suggestions for further improving the summer school in future years, along with a very strong vote for continuing to offer similar summer schools in the future.

The following is a summary of the analysis from 59 responses to the survey, or 98% of the participants. The participants felt that the following aspects of the Summer School were very beneficial:

- Ability to interact informally with the presenters in a comfortable and open environment
- Ability to learn about HPC challenges in a diverse range of fields
- Networking with other international students
- Learned a great deal that will benefit their own research spanning research methods, programming tools and new networks of colleagues

8.2.5 *Conclusions and lessons learnt*

The overwhelming consensus from attendees, presenters and support staff is that the summer school was extremely effective in allowing the attendees and presenters to achieve (or surpass) their reasons for attending, and that they should be continued with minor changes, and continue as an international endeavour.

The participants provided a number of good suggestions for improvements in the future. The major recommendations for improvements included:

- Provide both introductory and advanced sessions during the hands-on tutorials to accommodate the diverse background of the participants
- Provide more hands-on tutorials
- Encourage the talks to focus on technology challenges and solutions
- Lengthen the Summer School to 5 days and provide more free time for assimilating the information and talking with others
- Ensure very good Internet connectivity

8.3 **2013 International Summer School on HPC Challenges in Computational Sciences, New York City, USA**

8.3.1 *Basic information about the event*

Name: 2013 International Summer School on HPC Challenges in Computational Sciences

Dates: 23-28 June 2013

Location: New York City, USA

Organising sites: PRACE (RZG, Germany; ICHEC, Ireland), XSEDE (NCSA, USA), RIKEN AICS

8.3.2 *Organisational details*

Local organising committee

See programme committee below.

Venue

The location was selected to provide convenient access for European, Japanese and US attendees with ready access to tourist attractions, restaurants, as well as the advantages of a large city including mass transit. New York University (NYU) provided the necessary venue and facilities for the majority of the school's programme. Accommodation for almost all participants and presenters were arranged at NYU dorms nearby.

8.3.3 *Programme & content***Programme/organising committee**

Name	Affiliation, Country
Galen Arnold	NCSA, USA
Tricia Barker	NCSA, USA
Philip Blood	PSC, USA
Thomas Cheatham	University of Utah, USA
Lizanne Destefano	University of Illinois, USA
Jim Ferguson	NICS, USA
David Henty	EPCC, UK
Scott Lathrop	Shodor Education Foundation Inc./NCSA, USA
Hermann Lederer	RZG, Germany
Yuri Mazuka	RIKEN AICS, Japan
Lorna Ivette Rivera	University of Illinois, USA
Mitsuhisa Sato	University of Tsukuba, Japan
Barbara Tóth	NIIFI, Hungary
Simon Wong	ICHEC, Ireland

Table 16: Programme committee of the 2013 International Summer School on HPC Challenges in Computational Sciences

Final programme

The full programme is available at:

<https://www.xsede.org/web/summerschool13/agenda>

List of presenters and staff

Name	Affiliation, Country
Galen Arnold	NCSA, USA
Phil Blood	PSC, USA
Mark Bull	EPCC, UK
Scott Callaghan	University of Southern California, USA
Thomas Cheatham	University of Utah, USA
Gilles Civario	ICHEC, Ireland
Leroy Drummond	Lawrence Berkeley National Laboratory, USA
James Ferguson	NICS, USA
Lars Koesterke	Texas Advanced Computing Center, USA
Scott Lathrop	Shodor Education Foundation Inc./ NCSA, USA
Hermann Lederer	RZG, Germany
Erik Lindahl	KTH, Sweden

Name	Affiliation, Country
Yuri Mazuka	RIKEN AICS, Japan
Kengo Nakajima	University of Tokyo, Japan
Atsushi Oshiyama	University of Tokyo, Japan
Luciano Rezzolla	Albert Einstein Institute, Germany
Christian Rössel	JSC, Germany
Mitsuhisa Sato	University of Tsukuba, Japan
Thomas Schulthess	CSCS, Switzerland
Edward Seidel	Skolkovo Institute of Science and Technology, Russia
Amy Szczepanski	NICS, USA
Xavier Teruel	BSC, Spain
John Towns	NCSA, USA
Akira Ukawa	University of Tsukuba, Japan
John Urbanic	PSC, USA
Simon Wong	ICHEC, Ireland

Table 17: List of presenters and staff at the 2013 International Summer School on HPC Challenges in Computational Sciences

Designing the programme

Presenters were selected from the US, Europe and Japan to address a broader range of science topics, to cover the hands-on topics, and to engage experts in the field. They were also selected to mentor the attendees during the summer school. Support staff were selected from the US and Europe to provide assistance during the hands-on sessions, to provide mentoring to the attendees, and to coordinate logistics.

Description of the content

The 2013 participants were engaged in learning about:

- Long-term trends and strategies for advancing scientific discovery
- Availability of PRACE and XSEDE cyberinfrastructure in Europe and the United States to support computational science research and education
- Challenges and solutions for conducting leading-edge research across multiple fields of study
- Scientific programming and software development strategies
- Performance analysis and profiling
- Algorithmic approaches and numerical libraries
- Data-intensive computing
- Scientific visualization

Computer resources

All participants were asked to bring laptops for the hands-on tutorials. Course account access to both PRACE and XSEDE compute resources.

8.3.4 *Participants & feedback*

Number of participants by country

Country	Number of participants
Austria	2
Czech Republic	2
Finland	1
France	2
Germany	4
Italy	3
Japan	11
Netherlands	1
Portugal	1
Spain	5
Sweden	1
Switzerland	2
Turkey	3
UK	3
USA	32
Total	73

Table 18: Number of participants by country at the 2013 International Summer School on HPC Challenges in Computational Sciences

Process for selecting the participants

Applicants from Europe and the US were selected by PRACE and XSEDE, respectively. The European selection committee consisted of six scientists and HPC experts from Finland (CSC), France (CEA), Italy (CINECA), Germany (RZG), Spain (BSC) and the UK (EPCC). The selection criteria used include:

- Description of current research project and how it will benefit from the applicant learning about HPC
- Support of their faculty or research advisor to participate
- A basic understanding of computational science and high performance computing and experience with at least one of MPI, OpenMP, multi-core, or GPU programming
- Compelling statement of the applicant's reason for attending the Summer School
- A broad cross-section among the science and engineering communities from among the applicants
- A broad cross-section from institutions across the US and Europe
- Diversity among the participants

Statistics and analysis of the feedback survey

Participants were asked to fill out an online questionnaire agreed between PRACE, XSEDE and RIKEN AICS. 64 (88%) of the participants provided feedback. The following is a summary of the results in different categories:

- Overall: a general measure of the perceived quality of this event was the response to the statement “Overall I would rate my experience as successful”; to this an overwhelming 97% of respondents were in agreement, i.e. that the event was a successful experience for them.
- Learning outcome: 87% of respondents indicated that their goals of attending the event were achieved; 90% stated that the skills they’ve learnt will significantly contribute to their research; 91% are aware of the next step to build on what they have learned.
- Organisation: 96% of respondents found the school to be well organised. 90% of respondents were satisfied with the delivery format of the school.
- International audience: 90% of respondents indicated that participation of students from other countries contributed to their learning; 93% have meaningfully engaged with other students at the school. Many have also indicated in the comments that the diverse and international nature of other students and presenters very much enhanced their experience.
- Mentoring: notably a lower proportion of respondents (59%) have stated to have meaningfully engaged with their assigned mentor during the school, there is a general feeling that the (random) mentor assignment process should be replaced by a more guided process.
- Compute resources: 90% of respondents are interested in learning more about the resources/opportunities available through PRACE/XSEDE/RIKEN AICS as a result of their experience; 85% plan on obtaining access to PRACE/XSEDE/RIKEN AICS resources after the school.

