SEVENTH FRAMEWORK PROGRAMME
Research Infrastructures

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

PRACE-1IP

PRACE First Implementation Project

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Final Training Report
Final

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Table of Contents

List of Figures

List of Tables

References and Applicable Documents

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List of Acronyms and Abbreviations

BSC	Barcelona Supercomputing Center (Spain)
CaSToRC	Computation-based Science and Technology Research Center (Cyprus)
CEA	Commissariat à l'Energie Atomique (represented in PRACE by GENCI, France)
CINECA	Consorzio Interuniversitario, the largest Italian computing centre (Italy)
CSC	Finnish IT Centre for Science (Finland)
CSCS	The Swiss National Supercomputing Centre (represented in PRACE by ETHZ, Switzerland)
CUDA	Compute Unified Device Architecture (NVIDIA)
EPCC	Edinburgh Parallel Computing Centre (represented in PRACE by EPSRC, United Kingdom)
EPSRC	The Engineering and Physical Sciences Research Council (United Kingdom)
DEISA	Distributed European Infrastructure for Supercomputing Applications. EU project by leading national HPC centres.
GENCI	Grand Equipement National de Calcul Intensif (France)
GPU	Graphics Processing Unit
GRNET	Greek Research and Technology Network (Greece)

HPC	High Performance Computing; Computing at a high performance level at any given time; often used synonym with Supercomputing
HP-SEE	High-Performance Computing Infrastructure for South East Europe's Research Communities, an FP7 funded project
ICHEC	Irish Center for High-End Computing (Ireland)
KTH	Kungliga Tekniska Högskolan (represented in PRACE by SNIC, Sweden)
LinkSCEEM	Linking Scientific Computing in Europe and the Eastern Mediterranean, an FP7 Capacities funded project
MPI	Message Passing Interface
NCSA	National Centre for Supercomputing Applications (Bulgaria)
OpenCL	Open Computing Language
OpenMP	Open Multi-Processing
PATC	PRACE Advanced Training Centre
PGAS	Partitioned Global Address Space
PRACE	Partnership for Advanced Computing in Europe; Project Acronym
PSNC	Poznan Supercomputing and Networking Centre (Poland)
RZG	Rechenzentrum Garching (Germany)
SNIC	Swedish National Infrastructure for Computing (Sweden)
Tier-0	Denotes the apex of a conceptual pyramid of HPC systems. In this context the Supercomputing Research Infrastructure would host the Tier-0 systems; national or topical HPC centres would constitute Tier-1
VSB	Technical University of Ostrava (Czech Republic)
WP	Work Package

Executive Summary

This deliverable summarises the activities of the PRACE First Implementation Phase (PRACE-1IP) training programme - that is the task 3.2 in Work Package 3: 'Dissemination and Training' - during the project months 1 to 24 (July 2010 to June 2012), focusing on the latter half (months 12 to 24), the first half being described in an earlier deliverable (D3.2.2). The activities comprised the organisation and delivery of eleven large training events; the implementation of the PRACE Training Portal (an Internet hub in computational science training and education); and the groundwork involved with setting up the PRACE Advanced Training Centres.

The programme has been a great success and has had a major impact on the HPC skill level of European researchers. The training events addressed contemporary topics in high-performance computing, attracted international audiences, and received excellent feedback ratings from the participants. The online Training Portal was established, and its development continues in the subsequent PRACE Implementation Phase projects. The model for the PRACE Advanced Training Centres devised in this task has been put into practice by the PRACE-2IP project.

1 Introduction

Scientists utilizing high-performance computing (HPC) in their research need to harness the massive parallelism of computing architectures of today containing tens to hundreds of thousands of computational cores. This is of course highly nontrivial, but unavoidable for researchers who wish to gain a competitive edge from high-end computing. A comprehensive training and education programme is thus crucial for maximizing the impact of the PRACE research infrastructure [1].

The role of the training task in the PRACE first implementation phase (PRACE-1IP) project was to provide Europe with world-class HPC training and to establish best practices for pan-European HPC training in the future. The task was a part of the PRACE-1IP Work Package (WP) 3: 'Dissemination and Training'. The plan for the training program was published as the deliverable D3.2.1 [2] at the beginning of the PRACE-1IP project.

This report is a retrospect on the activities and accomplishments of the training task during the second half of the phase (months 12 to 24 of the project, or June 2011 to June 2012) as well as on the success of the programme as a whole. The realized initiatives range from traditional face-to-face training events, which we describe in Section 2, to the establishment of an online training portal, which is discussed in Section 3. Section 4 describes other activities, such as ambitions for educational outreach, and development of the concept of the "PRACE Advanced Training Centres", which have since been successfully implemented by the second implementation phase of PRACE. In Section 5 the coordination of work is described and in Section 6 we will compare the achievements to the plans set two years ago. Finally, detailed reports of each of the face-to-face events, authored by the respective organizing sites, are provided as annexes.

2 Face-to-face training events

2.1 Overview

The main cornerstone of the PRACE-1IP training programme was a series of eight seasonal schools addressing various topics and levels of HPC methodology. Special emphasis was put to topics related to scaling up codes to the Tier-0 level and other Tier-0 considerations. In addition to the seasonal schools, two discipline-specific workshops were organized, one in the first half and the other in the second half of the project. Furthermore, there was a special training event, the 2nd EU-US Summer School, organized in collaboration with the United States-based TeraGrid research infrastructure. This event was different in many respects to the PRACE-1IP seasonal school and is discussed separately. Detailed event reports are provided in the annexes of this document.

The target audience of the PRACE-1IP face-to-face training programme was European researchers working with computational sciences as well as the employees of PRACE partner supercomputing centres. The goal was to increase the awareness of the possibilities and challenges of large-scale HPC, and to improve the related set of programming and other skills. For the employees of the supercomputer facilities the series provided a chance to keep up with the latest developments in HPC and to meet the end users.

A full list of the events in the programme is presented in Table 1. The first four events of the list (indicated with grey colour) were documented in the First Training Report, D3.2.2 [3].