8.3.5 *Conclusions and lessons learnt*

The indication is that the school has been a very good success: it was well-received overall, perceived to be well-organised, and met the expectations/learning outcome of the participants. In addition, the many opportunities to interact with other international students and presenters from diverse backgrounds was highlighted as a unique, “value-add” feature of this school.

The one area where improvements can be made in future is the mentor assignment process. There was a general feeling that the random process that was used should be replaced by a more guided process so participants are assigned to mentors with similar research interests. However, this did not have a huge impact on the overall assessment of the school, as the participants had plenty of opportunities to engage with other mentors.

8.4 PRACE Autumn School 2012, Sofia, Bulgaria

8.4.1 Basic information about the event

Name: PRACE Autumn School 2012 on Massively Parallel Architectures and Molecular Simulations

Dates: 24 - 28 September 2012

Location: Sofia, Bulgaria

Organising sites: NCSA-BG

8.4.2 Organisational details

Local organising committee

- Krassimir Georgiev (NCSA-BG)
- Nedu Karaivanov (NCSA-BG)
- Georgi Prangov (NCSA-BG)

Venue

The PRACE Autumn School 2012 was held in Expo Hotel, Sofia, Bulgaria. The venue was chosen because it is only a few minutes away from Sofia Airport, provides modern facilities (including very good internet connection) and is not far from the Sofia city centre which makes it attractive for foreign students and researchers to attend. Additionally, the venue offered different conference rooms ranging in its capacity so that we were able to select the most appropriate one based on the final number of participants.

8.4.3 Programme & content

Programme committee

Name	Affiliation, Country
Giovanni Erbacher	CINECA, Italy
David Henty	EPCC, UK
Svetozar Margenov	IICT-BAS, Bulgaria
Stoyan Markov	NCSA-BG, Bulgaria

Table 19: Programme committee of the PRACE Autumn School 2012

Final programme

The final program can be found at:

<http://www.scc.acad.bg/ncsa/index.php/bg/2011-07-18-06-08-50?id=189>

List of trainers

Name	Affiliation, Country	Subject/expertise
Thomas Lippert	JSC, Germany	From Kepler to Supercomputing
Giovanni Erbacher	CINECA, Italy	Many Integrated Core Prototype EUROPA

Name	Affiliation, Country	Subject/expertise
Michael Stephan	JSC, Germany	JUQUEEN: System Architecture and Usage
Florian Janetzko	JSC, Germany	JUQUEEN: Application Stack and Best Practices
Ilian Todorov	Daresbury Laboratory, UK	DL_POLY – a Molecular Dynamics Engine; DL_POLY Packages – Differences and GUI; DL_FIELD – Force Field builder for DL_POLY
Michael Seaton	Daresbury Laboratory, UK	DL_MESO – Mesoscale Approaches via DPD & LBE; DL_MESO Applications & Demonstrations
Chin Yong	Daresbury Laboratory, UK	DL_POLY/FIELD Demonstrations; DL_POLY/FIELD/MESO Training Session I
Ivo Kabadshow	JSC, Germany	General Introduction to fast simulation methods; Scalable Fast Coulomb Solvers library ScaFaCoS; Analysis of the sequential Fast Multipole Method (FMM); Analysis of the parallel FMM
Rossen Apostolov	KTH, Sweden	Gromacs for Hybrid Systems -GROMACS, OpenMM and CUDA; GROMACS 4.6 Applications: Training

Table 20: List of trainers at the PRACE Autumn School 2012

Designing the programme

The program was designed with a target audience of people already familiar with standard parallel programming in mind such that they could expand their knowledge in multi scales/multi physics molecular simulation methods and software for high performance computing applications in molecular biology, biochemistry, microbiology, pharmacology research, cell medicine, immunology, chemical synthesis, atomic level material damage investigations and investigation of clusters of billions of nanoparticles.

In the first day it was presented two HPC architectures: Intel MIC based on the serious interest throughout HPC communities in Europe on this emerging technology and the new IBM system Blue Gene/Q as one of the PRACE Tier-0 system. In the next four days of the school it was put strong focus on molecular dynamics tutorials with some basic methods that could find strong practical implementation in areas such as drug design, new material, creation of new polymers with new structures, catalyst including their application in automobile and coal power station, nano foods and cosmetics.

Description of the content

Generally, the lectures were organised around the following topics: massively parallel architectures and molecular simulations.

Blue Gene/Q

Each rack contains 32 node boards with 32 compute nodes each. A node consists of a processor comprising 16 1.6 GHz 64 bit IBM PowerPC A2 cores for the execution of user applications, one additional core is used for the operating system. Every core can execute four processes/threads (fourfold Simultaneous Multi-Threading, SMT) and has a quad floating point unit (FPU) which can execute four double-precision Single Instruction Multiple Data (SIMD) Fused Multiply-Add operation (FMA) or two complex SIMD FMA per cycle. The maximal performance of the processor is 204.8 GFlop/s.

In order to use this architecture efficiently a hybrid parallelization strategy is necessary in general (e.g. MPI/OpenMP or MPI/Pthreads), especially since the main memory is limited to 16 GB per node (or 256 MB per process/thread with 4 processes/threads per core).

IBM Blue Gene/Q Characteristics

- Scales to 512 racks, achieving up to 100 PF at peak performance.
- Integrated 5D torus provides tremendous bisection bandwidth.
- Quad floating point unit (FPU) for 4-wide double precision FPU SIMD and 2-wide complex SIMD allows for higher single thread performance for some applications.
- “Perfect” prefetching for repeated memory reference patterns in arbitrarily long code segments achieves higher single thread performance for some applications.
- Multi-versioning cache with transactional memory eliminates the need for locks; and speculative execution allows OpenMP threading with data dependencies.
- Atomic operations, pipelined at L2 with low latency even under high contention, provide a faster handoff for OpenMP work.
- A wake-up unit allows SMT threads to sleep while waiting for an event and avoids register-saving overhead.
- A 17th core manages OS related tasks thus reducing OS related noise.

For more information see <http://www.redbooks.ibm.com/abstracts/sg247869.html?Open>

Intel® Many Integrated Core Architecture (Intel® MIC Architecture)

Following the growing interest in the Intel MIC architecture throughout Europe, it was decided to be presented a brief overview of MIC architecture.

Intel® MIC Architecture key specifications:

- 60 cores/1.053 GHz/240 threads
- 8 GB memory and 320 GB/s bandwidth
- Standard PCIe* x16 form factor, passively cooled
- Linux* operating system, IP addressable
- 512-bit single instruction, multiple data instructions
- Supported by the latest Intel® software development products
- Built using Intel’s 22nm process technology—Intel’s most energy efficient process yet - featuring the world’s first 3-D tri-gate transistors.

In the next four days the programme was designed around DL_POLY, Long-Range Interactions calculations, GROMACS ensuring full day lectures and hands-on sessions:

- ***DL_POLY Description***
 - DL_POLY: Molecular dynamics/mechanics is a theoretical tool for modeling the detailed microscopic behaviour of many different types of systems, including; gases, liquids, solids, polymers, surfaces and clusters. DL_POLY offers access to a generic implementation of this method by providing efficient machinery for solving numerically the classical equations of motion governing the microscopic time evolution of a many body system, subject to the boundary conditions appropriate for the geometry or symmetry of the system and well defined force-fields. Following the dynamics of a model system one

can monitor the microscopic mechanisms of energy and mass transfer in chemical processes, and dynamical properties such as absorption spectra, rate constants and transport properties can be calculated. Furthermore, it can be employed as a means of sampling from a statistical mechanical ensemble and determining equilibrium properties. These properties include average thermodynamic quantities (pressure, volume, temperature, etc.), structure, and free energies along reaction paths.

- DL_FIELD: DL_FIELD is a user-friendly tool for processing molecular information converting it from a user's specified atom models into file formats that are recognizable and ready to run by the DL_POLY program. It can handle any combination of molecules from a wide range of complex topological structures such as proteins, membranes, carbohydrates, large organic, poly-organic and networked molecules such as graphemes, organic cages, polymers and zeolites. Currently, the program has the capability to set up models using well-known force field schemes for organic molecules and biological molecules such as CHARMM, AMBER and OPLS-AA. More general force fields are also available such as DREIDING and PCFF (CFF93 consistent force field variant). DL_FIELD facilitates switching between these force fields representations without any modification to original configurations. Furthermore, the molecular structures and parameter databases for all force field schemes are presented in a single format. Thus allowing users to easily familiarise with any force field scheme and extend the existing standard databases with newly defined molecular structures and force field parameters.
- DL_MESO: The mesoscopic modeling methods available in DL_MESO (Lattice Boltzmann Equation, Dissipative Particle Dynamics) fit between those used for molecular dynamics and computational fluid dynamics. These operate at length and time scales suitable for modeling complex materials with both atom-like effects and bulk fluid properties such as viscosity. Examples of such systems include: flows through complex geometries, microfluidics, acoustic fields in mildly compressible fluids, solute diffusion, conductive and convective heat transfers, phase behaviour of fluids and polymers (e.g. surfactants, amphiphiles), self-assembly of chemical structures and adsorption onto surfaces.
- For more information see http://www.stfc.ac.uk/CSE/randd/ccg/software/DL_POLY/25526.asp
- **GROMACS** (from <http://www.gromacs.org/>)
 - GROMACS (Groningen Machine for Chemical Simulations), a molecular dynamics simulation package, was originally developed at the University of Groningen and is now maintained and extended at various institutions, including the University of Uppsala, the University of Stockholm, and the Max Planck Institute for Polymer Research. The application is a versatile package primarily designed to simulate the Newtonian equations of motion for systems with hundreds to millions of particles, for example, biochemical molecules such as proteins, lipids, and nucleic acids that have complicated bonded interactions. In addition, GROMACS is extremely fast at calculating non-bonded interactions (which usually dominate simulations), so many groups are also using it for research on non-biological systems (for example, polymers). The molecular dynamics simulations and energy minimization are two of the many techniques that belong to the realm of computational chemistry and molecular modeling. Computational chemistry is just a name to indicate the

use of computational techniques in chemistry, ranging from quantum mechanics of molecules to dynamics of large complex molecular aggregates. Molecular modeling indicates the general process of describing complex chemical systems in terms of a realistic atomic model, with the goal being to understand and predict macroscopic properties based on detailed knowledge on an atomic scale. Often, molecular modeling is used to design new materials, for which the accurate prediction of physical properties of realistic systems is required.

Macroscopic physical properties can be distinguished by (a) static equilibrium properties, such as the binding constant of an inhibitor to an enzyme, the average potential energy of a system, or the radial distribution function of a liquid, and (b) dynamic or non-equilibrium properties, such as the viscosity of a liquid, diffusion processes in membranes, the dynamics of phase changes, reaction kinetics, or the dynamics of defects in crystals. The choice of technique depends on the question asked and on the feasibility of the method to yield reliable results at the present state of the art. Ideally, the (relativistic) time-dependent Schrödinger equation describes the properties of molecular systems with high accuracy, but anything more complex than the equilibrium state of a few atoms cannot be handled at this *ab initio* level. Thus, approximations are necessary; the higher the complexity of a system and the longer the time span of the processes of interest is, the more severe the required approximations are. At a certain point (reached very much earlier than one would wish), the *ab initio* approach must be augmented or replaced by empirical parameterization of the model used. Where simulations based on physical principles of atomic interactions still fail due to the complexity of the system, molecular modeling is based entirely on a similarity analysis of known structural and chemical data.

The QSAR methods (Quantitative Structure- Activity Relations) and many homology-based protein structure predictions belong to the latter category. Macroscopic properties are always ensemble averages over a representative statistical ensemble (either equilibrium or non-equilibrium) of molecular systems. For molecular modeling, this has two important consequences:

- The knowledge of a single structure, even if it is the structure of the global energy minimum, is not sufficient. It is necessary to generate a representative ensemble at a given temperature, in order to compute macroscopic properties. But this is not enough to compute thermodynamic equilibrium properties that are based on free energies, such as phase equilibria, binding constants, solubility, relative stability of molecular conformations, etc.

The computation of free energies and thermodynamic potentials requires special extensions of molecular simulation techniques.

- While molecular simulations, in principle, provide atomic details of the structures and motions, such details are often not relevant for the macroscopic properties of interest. This opens the way to simplify the description of interactions and average over irrelevant details. The science of statistical mechanics provides the theoretical framework for such simplifications. There is a hierarchy of methods ranging from considering groups of atoms as one unit, describing motion in a reduced number of collective coordinates, averaging over solvent molecules with potentials of mean force combined with stochastic

dynamics, to mesoscopic dynamics describing densities rather than atoms and fluxes as response to thermodynamic gradients rather than velocities or accelerations as response to forces.

For the generation of a representative equilibrium ensemble two methods are available: (a) Monte Carlo simulations and (b) Molecular Dynamics simulations. For the generation of non-equilibrium ensembles and for the analysis of dynamic events, only the second method is appropriate. While Monte Carlo simulations are more simple than MD (they do not require the computation of forces), they do not yield significantly better statistics than MD in a given amount of computer time. Therefore, MD is the more universal technique. If a starting configuration is very far from equilibrium, the forces may be excessively large and the MD simulation may fail. In those cases, a robust energy minimization is required. Another reason to perform an energy minimization is the removal of all kinetic energy from the system: if several “snapshots” from dynamic simulations must be compared, energy minimization reduces the thermal noise in the structures and potential energies so that they can be compared better.

- **Long-Range Interactions**

- Long-Range Interactions are an essential part of molecular simulations. In practice they often involve important physical forces: gravity and the electromagnetic interaction, the basis for the propagation of light, electricity, chemical reactions and the structure of solids, molecules and atoms. Since in such systems, each particle interacts with all other particles, the calculations that need to be carried out increase to extremely big numbers. For example, if a super computer such as JUGENE with its 294,912 processors were to calculate the interactions between three trillion particles directly, it would require more than 32,000 years. One of the methods, which swingeing cuts the calculation times is the fast multipole method (FMM). With the help of the FMM distant particles may be combined into clusters, which are described by the so-called multipole moments. Thus one no longer needs to calculate each interaction individually. On the basis of FMM Jülich scientists Ivo Kabadshow and Holger Dachsel created a new algorithm and solved the same task on the JUGENE supercomputer with its 294,912 processors for less than 695 seconds, from “World-Record Algorithm from Jülich Calculates Over Three Trillion Particles”:

<http://www.research-in-germany.de/73280/2011-08-02-world-record-algorithm-from-j-lich-calculates-over-three-trillion-particles.html>

Sufficient details of the Fast Multipole Methods can be found in “An Overview of Fast Multipole Methods”:

http://www.ics.uci.edu/~ihler/papers/ihler_area.pdf

Computer resources

For the school it was granted NCSA-BG resources to the Bulgarian Blue Gene/P system as well in order to be ensuring the training process some of the hands-on examples were run on Daresbury Laboratory Blue Gene/P system and KTH Cray system. Participants agreed to bring their own laptops. Laptops were mainly used as ssh terminals to login to supercomputer resources available for the school.