School	Time	Location	Organizer(s)
1st Autumn school	Oct 25-29, 2010	Barcelona, Spain	BSC
1st Winter school	Jan 24-27, 2011	Nicosia, Cyprus	CaSToRC & GRNET
1st Scientific seminar	Feb 20-22, 2011	Stockholm, Sweden	SNIC
1st Spring school	Mar 29-31, 2011	Edinburgh, UK	EPCC & ICHEC
EU-US Summer School	Aug 7-12, 2011	Lake Tahoe, USA	CSC, ICHEC, RZG[1]
1st Summer school	Aug 28-Sep 1, 2011	Espoo, Finland	CSC & SNIC
2nd Autumn school	Oct 25-27, 2011	Paris, France	GENCI
2nd Winter school	Feb 6-10, 2012	Bologna, Italy	CINECA
2nd Scientific seminar	Feb 17-18, 2012	Sofia, Bulgaria	NCSA
2nd Spring school	May 16-18, 2012	Cracow, Poland	PSNC & VSB
2nd Summer school	Jun 21-23, 2012	Lugano, Switzerland	CSCS

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

2.2 Seasonal schools

The series of seasonal schools aimed at addressing various competence levels from beginner to advanced, and focussed particularly on best practises in developing, optimizing an scaling applications to run on Tier-0 facilities.

[1] Contributing PRACE partners listed here. Most of the organization work was carried out by the TeraGrid project.

All but one of the seasonal schools were fully subscribed, and in some cases, a selection process had to be implemented due to oversubscription.

The geographic distribution of the participants in the seasonal schools is presented in Table 2. We provide for reference also the figures from the first three schools as documented in D3.2.2. The training events have attracted participants from nearly all PRACE member countries, but also from countries outside of PRACE. It is evident that most of the participants of a given school were from the hosting country or its neighbouring countries – this assumption was part of the underlying reasoning behind the geographical distribution of the schools – but the participation of students from external countries is very positive, as the events serve to promote PRACE and foster international collaboration and networking. Our target of having at maximum 50% of the participants from the hosting country [3] was met by the both Summer schools and the Winter school in 2012; the Spring School in 2012 had 59% of its participants from the hosting country.

Each of the schools had a slightly different theme or focussed on particular areas within the broader topic of contemporary HPC. The Summer School 2011 in Finland was focussed towards application optimization as well as the programmer's productivity. The Autumn School 2011 in France was GPU-centric, while the Winter School 2012 focussed on hybrid architectures other than GPU clusters. The Spring School 2012 addressed HPC application design and the use of frameworks and libraries. The Summer School 2012 focused on programming the novel Intel MIC architecture.

All of the schools gathered feedback from the participants using the same feedback form, for ease of analysis and comparison.[2] From the participant feedback it is obvious that the training schools were well organised and proceeded without serious incident. The high quality of practical arrangements and programme content is visible in the feedback. After the first training report the feedback survey form was augmented by a question regarding the social events of the schools. The average scores in response to the question "*Overall, how would you rate this school? [0 = waste of time, 10 = excellent]"* is one of the key metrics for our analysis. All eight schools received similar overall rating from the participants, with only the Autumn School 2011 receiving a slightly lower score. The distribution of individual ratings of the five last schools is presented in Figure 1, and the corresponding graph from the first three schools is provided in D3.2.2. The average scores are provided in the legend; as scores of less than five were not observed, the scale of the figure has been adjusted accordingly for the sake of clarity. The median score in all these events was 8 besides the Autumn School that had 7.

[2] The feedback from the Summer School 2012 was not included to this document since the school was concluded after the deadline of the document.

Country	Autumn 2010	Winter 2010	Spring 2011	Summer 2011	Autumn 2011	Winter 2012	Spring 2012	Summer 2012
Albania	0	3	0	0	0	0	0	0
Austria	0	0	0	0	0	0	0	2
Bulgaria	0	0	0	0	0	0	2	1
Croatia	0	1	0	0	0	1	0	0
Czech Rep.	3	0	6	7	0	2	13	0
Cyprus	0	18	2	0	0	0	0	0
Finland	0	0	3	15	1	0	0	0
France	0	1	0	0	6	2	0	0
Egypt	0	14	0	0	0	0	0	0
Greece	0	4	3	0	0	0	0	0
Germany	1	1	3	2	1	4	1	4
Ireland	0	0	7	2	0	1	0	0
Israel	0	3	0	0	0	0	1	0
Italy	1	0	3	1	2	19	0	1
Jordan	0	8	0	0	0	0	0	0
Lebanon	0	4	0	0	0	0	0	0
Makedonia	0	0	0	0	0	0	1	0
Netherlands	0	1	0	2	1	0	0	2
Norway	0	0	3	1	0	1	0	0
Poland	0	0	2	2	0	1	32	0
Romania	0	0	0	0	0	2	0	0
Saudi Arabia	0	1	0	0	0	0	0	0
Serbia	0	0	2	0	0	2	4	1
Slovenia	0	0	0	1	0	0	0	0
Spain	42	2	2	0	1	3	0	4
Switzerland	0	0	0	1	1	1	0	14
Sweden	1	0	0	0	0	1	0	0
Syria	0	1	0	0	0	0	0	0
Turkey	2	0	2	0	1	0	0	0
UK	1	1	33	1	0	0	0	1
USA	0	0	3	1	0	0	0	2
Total	**51**	**63**	**74**	**38**	**14**	**40**	**54**	**32**