8.4.4 *Participants & feedback*

Number of participants by country

Country	Number of participants
Bulgaria	33
Czech Republic	2
Egypt	2
Germany	1
Greece	1
Ireland	1
Poland	2
Slovenia	2
Turkey	3
UK	1
Total	48

Table 21: Number of participants by country at the PRACE Autumn School 2012

Process for selecting the participants

Initially after the registration deadline there were around 64 participants registered. 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.

Statistics and analysis of the feedback survey

From the PRACE survey: as regards the question “Overall, how would you rate this school? [0 = waste of time, 10 = excellent]”, the average score was 8.4 basing on answers from 27 participants which represents 56% of the total number of the participants.

The venue and overall organisation were rated very highly with a mark between Good and Excellent above 90% of all responses; the catering was slightly lowest score with 74% rated with mark between Good and Excellent. The feedback on the lectures was also very good.

In general, the feedback was very good and the participants were very satisfied with the event. The schedule should have contained more space for exercises “practice of examples and applications of the programs”.

8.4.5 *Conclusions and lessons learnt*

We had some unexpected moments with the high level of initially registered participants outside Bulgaria that then withdrew from the event at confirmation stage just before the event. In that sense, it is necessary to be taken into consideration some measures that could prevent last moment withdrawal.

There were some issues related to visa application times for non-EU nationals and non-PRACE members. There should be some clear recommendations on such applicants and based on this guidelines each organizing site can simply encourage non-EU nationals through different mechanisms e.g. to apply as early as possible or providing some funding support.

Despite the fact that the school went very smoothly and successfully, it was the first such big event here in Sofia, Bulgaria so that we will continue looking for improvement in all aspects in order to achieve some level of sustainability.

8.5 PRACE Winter School 2013, Dublin, Ireland

8.5.1 Basic information about the event

Name: PRACE Winter School 2013 on Scientific Visualisation

Dates: 19-22 March 2013

Location: Dublin, Ireland

Organising sites: ICHEC

8.5.2 Organisational details

Local organising committee

- Simon Wong (ICHEC)
- Emma Hogan (ICHEC)

Venue

The premises of Chartered Accountants House was hired for the purpose of the school. The venue was chosen due to various reasons: (a) it is centrally located in Dublin city centre with good accessibility by public transport. (b) reliable network connectivity: the organising site had used the same venue for a local event prior to this school. The venue had also hosted large conferences with hundreds of attendees who carried laptops and smartphones. (c) it provides a suitably-sized classroom for ~50-60 people, as well as catering areas for breaks and lunches in the same building. It also provides state-of-the-art audio-visual equipment.

8.5.3 Programme & content

Programme committee

Name	Affiliation, Country
Simon Wong	ICHEC, Ireland
Sean Delaney	ICHEC, Ireland
Pekka Manninen	CSC, Finland

Table 22: Programme committee of the PRACE Winter School 2013

Final programme

Tuesday, 19 March	
13:00 - 14:00	LUNCH
14:00 - 14:10	Welcome
14:10 - 15:00	Introduction to Scientific Visualisation Nicolas Rougier, LORIA, France
15:00 - 15:30	Introduction to R Adam Ralph, Irish Centre for High-End Computing

15:30 - 16:00	<i>AFTERNOON BREAK</i>
16:00 - 17:30	R: Basics and Plotting I Adam Ralph & Bruno Voisin, Irish Centre for High-End Computing
19:00 - 22:00	<i>SOCIAL DINNER</i>
Wednesday, 20 March	
09:00 - 09:30	<i>MORNING TEA/COFFEE</i>
09:30 - 11:30	R: Plotting II Bruno Voisin, Irish Centre for High-End Computing
11:30 - 12:00	<i>MID-MORNING BREAK</i>
12:00 - 13:00	Introduction to Python Nicolas Rougier, LORIA, France
13:00 - 14:00	<i>LUNCH</i>
14:00 - 15:30	Python: Matplotlib Nicolas Rougier, LORIA, France
15:30 - 16:00	<i>AFTERNOON BREAK</i>
16:00 - 17:30	Python: Matplotlib Nicolas Rougier, LORIA, France
Thursday, 21 March	
09:00 - 09:30	<i>MORNING TEA/COFFEE</i>
09:30 - 11:00	Visit Jean Favre, CSCS, Switzerland
11:00 - 11:30	<i>MID-MORNING BREAK</i>
11:30 - 13:00	Visit Jean Favre, CSCS, Switzerland
13:00 - 14:00	<i>LUNCH</i>
14:00 - 15:30	Visit Jean Favre, CSCS, Switzerland
15:30 - 16:00	<i>AFTERNOON BREAK</i>
16:00 - 17:00	Visit Jean Favre, CSCS, Switzerland
Friday, 22 March	
09:00 - 09:30	<i>MORNING TEA/COFFEE</i>
09:30 - 11:00	Paraview Jean Favre, CSCS, Switzerland
11:00 - 11:30	<i>MID-MORNING BREAK</i>
11:30 - 13:00	Paraview Jean Favre, CSCS, Switzerland
13:00 - 14:00	<i>LUNCH</i>

Table 23: Final programme of the PRACE Winter School 2013

List of trainers

Name	Affiliation, Country	Subject/expertise
Adam Ralph	ICHEC, Ireland	General R usage
Bruno Voisin	ICHEC, Ireland	R plotting tools and libraries
Jean Favre	CSCS, Switzerland	VisIt and Paraview
Nicolas Rougier	LORIA, France	Python, matplotlib library

Table 24: List of trainers at the PRACE Winter School 2013

Designing the programme

The programme was designed to provide some basic introduction and tutorials of both 2-D (graphs and diagrams), and 3-D (manipulation/representation of 3-dimensional data) visualisation tools and techniques. The committee selected some of the most popular tools used in this regard. For 2-D visualisation, the statistical package R and the Python matplotlib library were chosen; they are widely used, e.g. for generating figures in publications. For 3-D visualisation, the VisIt and Paraview packages were chosen as the focus of teaching. In the selection of trainers for the programme, the database of trainers (constructed during earlier work in the project, see Section 2) was utilised to seek experts in the field of scientific visualisation.

Description of the content

The school opened with a general talk on scientific visualisation. This was followed by a series of talks and hands-on tutorials on the R statistical package along with built-in functions and libraries used for plotting common figures (e.g. histograms, boxplots, and more complex visual representation of data, etc).

Attendees were then given a brief introduction to the Python programming language. An afternoon was then spent on the Python matplotlib library, which provides the ability to embed plotting functions into Python programs. The session includes both live demonstrations as well as hands-on exercises on the use of different matplotlib routines.

The second half of the school focused on the VisIt and Paraview packages, both commonly used to conduct 3-D data manipulation and exploration. This consisted of a 1-day tutorial on VisIt and a half-day tutorial on Paraview - many concepts are common between the two packages - hence the latter aimed to highlight some key differences. Again, the format of the tutorials consists of a mix of talks, live demonstrations and hands-on tutorials carried out by attendees.

Computer resources

This school did not require access to supercomputers, all attendees brought laptops to the school for the hands-on exercises. While access to local supercomputing facilities was arranged as a fail-safe option, attendee laptops were sufficiently equipped to conduct the hands-on exercises. Some live demonstrations were conducted by remote connections to supercomputing facilities at CSCS.

8.5.4 *Participants & feedback*

Number of participants by country

Country	Number of participants
France	1
Germany	1
Ireland	38
Italy	2
Romania	1
Total	43

Table 25: Number of participants by country at the PRACE Winter School 2013

Process for selecting the participants

Participants were selected on a first come, first served basis.

Statistics and analysis of the feedback survey

A total of 26 participants responded to the feedback survey as developed by PRACE for most of its training events. The school achieved an overall rating of 8.5 (0: worst, 10: best). Many aspects of the school, from information, registration venue, catering and organisation were all deemed to be either good or excellent by the participants. There were overwhelming agreement (>96%) that the topic being taught were relevant to the participants' research, 92% agree that the teaching aides used were well prepared.

The only issues a few participants found were that the pace of teaching may have been too fast for some, and that instead of having a comprehensive course covering a variety of visualisation tools and techniques, it may be more useful to have more in-depth, longer courses on individual tools.

8.5.5 *Conclusions and lessons learnt*

In general the PRACE Winter School 2013 was a very successful event. It provided a good introduction to a number of free and open source tools for scientific visualisation. The school was implemented smoothly and most participants have rated the it very highly, with some minor criticisms (see above) that can be addressed in future by delivery of longer, more focused events on specific scientific visualisation tools.

8.6 PRACE Spring School 2013, Umeå, Sweden

8.6.1 *Basic information about the event*

Name: PRACE Spring School 2013 on New and Emerging Technologies - Programming for Accelerators

Dates: 23 - 26 April 2013

Location: Umeå, Sweden

Organising sites: SNIC-UmU (HPC2N, Umeå) and SNIC-LiU (NSC, Linköping), Sweden

8.6.2 Organisational details

Local organising committee

- Jerry Eriksson (HPC2N, Sweden)
- Peter Münger (NSC, Sweden)
- Torben Rasmussen (NSC, Sweden)
- Mikael Rännar (HPC2N, Sweden)

Venue

The MIT building in Umeå University, Umeå, Sweden. The venue was chosen because HPC2N is located in that building and there exists good lecture halls and there is also an existing IT infrastructure (wireless network, workstations) available. Everyone brought their own laptop so there was no need to use the workstations. The wireless networks worked without any problem.

8.6.3 Programme & content

Programme committee

Name	Affiliation, Country
Jerry Eriksson	HPC2N, Sweden
David Henty	EPCC, UK
Nick Johnson	EPCC, UK
Peter Münger	NSC, Sweden
Torben Rasmussen	NSC, Sweden
Mikael Rännar (chair)	HPC2N, Sweden

Table 26: Programme committee of the PRACE Spring School 2013

Final programme

The course was split into three parts covering different types of architecture and accelerators. The first two days focused on the Intel Many Integrated Core (MIC) architecture with hands-on using the Xeon Phi system at CSC in Finland. The third day was dedicated to learning how, and when, to offload computations to accelerators using OpenACC, with hands-on using the GPU cluster at LUNARC, Sweden. The final day BSC presented a comprehensive view of their ARM-based prototypes and how to program these machines efficiently. The hands-on session used the prototype system at BSC, Spain. For the full program see Appendix A. There is also a schedule available online (<http://www.hpc2n.umu.se/node/884>) with links to the slides for each lecture.

List of trainers

Name	Affiliation, Country
Mikko Byckling	CSC, Finland
Gabriele Carteni	BSC, Spain
Nick Johnson	EPCC, UK

Name	Affiliation, Country
Michael Klemm	Intel, Germany
Olli-Pekka Lehto	CSC, Finland
Nicola Rajovic	BSC, Spain

Table 27: List of trainers at the PRACE Spring School 2013

Designing the programme

The idea was to have a connection with WP11 (Prototyping) and the theme was therefore chosen to be accelerator related. We wanted an introduction to, but at the same time some state-of-the-art, trends in programming for accelerators. This resulted in a program where we are introduced to programming for different types of accelerators including MIC, GPU, and ARM processors. When we started to look for speakers it was natural to look first at the different PATCs, and later we also invited Intel to the MIC sessions.

8.6.4 Participants & feedback

Number of participants by country

Country	Number of participants
Bulgaria	2
Czech Rep.	1
Finland	1
France	2
Norway	1
Sweden	34
UK	2
Total	43

Table 28: Number of participants by country at the PRACE Spring School 2013

Process for selecting the participants

At first we had a limit of 30 participants, but since the lecture halls were big enough we decided to accept 40 participants instead of having to do a rather late selection which we wanted to avoid since Umeå is not the easiest place to get cheap travels to. Using the online registration, 59 people registered for the course and we accepted everyone that answered our acceptance mail. After some late drop outs the number of participants ended on 43.

Statistics and analysis of the feedback survey

A total of 28 participants completed the standard PRACE feedback survey for training events. The results of the survey are summarised in Figure 11, Figure 12 and Figure 13.