Table 2: Number of participants per country in the seasonal schools

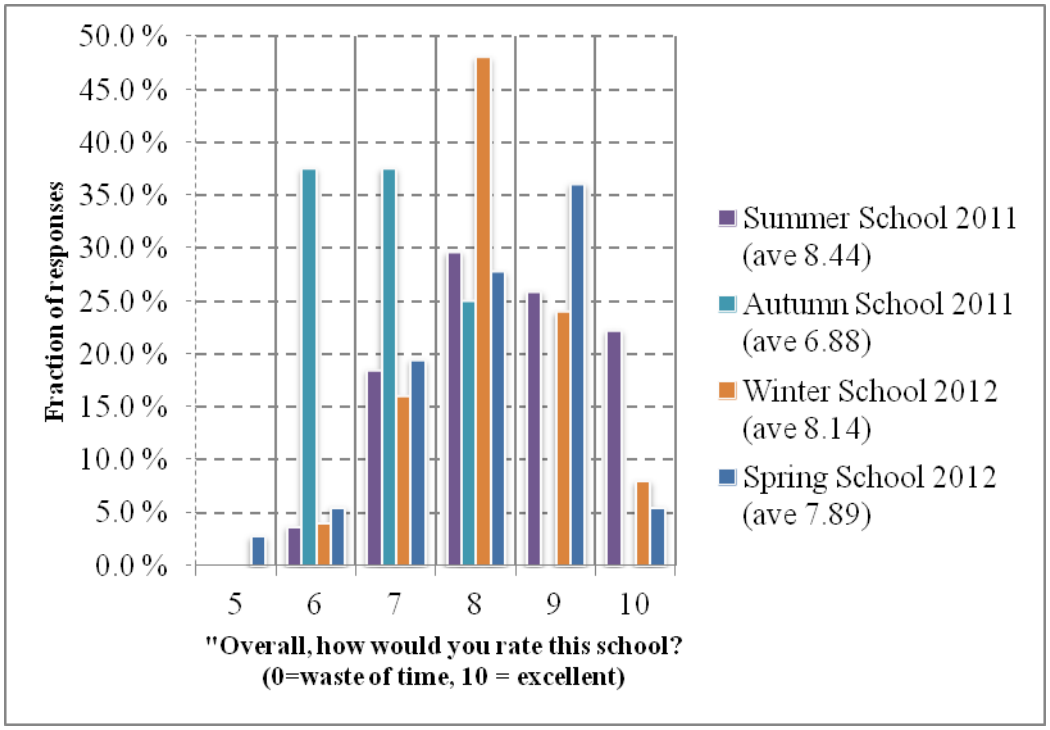


Figure 1: Overall impression scores for the seasonal schools in the second half of PRACE-1IP.

2.3 Scientific workshops & local training events

The PRACE-1IP training programme contained two scientific workshops targeted at specific domain science communities. The first workshop was held in Sweden and documented in D3.2.2. The second was held in Sofia, Bulgaria, and it focused on HPC approaches for life sciences and chemistry. This workshop had 55 participants, mostly from Bulgaria.

As described in the training plan, the training programme provided sites with the possibility to organize training events beyond the designated list of seasonal schools and workshops. The funding model was such that the organizers were able to utilize a small amount of PRACE-1IP WP3 person work, but no direct funding was provided. This opportunity was utilized in a large HPC training event held in Athens in July 2011. This event was organized in collaboration with the HP-SEE [4] and LinkSCEEM [5] projects. Also two six-day workshops, "Parallel programming with MPI on the BlueGene supercomputer and high-performance computer clusters" and "Applied software for programming the Bulgarian supercomputer" in Bulgaria during spring 2012 were organized with the help of PRACE-1IP WP3 funding. In addition, a lecture series "Supercomputer applications in natural sciences" was held in the University of Sofia, Bulgaria, during the academic year 2011-2012 with the help of this support. These training events and the lecture series are described in more detail in annexes 7.8-7.10.

2.4 EU-US Summer School

The second EU-US Summer School on HPC Challenges in Computational Sciences was held from 7-12 August 2011, at Lake Tahoe, California. In attendance were graduate students and postdocs from Europe and the United States, along with instructors and support staff from Europe and the United States. A total of 60 participants were selected from a total of 236 applications. The participants selected were from 17 different countries, and 30% were women. There were 26 instructors and support staff from diverse disciplines and backgrounds to provide a broad spectrum of HPC content as well as mentoring for the students.

The primary goal of the school was to extend the attendees' knowledge of high performance computing (HPC) and its applications in various fields of science and engineering. A secondary goal was to foster new collegial friendships and partnerships (nationally and internationally) among the presenters and attendees.

A survey conducted after the event showed that 90% of the attendees, and 100% of the presenters and support staff, considered the summer school to be excellent or very good.

3 PRACE Training Portal development

The PRACE Training Portal, a central location on the Internet for the delivery of high-quality HPC training materials and information about training opportunities, is an important aspect of the PRACE training program. The training portal was opened in autumn 2011 and its development and implementation was described in D3.1.5 [6].

To meet the training needs of the PRACE user community, the PRACE Training Portal will contain in time:

- Static training material, including video, audio and slides.
- A training opportunities calendar, which lists seminars, workshops and other events relating to HPC and computational science in Europe. This is accomplished by integrating the portal to the events.prace-ri.eu service based on the Indico software.
- Interactive training material, where progress can be monitored via tests or quizzes.
- Discussion forums for peer-to-peer discussion and problem solving.
- A blog, contributed to by multiple authors from PRACE sites.
- Regular news items on the state of the art in HPC technology.

Portal users have the ability to log in to the site to rate and comment on the training materials and blog entries. These features together with the discussion forum provide a dynamic framework to increase the social interactions both amongst the PRACE users themselves and between PRACE staff and their users.

The portal framework is based on open source web technologies (TYPO3 and WordPress) and is extensible such that additional functionality can be added as and when required. All partner sites are expected to contribute to the development of the portal contents. The development work for the portal is an ongoing task, currently led by task 4.3 of the PRACE-2IP project, and the portal will be offered to the PRACE AISBL as a candidate for permanent service after the PRACE-3IP project.

4 Other activities

4.1 Developing the concept of PRACE Advanced Training Centres

While planning the PRACE-1IP training programme, an idea emerged of setting up more permanent sites for HPC training. The concept and models for operation of these "PRACE Advanced Training Centres" (abbreviated as PATCs) were designed during the PRACE-1IP project, and the guidelines for the establishment of the PATCs, covering issues such as their management, business models and processes for hosting the centres and their locations were documented in the deliverable D3.2.3 [7].

The mission of the PATCs is to serve as European hubs of advanced, high-quality HPC training and education for researchers and students. The PATCs provide and coordinate training and education activities necessary to achieve the best utilisation of the PRACE research infrastructure by the community. The geographical locations of the PATC sites may and will vary over time, but the network itself is intended to be permanent. The long-term goal of the centres is to become the driver in European HPC education.

The PATC network has been successfully implemented by the task 4.2 of the PRACE-2IP project (this process has been documented in the deliverable D4.2 of PRACE-2IP [8]). Task 4.2 of PRACE-2IP will continue to coordinate the development of the PATC concept, task 4.1 of PRACE-3IP will produce the permanency plan for the PATCs, and the PRACE AISBL will take the control of PATCs during 2013.

4.2 Remote learning initiatives

Initiatives regarding remote learning, both in terms of virtual learning environments (e.g. Moodle) and webinars were observed to be less important in the survey of training needs carried out in the PRACE-2IP project. Therefore, all tasks related to remote learning were passed to the PRACE Advanced Training Centres to realize in the format and volume they consider the best.

4.3 Education outreach initiatives

The importance of reaching out to the secondary and tertiary education sectors was identified during the PRACE preparatory phase and stressed in the training plan for PRACE-1IP. However, these activities did not receive the attention they deserved during the PRACE-1IP project. The completed actions – one piloting event and a video for school classes – will be documented in a separate PRACE-1IP deliverable, D3.2.4 Education Outreach Report. The Education Outreach Report will also contain a more general discussion of best practices in education outreach, which will assist in planning these activities in latter PRACE projects and by the PRACE AISBL.

4.4 Training preparation checklist

During the course of work, it became necessary to set up more well-defined processes for PRACE training events organization to ensure good quality of the events. Committing to this checklist is a prerequisite for using the PRACE brand and resources for organizing a local training event. The list was devised by George Karagiannopoulos and Ioannis Liabotis.

This checklist presents the major points that the coordinators responsible for the PRACE schools and the on-site organizations should consider before, during, and after each training

event. These considerations ensure a well prepared and complete process for organizing training events. The upcoming PRACE events will follow a checklist based on this process.

A - Set the scope (6 months in before the event)

A1 - Design a detailed training plan

A2 - Agree upon the training title

A3 - Determine the training objectives

A4 - Identify the Target Audience

A5 - Propose a Date – Time & Duration

A6 - Propose a Location

A7 - Determine and take the approval from PRACE-2IP or 3IP WP4 leader of a rough estimation of the cost of training

B - Before the training event (6 months – 2 weeks before the event)

The following tasks should be completed before the training is held:

B1 – Set up committees and roles (6 months in advance)

- Assign a responsible person for the overall coordination of the training event.
- Training Programme Committee (this should contain at least one person from a PRACE partner other than the organizing country, e.g. from one of the PRACE Advanced Training Centres)
- Admission Committee
- Local Organizing Committee

B2 - Advertise the training event (6 months in advance)

- Design an efficient and effective advertising plan.
- Prepare a special website for the training event (overview of the event, registration page, the detailed program, useful links, and logistic information).
- Decide the recipients for advertisement emails.
- Send emails announcing the course and the dates. PRACE-2IP WP4 list should be informed so that other PRACE partners advertise the event.
- Discuss with PRACE press-team about making a press release on the event.

B3 – Event details (6 months in advance)

- Determine the course description
- Training Outline and structure
- Decide on the mixture of lectures and hands-on sessions
- Determine the Pre-requisites for accepting the applicants
- Decide upon the duration of the training event (3 days training course is necessary to cover the most important HPC topics according to the outcomes of the training survey)

B4 - Trainers (6 months in advance)

- Determine selection criteria for trainers (scientific skills, ability to communicate their knowledge to the audience).

- Consult PRACE trainer's database and consider also industrial trainers.
- Contact the wanted trainers and ensure availability.
- Collect necessary trainers documentation (resume, short biography, presentation outline etc).
- Arrange the travel details of the trainers.
- Review the training documents handouts and the PowerPoint presentation.

B5 - Audience (6 months in advance)

- Participants application process – create registration form
- Evaluation process of the training participants
- Consideration of possible special needs of the participants
- Create a final participants mailing list
- Prepare handouts for the training and arrange them into participant training kit – it is advised that training material (presentations etc) is given also in electronic form
- Prepare nametags for participants
- Prepare a sign-in form to verify attendance

B6 - Venue (6 months in advance)

- Search for the appropriate venue that will best facilitate the training
- Find and prepare public transportation details for the individuals
- Arrange the transportation for the foreign participants and trainers from the hotel to the venue, as well as from the venue to the social events
- Arrange lunch, refreshment/beverage arrangements, social events
- Prepare directions from key places (airport etc) for the venue
- Ask for a list of venue contacts for
    - Booking
    - Emergency
    - Technical issues
    - Maintenance
    - Security
- Ask for the training room to be available 1 hour before/ after the training

B7- Hotels (4 months in advance)

- Prepare of a possible list for the hotels
- Arrange the accommodation of all the participants by negotiating with the hotels for relevant discounted rates

B8 - Other actions (1-3 months in advance)

- Prepare of a questionnaire for collecting the trainees evaluation – the existing PRACE events evaluation form should be used
- Arrange for PRACE dissemination material to be delivered to the venue. Ask PRACE dissemination team for posters, brochures etc
- Prepare detailed event budget including all possible items that are to be paid for
- Get approval from WP4 on the estimated budget

C- During the training event

The following tasks should be completed during the training:

C1 - Identify actual participants. Count changes made for supplies, food arrangement, etc.

C2 - Room set-ups as specified by trainers are confirmed with facility coordinator.

C3 - All facility arrangements are completed and confirmed.

C4 - Participant names placed on name badges or name tents (as applicable).

C5 - All transferable equipment, supplies and materials are organized, boxed and transported to facility.

C6 - Load the presentations slides on the classroom computer.

C7 - Arrange that all presentations are online so that students have access to them.

C8 - Check the equipment to ensure that it is working properly. Check to ensure the slides can be seen clearly from the back of the room.

C9 - Registration table is set-up with necessary supplies.

C10 - Last considerations before the start

- Make sure all equipment, supplies, materials and room set-up is according to specifications.
- Check that everything is all right with catering

C11- Give and collect the evaluation form.

D - After the event (within 2 weeks after the event)

The following tasks should be completed after the training:

D1 – Training event debriefing

- Success, pitfalls, areas for improvement, suggestions for future training events

D2 - Completion of last remaining practicalities

- Payments to vendors of services and supplies
- Payment of expenses to trainers
- Return any borrowed material, equipment, etc

D3 - Upload all the presentation material on the website.

D4 - Process the outcomes of the feedback.

D5 - Prepare and send a thank-you note to participants, trainers and vendors.

D6 - Calculate the final cost of the training and inform WP4 leader about it.

D7 - Send a thank-you note to the people who contributed to the event.

D8 - Prepare training report for inclusion in PRACE deliverables.

5 Coordination of work

In the PRACE-1IP training task, work was coordinated based on progress reports, discussion and designated action points, and their review in regular video- or teleconferences. From the beginning of the PRACE-2IP project, i.e. for the period that this document describes, a training-specific videoconference was held every two weeks. This meeting discussed training topics from both the PRACE-1IP and PRACE-2IP projects. In general, the videoconferences were well attended and discussions were useful and lively.