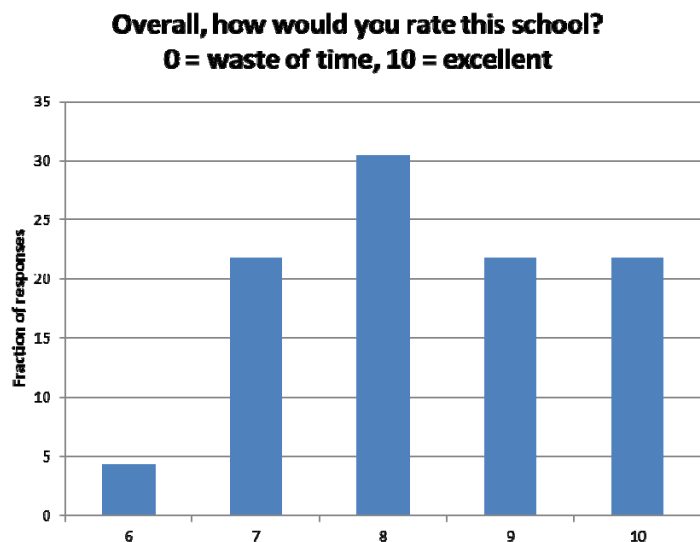


Figure 11: PRACE Spring School 2013 feedback - overall rating

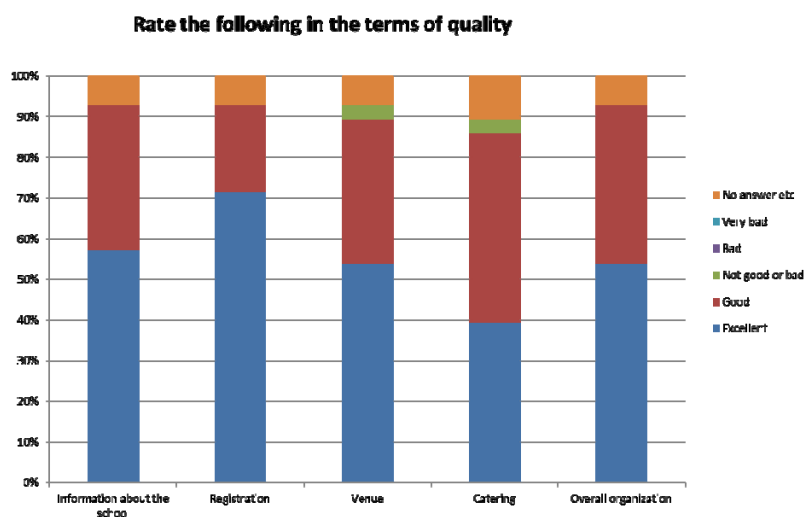


Figure 12: PRACE Spring School 2013 feedback - various aspects of the event

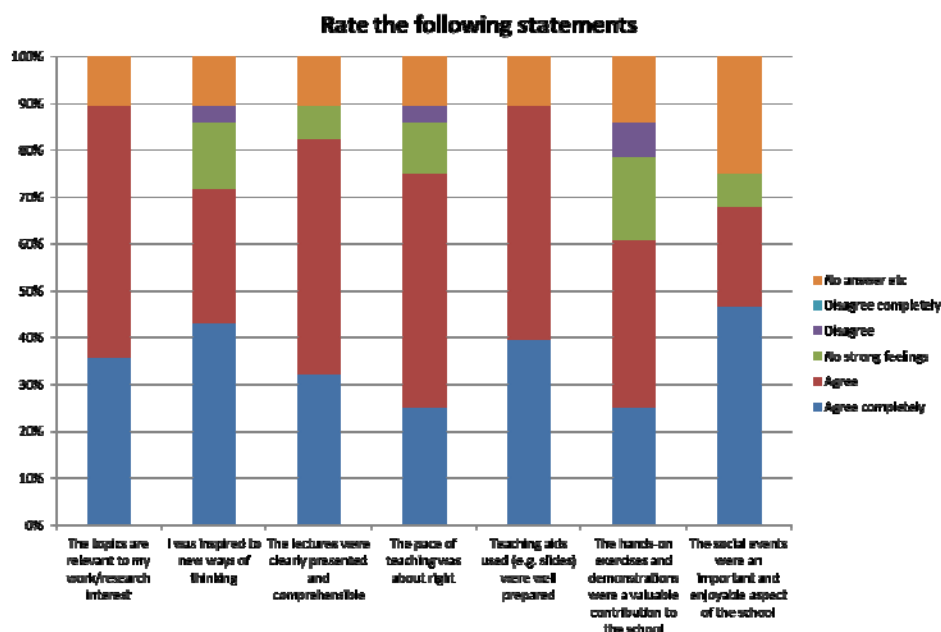


Figure 13: PRACE Spring School 2013 feedback - agreement with various statements

The overall impression from the feedback forms are that the participants were very satisfied with the school, especially the two first days, which was about the Intel Xeon Phi, received several positive comments. A couple of participants thought that the hands-on were lacking in explanation and wanted more feedback on the exercises.

8.6.5 Conclusions and lessons learnt

One thing is to think about the length of the school, maybe four days is a bit long especially if the hosting city is far to the north (travelling home after the school could take some time). Another point is in order to be able to provide better feedback on the hands-on the number of students must not be too many (or you have to increase the number of tutors).

8.7 PRACE Summer School 2013, Ostrava, Czech Rep.

8.7.1 Basic information about the event

Name: PRACE Summer School 2012 on Frameworks for Scientific Computing on Supercomputers

Dates: 17 - 21 June 2013

Location: Ostrava, Czech Republic

Organising sites: VŠB-Technical University of Ostrava and IT4Innovations Centre of Excellence, Czech Republic

8.7.2 Organisational details

Local organising committee

Name	Function
O. Jakl	chair and overall coordination
D. Horák	deputy, technical organization
K. Pešatová	dissemination and media, technical organization (coordinator)

Name	Function
A. Němcová	accounting
D. Hrbáč	computing resources
V. Hapla	tutor's contact
M. Merta	tutor's contact
M. Stachoň	tutor's contact
V. Vondrák	head of the local PRACE team

Figure 14: Local organising committee of the PRACE Summer School 2013

Venue

The PRACE Summer School 2013 took place in the Lower area of Vítkovice, Ostrava (<http://www.dolniblastvitkovice.cz/default/index/index/lang/en/site/56>), more precisely in its multifunction auditorium Gong. We gave precedence to the Lower area of Vítkovice over some conventional university environment because of the uniqueness of this place and high standards it provides: As a national cultural monument, it tells the story of the heavy industry (mining and metallurgy) characteristic for Ostrava and its region, in an extent hardly to be found elsewhere. At the same time, Gong, a former gasholder, is a perfect example how this precious industrial heritage is being transformed to a modern cultural and educational site. That immense construction was converted to an architecturally impressive convention centre prepared to host conferences, concerts, workshops and exhibitions. The School made use of one of its smaller, nevertheless spacious halls, suitable for up to 80 participants, offering flexible partitioning, full multimedia equipment, air conditioning, wireless connectivity and other modern features. Moreover, the venue is located very close to the centre of Ostrava with hotels of different standards available for participants. Also after the event we consider the choice of the Lower area of Vítkovice and Gong in particular for the venue of the PRACE Summer School 2013 as very appropriate, as it fulfilled all our expectations and enriched the participants with unusual experience (e.g. visit of the blast furnace – c.f. the School's programme and social events).

8.7.3 Programme & content

Programme committee

Name	Affiliation, Country
D. Horák	VŠB-TUO & IT4Innovations, Czech Rep.
V. Hapla	VŠB-TUO & IT4Innovations, Czech Rep.
M. Merta	VŠB-TUO & IT4Innovations, Czech Rep.
T. Karásek	VŠB-TUO & IT4Innovations, Czech Rep.
V. Vondrák	VŠB-TUO & IT4Innovations, Czech Rep.
S. Wong	ICHEC, Ireland

Table 29: Programme committee of the PRACE Summer School 2013

Final programme

The full programme of the school is available at:

<http://events.prace-ri.eu/conferenceTimeTable.py?confId=140#all>

List of trainers

Name	Affiliation, Country	Subject/expertise
Jed Brown	Argonne National Laboratory, USA	PETSc
Mathieu Faverge	INRIA Bordeaux, France	Magma & Plasma
Tomáš Karásek	VŠB-TUO & IT4Innovations, Czech Rep.	Paraview
Benjamin Kirk	NASA Lyndon B. Johnson Space Center, USA	libMesh
Nico Schlömer	Technical University of Berlin, Germany	Trilinos

Table 30: List of trainers at the PRACE Summer School 2013

Designing the programme

The Programme committee decided to focus the School on the “Frameworks for Scientific Computing on Supercomputers”, in accordance with the scientific interests of the hosting IT4Innovations Centre. In this context, the aim, reflected in the programme design, was to acquaint the students (scientists and developers who wish to use high-level tools but at the same time require fine-grain control over the solution process) with a set of high-quality and open-source tools suitable for solving large-scale engineering and scientific problems on high performance computing systems. This set was “complete” in the sense that it covered the whole "life cycle" of such projects: preprocessing, solution and postprocessing. However, the focus was on the solution phase (PETSc, Trilinos). We also wanted to reflect the advances in the computer architectures and their impact on the numerical libraries (Magma & Plasma). In general, our effort was to invite outstanding specialists as trainers, preferably leaders or members of the tool/library developer teams.

Description of the content

The School started with a short introduction covering its programme, organization, venue, hosting institution and PRACE presented by local organisers. The first tutorial addressed preprocessing and introduced libMesh, a library for the numerical simulation of partial differential equations using arbitrary unstructured and adaptive discretisations on serial and parallel platforms. The second and third days were devoted to the solution of the arising linear systems through the PETSc or Trilinos frameworks, which provide building blocks for the development of parallel and scalable applications for the solution of partial differential equations. The fourth day offered a more in-depth coverage of linear algebra algorithms for emerging computer architectures (multicore, GPU, heterogeneous, hybrid), as they are being developed in the Plasma and Magma projects at the Innovative Computing Laboratory of the University of Tennessee. The last day, devoted to postprocessing, delivered a tutorial on ParaView, a highly respected data analysis and visualization tool designed to run on massively parallel platforms. To get the most out of the School, all lectures were accompanied by hands-on exercises ("labs") carried out on a supercomputer.

The contents of the tutorials can be characterised as follows:

- **libMesh:** This tutorial covered the fundamental design principles and usage of the libMesh finite element library. Key data structures and algorithms were presented, along with a series of example programs of increasing complexity. Domain discretization, finite element approximation, and adaptive solution strategies were discussed for a range of physical applications. Implementation examples demonstrated the hybrid multilevel parallel capabilities of the software library. Interfaces to high-

quality external software packages, such as PETSc and Trilinos, are key components of the libMesh functionality and were also highlighted.