Training topics were also discussed at the monthly PRACE-1IP WP3 all-hands teleconferences, at the PRACE-1IP all-hands meeting in Barcelona, and at the joint PRACE-1IP WP3 and PRACE-2IP Pillar 4 face-to-face meeting in Dublin.

6 Concluding remarks

Planning training activities two years in advance turned out to be a challenging task in this rapidly developing field of HPC. Despite this, the main considerations of the D3.2.1 Training Plan – the series of face-to-face training events, the Training Portal, and outlining the PATCs – were all completed successfully.

The deviations from the plan were mostly the following:

- The education outreach activities were not as pronounced as planned. In retrospect, it is clear that this activity should have been the responsibility of task 3.1 (dissemination) rather than task 3.2.
- The remote learning initiatives – providing webinars and real-time broadcasts of courses – were not realised in the volume envisaged. Only the Spring School 2012 was available online in real time, although the others were recorded for later reference. The lack of enthusiasm for these activities was very much due to the observation that the user demand for these services is not very pronounced [9].

Overall, the PRACE-1IP training programme can be considered as being completed very successfully. The training programme trained well over 500 scientists and without doubt had a major impact in the HPC skills among the research community. The training portal will very likely establish itself as an important service, and the plan for the PATCs was a valuable input for the PRACE-2IP project. The first PATCs are in operation and several PATC courses have already been presented.

Training and education activities play a crucial role in ensuring that the end-users of the PRACE infrastructure are able to fully exploit the strengths of existing and future high-performance computing hardware and software resources. This task has fulfilled the expectations set to it and the PRACE training programme will continue its important work in the latter PRACE phases.

7 Annex

7.1 Report on the first Summer School

Pekka Manninen

Name: PRACE Summer School – Taking the Most out of Supercomputers

Dates: August 28 to September 1, 2011

Location: Espoo, Finland

Organizers: CSC (Finland) and SNIC (Sweden)

Organizational details

Local organizing committee

Name	Institution
Pekka Manninen (chair)	CSC
Lilit Axner	SNIC-KTH
Anni Jakobsson	CSC
Tiina Timonen	CSC
Paula Pesonen	CSC

Venue

Premises of CSC in Keilaniemi, Espoo, Finland. The venue was selected for the good value in rental cost, existing IT infrastructure (laptops, workstations) and the availability of local processes for event organization. The day program was held in the venue, together with the poster session and welcoming drinks. Only the conference dinner was organized outside of the CSC premises.

Budgeting

The starting point for the event was to have world-class speakers; therefore quite a lot of the budget was reserved for travel expenses of the US-based speakers. In addition, we wanted to provide the attendees a memorable school and faultless organization. Therefore there were three social events with sufficient budgets. For these starting points, we were enforced to limit the number of attendees to 40.

The budget figures and realized expenses (VAT including) were as follows:

Expense	Budgeted	Actual
Speakers' travel & accommodation	3,805 €	4,569 €
Coffees & lunches (at CSC)	3,825 €	3,698 €
Social events	4,295 €	5,039 €
Venue rental & services (e.g. poster boards)	2,256 €	2,256 €
Video recordings	3,000 €	3,000 €
Total	17,181 €	18,562 €

Program & content

Program committee

Name	Institution
Pekka Manninen (chair)	CSC
Lilit Axner	SNIC-KTH
Jussi Enkovaara	CSC
Sebastian von Alfthan	CSC

Final programme

The final programme can be found at *http://www.csc.fi/courses/archive/prace-summer-school*

List of trainers

- Dr. Sebastian von Alfthan (FMI, Finland)
- Dr. Jussi Enkovaara (CSC, Finland)
- Prof. William Gropp (University of Illinois, USA)
- Dr. Sami Ilvonen (CSC, Finland)
- Prof. Lennart Johnsson (KTH, Sweden and University of Houston, USA)
- Prof. Erik Lindahl (Kunglika Tekniska Högskolan, Sweden)
- Prof. Kai Nordlund (University of Helsinki, Finland)
- Dr. Rolf Rabenseifner (HLRS, Germany)
- Prof. Kari Rummukainen (University of Helsinki, Finland)
- Prof. Jan Westerholm (Åbo Akademi University, Finland)
- Dr. Brian Wylie (FZJ, Germany)

Designing the program

The theme of the school, "taking the most out of supercomputers", was realised by having thorough tutorials on three important aspects associated with scaling codes: advanced message-passing interface (MPI) programming; hybrid MPI+OpenMP programming; and using CUDA+MPI to utilize supercomputers based on GPGPUs. These were supplemented with three shorter tutorials on using Python programming language in HPC, performance analysis with Scalasca software, and low-level code optimization. In addition to the tutorials combining lectures and hands-on exercises, the school provided four "scientific case" presentations (60 min each) on high-end supercomputing. In other words, we wanted to expose the participants to the most relevant skills in advanced HPC as well as to provide the scientific point-of-view through the scientific cases. The timetable was constructed such that the first day would begin at lunchtime and the last day would end at lunchtime to make it as convenient as possible for participants to reach Helsinki.

Description of the contents

Full contents can be found from the school page given above, and the video recordings are available through the PRACE Training Portal *http://www.prace-ri.eu/training*

Computer resources

The participants had accesses to Lindgren, a 300 Tflop/s Cray XT6 system at PDC, Sweden, as well as to Louhi, a 100 Tflop/s Cray XT4/XT5 system at CSC. Most of the participants used their own laptops to access these machines remotely. Participants who came without laptops were able to borrow them from CSC. The network speed of the auditorium was boosted for the event by several additional powerful wlan stations.

Participants & feedback

Number of participants by country

Country	Number of participants
Finland	15
Czech Republic	7
Germany	2
Netherlands	2
Ireland	2
Poland	2
Slovenia	1
UK	1
US	1
Italy	1
Spain	1
Switzerland	1
Norway	1
Total	38

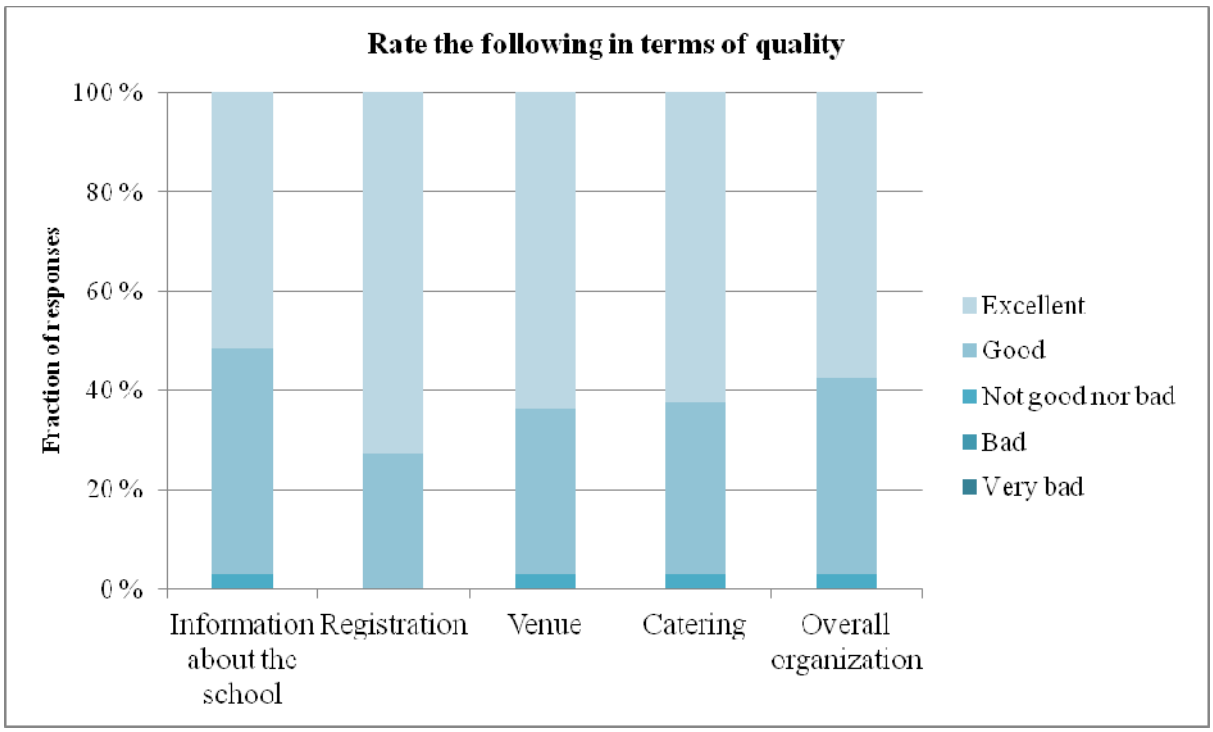
Table 3: Participants First Summer School

Process for selecting the participants

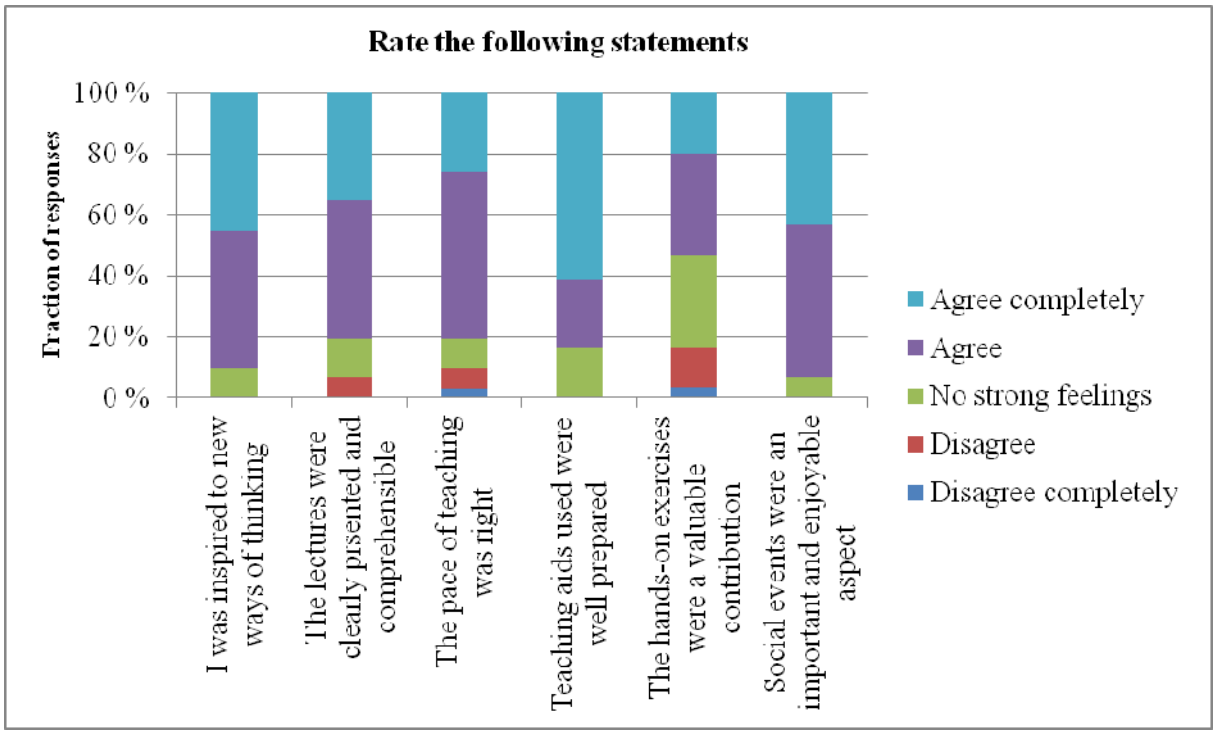
At the time of close of registration there were 62 applicants for the 40 places available. The main responsible persons from each organizing site (Pekka Manninen and Lilit Axner) independently assessed the participants and gave them ratings from 0 = "this school is definitely not for this person for many reasons" to 3 = "this applicant exactly fits the target audience". The final participant list was based on a score equal to the two rankings plus a possible 2 extra points for committing to bring a poster. The initial cut-off was a total score of 5, but as some cancellations occurred, in practice the cut-off went down to four points, yielding the final number of 38 participants.