- **PETSc:** The tutorial presented scalable linear and nonlinear solver methodology within the context of the Portable Extensible Toolkit for Scientific computing (PETSc). It covered the underlying principles of Krylov, domain decomposition, and multigrid methods, as well as field-split methods for coupled multiphysics problems. Throughout the tutorial, library interfaces were presented, along with opportunities for solver composition, convergence diagnostics, and performance considerations for modern hardware.
- **Trilinos:** This tutorial made the students familiar with the high-performance numerical toolkit Trilinos. They got insight into the core capabilities of Trilinos and some of its more than 50 packages, covering almost every aspect of numerical computation. On the low level, data organization and the architecture of Trilinos were discussed. On a higher level, numerical methods such as Krylov and LU solvers for linear problems, nonlinear solvers, optimization packages, multigrid preconditioners, and discretization capabilities were introduced.
- **Magma & Plasma:** This tutorial presented libraries developed by ICL to optimise the solution of large dense linear problems on today's heterogeneous parallel computer architectures. The course started with revision on dense linear algebra algorithms. Later the Plasma library, targeting shared memory multi-core architectures, was presented, including the dataflow programming model. Then, as the main interest nowadays is in accelerators, the Magma library and the development of GPU kernels was focused on. Finally, the students learned how to extend those libraries to distributed heterogeneous environment thanks to the PaRSEC runtime.
- **Paraview:** In this half-day tutorial the visualization tool ParaView was introduced, mostly on examples. Basic structure and usage of ParaView were covered, including key data structures and basic functions for visualization of large data sets. Different visualization concepts such as isosurfaces, streamlines and glyphs on different data types such as structured grids, unstructured grids and polygonal data were presented to give feel and taste of the ParaView's capabilities. A short introduction to the parallel features of ParaView was also attached.

Computer resources

Although the School has been shifted to the latest possible term, the organization was partially endangered by the delayed installation and deployment of the new IT4Innovation's supercomputer. That is why we asked the PRACE Advanced Training Centres to provide the School with some backup machine. It was Francesco Falciano from Italy, who helped a lot in this respect and arranged access for the tutors and students to the CINECA's PLX cluster. Thus, the use of the computing facilities during the School was as follows:

- **Anselm (IT4Innovation/VŠB-TUO):** This newly installed Bull cluster was the main computing resource, especially for the libMesh and PETSc tutorials. After intensive preparatory work of the organisers and Anselm's administrators this platform could meet very well the requirements of the School.
- **PLX cluster (CINECA):** This machine was employed for some comparisons during the Magma & Plasma tutorial (GPU accelerators).
- **Participants' laptops:** We experienced insufficient performance with graphically demanding applications on remote machines. That is why especially for ParaView the students were recommended to perform local installation of the software before the tutorial. Local installation was the preferred choice also for Trilinos.

Networking and Internet connection in Gong was realised through a dedicated local wireless infrastructure. Despite of some drop-outs the connectivity was sufficient for the purposes of the School.

8.7.4 *Participants & feedback*

Number of participants by country

Country	Number of participants
Bulgaria	2
Czech Republic	31
Denmark	5
France	2
Germany	2
Ireland	3
Italy	1
Poland	1
Slovakia	1
USA	2
Total	50

Table 31: Number of participants by country at the PRACE Summer School 2013

Process for selecting the participants

During the registration, the applicants were asked to provide quite a lot of information about their motivation and background to attend the School, so we were prepared to perform a rigorous selection procedure, if necessary. However, the number of registered people was within reasonable limits, so we were able to accept all candidates (except 1-2 persons not fulfilling elementary criteria). Moreover, for those who might not be able to attend the School, an on-line video transmission from the event was available.

Statistics and analysis of the feedback survey

22 participants provided feedback for the school. On average, the respondents gave the school an overall rating of 8.5 out of 10 (0: worst, 10:best). 82% of the respondents considered the overall organisation of the School at least good (64% excellent). In particular the venue and catering, and also social events were highly appreciated. On the contrary, one critical remark mentions lack of (web) information related to the School. As far as the tutorials themselves is concerned, the respondents were also very positive, there are only rare (not more than 2) negative marks among the responses to the individual questions. With respect to the complexity of the objects of study (e.g. Trilinos as such could saturate the whole School extent), this seems to be a good result.

8.7.5 *Conclusions and lessons learnt*

The organisers share a positive feeling after the School. On one hand, the preparations were considerably more demanding than we expected at the beginning. On the other hand, this challenge brought up a team of collaborators that proved to be competent to organise international educational events. We believe that we have done a good job for PRACE, but also for IT4Innovations: Not only because the School accelerated the deployment of the new

Anselm cluster, but with progressing computer capacities it urgently needs to develop local training programme in HPC. The PRACE Summer School 2013 paved the way to achieve this goal.

8.8 PRACE Tier-1 Workshop 2011, Amsterdam, The Netherlands

8.8.1 Basic information about the event

Name: PRACE Tier-1 Workshop

Dates: 29 - 30 November 2011

Location: Amsterdam, The Netherlands

Organising sites: SARA

8.8.2 Organisational details

Local organising committee

- Wim Rijks (SARA)

Venue

The facilities at SARA were chosen to host this event as (a) their location is conveniently accessible by the majority of the target audience, i.e. PRACE Tier-1 users, and (b) that SARA had the appropriate facilities to host this event such as rooms and audiovisual equipment, and (c) they were able to make their facilities available on short notice, as the event was aimed to coincide shortly after the DECI-7 call awards were announced.

8.8.3 Programme & content

Programme committee

Name	Affiliation, Country
David Henty	EPCC, UK
Ioannis Liabotis	GRNET, Greece
Simon Wong	ICHEC, Ireland

Table 32: Programme committee of the PRACE Tier-1 Workshop 2011

Final programme

29 November 2011

12:30 - 13:30 Reception and Lunch

13:30 - 13:45 Welcome and Introduction to SARA (Axel Berg)

13:45 - 14:30 PRACE hardware, software and services (David Henty)

14:30 - 15:30 Use of Certificates, Using gsi-ssh and gridftp (Cerlane Leong)

15:30 - 16:00 Coffee Break

16:00 - 17:30 Hands on session (practical examples)

17:30 CLOSE

20:00 Dinner for all participants

30 November 2011

09:30 - 10:15 PRACE support for the accepted DECI projects (Lilit Axner)
 10:15 - 10:30 Remote Visualization (Paul Melis)
 10:30 - 11:00 Hands on Sessions (users' own application codes)
 11:00 - 11:30 Coffee Break
 11:30 - 12:30 Hands on Sessions (users' own application codes)
 12:30 - 13:30 Lunch
 13:30 - 15:30 One-to-one sessions (optional)
 15:30 CLOSE

Table 33: Final programme of the PRACE Tier-1 Workshop 2011**List of trainers**

Name	Affiliation, Country
Lilit Axner	KTH, Sweden
David Henty	EPCC, UK
Cerlane Leong	JSC, Germany
Paul Melis	SARA, the Netherlands

Table 34: List of trainers at the PRACE Tier-1 Workshop 2011**Designing the programme**

The programme was designed to provide practical guidelines and experience on utilising various European Tier-1 systems through DECI, highlighting the hardware, software, services and support that are available. There was a heavy emphasis on the hands-on sessions where participants had the opportunity to implement codes, including their own, on target architectures with the assistance of PRACE staff. Grid certificates and their use in facilitating data transfer was also covered.