Statistics of the feedback survey

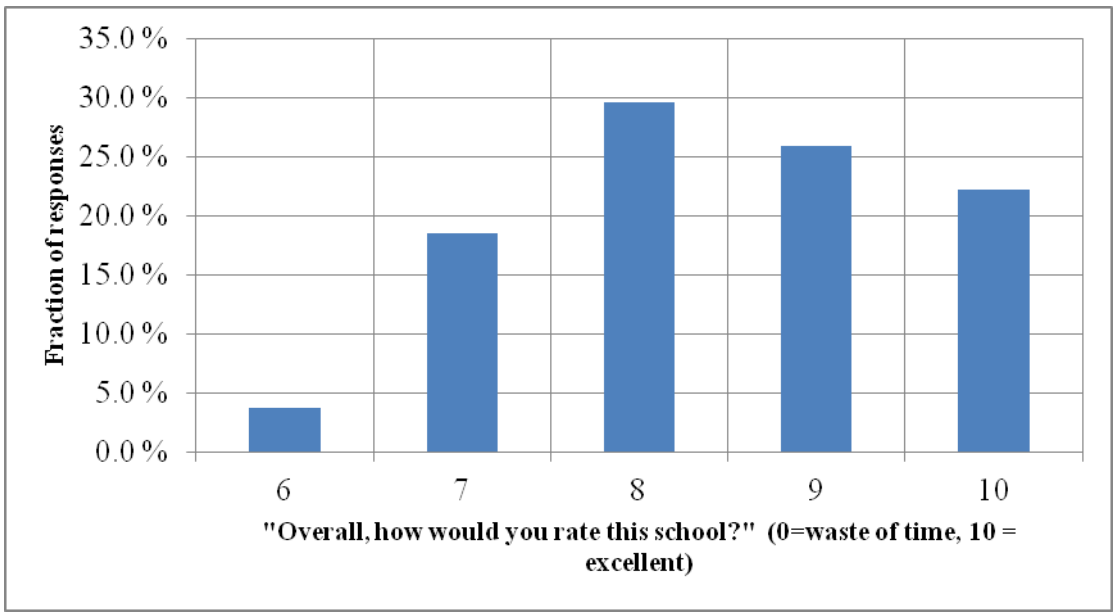
Participants' view on practical arrangements as an agreement with the question "please rate the following in terms of quality" (very bad / bad / not good nor bad / good / excellent):



Participants' view on the contents and delivery of the school as a response to the question "please rate the following statements" (statements given in the graph):



Finally, the distribution of the overall impression ratings of the event ("Overall, how would you rate this event? 0 = Waste of time, 10 = Excellent"). The average score was 8.44.



Analysis of the feedback

In general, the feedback was very good and the participants were very satisfied with the event, especially its arrangements. Indeed, there is very little to improve on with the arrangements, as all attendees rated all categories as 'good' or 'excellent', and over 50% of the participants rated overall organization as being excellent. From the content-related feedback (and from the free-text comments not reported here) it is visible that the program was designed too tightly: much more time should have been reserved for hands-on exercises.

Conclusions & lessons learned

The most important lessons learned belong to the planning stage. The schedule should have contained fewer speakers and topics, with more time to spend on each topic and especially the related hands-on exercises. A smaller number of speakers would also have provided savings in travel expenses: the budget was slightly exceeded, mostly due to unexpectedly large travel expenses from some of the speakers. The school itself was carried out very smoothly; hence there was little room for improvement in aspects related to local arrangements.

7.2 Report on the second Autumn School

Laetitia Baudin and Guillaume Colin de Verdière

The PRACE 2011 Autumn School has been held on 25-27 October in Bruyères-le-Châtel, France. The school was hosted at CEA's Very large Supercomputing Centre (TGCC) where CURIE, the French PRACE Tier-0 system, is located and operated.

This seasonal school has been organized by CEA, in link with GENCI.

Organizational details

Local organizing committee

Name	Affiliation	Responsibility
Guillaume Colin de Verdière	CEA	Program, lectures and hands-on
Patrick Allal	CEA	TGCC logistics
Laetitia Baudin	GENCI	General logistics (registration, rooms, catering…)

Venue

CEA's Very Large Supercomputing centre (TGCC) is a new "green infrastructure" for high computing performance, welcoming the CURIE supercomputer, funded by GENCI and being the French commitment in PRACE.

Located in Bruyères-le-Châtel, at 20 km from Paris, TGCC is especially designed to provide a communication and exhibition space for scientific events (conferences, seminars...).

During the 2011 fall semester, CURIE has been upgraded with a partition of x86 thin nodes, after being extended with a hybrid partition based on the latest NVIDIA M2090 GPUs. Altogether this has lead to a global peak performance of 2 Pflop/s.

CURIE hybrid partition, which has been opened to European scientists through PRACE preparatory access calls late 2011, is the first large scale hybrid system available into the PRACE Research Infrastructure.

The state-of-the-art technological environment provided by TGCC and the performances of CURIE led CEA and GENCI to welcome the PRACE Autumn School and propose a three-day training session focused on advanced hybrid programming, benefiting from the CURIE GPU partition for hands-on exercises. The students had the exceptional opportunity to be the first real users of this new addition to Curie.

Budgeting

As well as the other PRACE seasonal schools, the PRACE 2011 Autumn School was free of charge for PRACE country members, regarding accommodations and catering. Morning and afternoon coffees have been served as well as lunches and some of the evening caterings (welcoming drinks, refreshments and the dinner on the 26th evening).

The budget was spent on accommodations, transportation and catering in order to facilitate people's stay.

All the trainees were hosted in a unique hotel, Le Relais des Chartreux, where a dinner took place on the second day of the school, on the 26th of October.

A bus has been hired for transportation between the hotel and TGCC during the three-day session.

On the first evening (25th of October), an opportunity was given to visit or simply have a dinner in Paris.

An extra-night has been finally booked on the 24th of October.