Description of the content

The first day of the event was aimed to give a brief overview of PRACE Tier-1 systems, followed by practical tutorials on how Tier-1 users may gain access to their target machines, avail of tools/services (e.g. data transfer) using certificates, and be able to implement example codes. The second day focuses on PRACE support for Tier-1 projects and remote visualisation tools; this was then followed by hands-on sessions where participants are encouraged to implement their own or other codes on their target systems.

Computer resources

Since this event required that participants log into their target machines/architectures, there was a coordinated effort with several Tier-1 partners to ensure that participants, many of whom are new Tier-1 users who had never logged into their target machines, were able to successfully log in and carry out practical exercises (e.g. submission of test jobs).

8.8.4 *Participants & feedback*

Number of participants by country

Country	Number of participants
Finland	2
France	3
Germany	3
Greece	1
Hungary	1
Italy	1
Portugal	2
Serbia	2
Spain	2
Sweden	1
Switzerland	1
Total	19

Table 35: Number of participants by country at the PRACE Tier-1 Workshop 2011

Process for selecting the participants

No selection process was required as the venue was able to accommodate everyone who had applied.

Statistics and analysis of the feedback

A total of 16 (84%) of the participants provided feedback responses. Overall, they have given the school a rating of 7.3 (0 = worst; 10 = best), which is a somewhat acceptable score. While there is still general agreement that the hands-on components were valuable contributions to the workshop, the extent to which this is reflected in the feedback is perhaps not as pronounced as seen in other PRACE training events. This may be explained by a lack of time to focus on specific architectures (as expressed by one participant as free text comment), and/or the fact that the hands-on component in this workshop was more dependent on the participants to bring their own code to the event.

8.8.5 *Conclusions and lessons learnt*

The event was very successful in attracting 14 PRACE Tier-1 users, or 74% of the participants, to come from 11 European countries to attend this event (a number of travel subsidies were provided). Many participants, i.e. the Tier-1 users, found it useful to have the opportunity to gain hands-on experience on their target system architectures.

It took a lot of effort to organise access and adapt/test exercises on many different target systems, it was also mentioned in the feedback responses that more time be devoted on specific architectures. Hence in future it may be more advisable to organise multiple events each focused on different HPC architectures, and invite different cohorts of Tier-1 users to such courses.

8.9 PRACE Scientific Workshop 2012, Coimbra, Portugal

8.9.1 Basic information about the event

Name: PRACE@COIMBRA 2012

Dates: 4 - 5 October 2012

Location: Coimbra, Portugal

Organising sites: UC-LCA, Portugal

8.9.2 Organisational details

Local organising committee

- Myrta Grüning (Universidade de Coimbra)
- Fernando Nogueira (Universidade de Coimbra)
- Pedro Vieira Alberto (Universidade de Coimbra)

Venue

Physics Department of the University of Coimbra. The University of Coimbra (UC) is one of the oldest universities in Europe and has been a pioneer in Portugal in deploying HPC systems for use in scientific research, namely in condensed matter physics and high energy physics. In those and other domains there are strong international connections with similar groups developing and/or using scientific applications for HPC systems. Today UC is a reference in Portugal as far as HPC services and usage are concerned, and is Portugal's representative in PRACE. The opportunity for a PRACE training event presented itself when UC organised the 17th ETSF Workshop on Electronic Excitations (<http://www.tddft.org/ETSF2012/>), thus providing an excellent opportunity to interface with a community of scientists who are also experts in computer simulations in their field of expertise.

8.9.3 Programme & content

Programme committee

Name	Affiliation, Country
Myrta Grüning	Universidade de Coimbra, Portugal
Fernando Nogueira	Universidade de Coimbra, Portugal
Pedro Vieira Alberto	Universidade de Coimbra, Portugal

Table 36: Programme committee of PRACE@COIMBRA 2012

Final programme

October 4, 2012

11:00 Overview of the PGAS programming model (Montse Farreras)
 11:15 Programming in Unified Parallel C – Introduction (Montse Farreras)
 12:30 Lunch break
 14:30 Hands-On session (Montse Farreras)
 16:30 Scalability and performance considerations (Montse Farreras)

17:15 Conclusions (Montse Farreras)	
<u>October 5, 2012</u>	
14:30	PRACE presentation (Pedro Alberto)
14:45	Accelerated QE-PWscf code for hybrid system equipped with NVIDIA GPU: development experience and performance analysis (Ivan Girotto)
15:15	Bluegene/Q for material science. First experiences with FERMI (Fabio Affinito)
15:45	High performance computing with Abinit and Bigdft: performance analysis and code refactoring within the PRACE project (Matteo Giantomassi)

Table 37: Final programme of PRACE@COIMBRA 2012

List of trainers

Name	Affiliation, Country	Subject/expertise
Fabio Affinito	CINECA, Italy	HPC for scientific applications
Montse Farreras	BSC, Spain	Programming models, UPC
Matteo Giantomassi	Université Catholique de Louvain, Belgium	HPC, ab-initio simulations
Ivan Girotto	International Centre for Theoretical Physics, Italy	HPC for scientific applications

Table 38: List of trainers at PRACE@COIMBRA 2012

Designing the programme

The UPC course was thought out based on the previous experience of the trainer (Montse Farreras) which suggested its contents and schedule. The contents and lecturers of the PRACE session in the ETSF meeting were designed based on the particular interests of the audience of the workshop, which are concerned mainly with condensed matter/material science codes, including porting, tuning and performance issues in HPC systems and using accelerators like GPGPUs with those codes.

Computer resources

The computer resources used for the event, namely the UPC course, were desktops (iMacs) in a classroom at the Physics Department in the UC. They were sufficient for the course purpose.

8.9.4 Participants & feedback

Number of participants by country

UPC course

Country	Number of participants
Portugal	17
Total	17

Table 39: Number of participants by country at the UPC course of PRACE@COIMBRA 2012

ETSF Workshop

Country	Number of participants
Austria	1
Belgium	24
France	24
Germany	16
Italy	14
Japan	1
Luxembourg	1
Portugal	7
Spain	9
Sweden	3
United Kingdom	2
USA	1
Total	103

Table 40: Number of participants by country at the ETSF Workshop of PRACE@COIMBRA 2012

Process for selecting the participants

Not applicable; there was no requirement for a selection process.

Statistics and analysis of the feedback

The main comments were very positive about the UPC course, both for the material presented, the way it was presented, and the interest of the course. Most participants expressed the desire that such events could be done again.

Regarding the PRACE session “High Performance Computing for ab-initio Condensed Matter Physics” at the ETSF meeting, in spite of the fact there was no survey at the end, some private discussions with scientists in the audience after PRACE talks were in general very positive regarding the contents and usefulness of this kind of interaction between PRACE collaborators and members of this particular scientific community.

8.9.5 *Conclusions and lessons learnt*

We believe both events were very successful.

In the case of the UPC course, more than 30 people had registered, but unfortunately there was a strike by workers of the Portuguese railroad company on the day of the course, which prevented many registered people to participate. More than half of the participants were university students. As explained above, the feedback from the course was very positive and people expressed the wish that it may be repeated in the future.

In the case of the ETSF workshop, again as mentioned above, we had also a positive feedback, with the added value that in this case there was a interaction with a particular scientific community from condensed matter/material science, which is not so common in PRACE. We believe that this particular kind of events, focusing not so much on training, but providing useful interactions between PRACE experts and developers of scientific applications from a particular scientific community, should be promoted by PRACE in a regular basis. This would improve PRACE ties with European scientific communities who are

or can be users of PRACE systems. For instance, these interactions may help them to enhance the applications they develop, either by tuning or scaling them to high end PRACE supercomputers, thus, in the end, making these communities more competitive scientifically worldwide.