Purpose	Company	Amount	Price
Accommodations and Dinner	Le Relais des Chartreux	31 rooms	€3901.80
Catering	Millessence		€1221.93
Transportation	Les Cars Jouquin	10 p.	€915
Total			**€6038.73**

Program and contents

Program Committee

Name	Affiliation
Guillaume Colin de Verdière	CEA
Stéphane Requena	GENCI
Sadaf Alam	CSCS
Eric Boyer	CINES

Final program

Tuesday, October 25th

Time table	Subject	Contents	Teacher
09.00 10.30	Introduction & methodology	What should be done to transform a C/Ftn code to get ready for hybrid programming	Guillaume Colin de Verdière (CEA)
Break			
11.00 13.00	Performance analysis	Understand a program behavior in order to get prepared to efficient hybrid programming	Jesus LABARTA and Judit GIMENEZ (BSC)
Lunch			
14.00 15.30	Performance analysis	[same]	Jesus LABARTA and Judit GIMENEZ (BSC)
Break			
16.00 17.30	Advanced OpenCL	How to get real performances out of an OpenCL code on CURIE	Julien DEMOUTH (NVIDIA)

Wednesday, October 26th

Time table	Subject	Contents	Teacher
09.00 10.30	Advanced OpenCL	How to get real performances out of an OpenCL code on CURIE	Julien DEMOUTH (NVIDIA)
Break			
11.00 13.00	Advanced OpenCL	[same]	Julien DEMOUTH (NVIDIA)
Lunch			
14.00 15.30	Debugging	[same]	Patrick Wohlschlegel (ALLINEA)
Break			
16.00 17.30	Debugging	Debug CUDA and MPI C code	Patrick Wohlschlegel (ALLINEA)

Work dinner (19.00 - 22.00)

Thursday, October 27th

Time table	Subject	Contents	Teacher
09.00 10.30	Advanced HMPP	Using pragmas is easy at the beginning on a simple code. Getting performance out of a large code can be tricky. It will require performance analysis (link to session 1) and debugging (session 3) as well as understand OpenCL (session 2) for this specific target.	Jean-Charles VASNIER (CAPS)
Break			
11.00 13.00	Advanced HMPP	[same]	Jean-Charles VASNIER (CAPS)
Lunch			
14.00 15.30	Advanced HMPP	[same]	Jean-Charles VASNIER (CAPS)
Break			
16.00 17.30	Preparing emerging systems	Investing in GPU development efforts would be useful for emerging systems (next 3-5 years).	Sadaf ALAM (CSCS)
	Wrap-up and adjournment		Guillaume Colin de Verdière

List of trainers

Name	Affiliation	Contact
Guillaume Colin de Verdière	CEA	guillaume.colin-de-verdiere@cea.fr
Jesus Labarta	BSC	jesus.labarta@bsc.es
Judit Gimenez	BSC	Judit.gimenez@bsc.es
Julien Demouth	NVIDIA	jdemouth@nvidia.com
Jean-Charles Vasnier	CAPS Entreprise	jvasnier@caps-entreprise.com
Patrick Wohlschlegel	ALLINEA	patrick@allinea.com
Sadaf Alam	CSCS	alam@cscs.ch

Designing the program

The program was designed based on the evolutions of users' needs. Many GPGPU schools for beginners are available (even within PRACE). CEA has hosted the first PRACE School on GPGPU back in 2009. In 2011, it was high time to design and implement a school on advanced topics, more related to real life problems of large code evolution.

The pattern used to actually build the school was to follow the process of code migration from a classical MPI version to a more modern highly optimized GPGPU code. Therefore you need to have a methodology, a good understanding of the current code's behavior, understand how to get performances out of the new programming languages and debug your first versions of the new code. The layout of the school was then straightforwardly set, taking into account teachers' availabilities.

Computer resources

The hands-on exercises have been successfully made on the hybrid partition of CURIE.

Participants and feedback

Number of participants by country

People coming from PRACE countries represent 57% of the trainees.

Country	Participants
Finland	1
France	6
Germany	1
Italy	2
Spain	1
Switzerland	1
Turkey	1
The Netherlands	1
Total	**14**

Process for selecting the participants

The PRACE Autumn School announcement has been released On August 30th, 2011.

Since the school was focused on advanced hybrid programming, when they register, people were asked to describe:

- their scientific background and current HPC skills,
- the scientific project they were working on,

- the project on which they will use the knowledge learned during the school.

On the basis of this information, and of TGCC security rules, the program committee has selected the trainees: 14 from around 20.

In link with PRACE-1IP/WP5, in charge of conceiving an industrial access to the PRACE resources, the PRACE 2011 Autumn School has also be opened, for the first time, to a French SME (Audionamix), an innovative technology company involved in the field of audio signal processing (see online: *http://www.audionamix.com*).

Statistics of the feedback survey

Only 6 answers were received, representing 43% of the trainees.

Level of expertise prior to attending the school

	Unskilled	Fair	Good	Excellent	No answer
HPC programming languages	0	0	2	4	0
Message-passing interface	0	1	3	2	0
Shared-memory parallel programming	1	3	1	1	0
Performance analysis	0	1	3	2	0
Code optimization techniques	0	0	6	0	0
Parallel program debugging	0	2	2	2	0
Next generation HPC prog. languages	4	1	1	0	0
Accelerator programming	2	3	1	0	0

Organization of the school

	Very bad	Bad	Not good Not bad	Good	Excellent	Don't know
Information about the school	1	0	1	4	0	0
Registration	0	0	1	3	2	0
Venue	1	0	1	4	0	0
Catering	0	1	0	4	1	0
Overall organization	1	0	0	5	0	0

Program and contents

	Disagree completely	Disagree	No strong feelings	Agree	Agree completely	Don't know
Relevant topics	0	0	0	3	3	0
Inspiring new ways of thinking	0	0	0	3	3	0
Clear and comprehensible lectures	0	0	1	3	2	0
Right pace of teaching	0	0	1	4	1	0
Well prepared teaching aids	0	0	0	3	3	0
Valuable contribution of hands-on	0	0	1	2	3	0

Conclusions and lessons learned

We were somewhat disappointed by the quite small number of applicants. One reason could be that we have advertised the school somewhat late; another one is probably the high level of the program we proposed. However, 14 students (even if we were ready to have 40 of them) is an ideal number to foster interactions with the different teachers as well as between students, yet still having a manageable group. Larger groups are less prone to such interactions.

The selection process of the trainees should be made stricter to maximize effectiveness of the seasonal schools. The levels of the attendees were too widespread. Some of them where real beginners and had nothing to do in this school. Globally speaking, the level of students was mixed and it was a difficulty for the management of the sessions.

The program of each school should be discussed amongst PRACE for a better coordination and homogeneity of the groups.

7.3 Report on the second Winter School

Marzia Rivi

Name: PRACE Winter School 2011

Dates: February 6-10, 2012

Location: CINECA, Bologna, Italy

Organizer: CINECA

Organizational details

Local organizing committee

- Marzia Rivi (CINECA)
- Silvia Giuliani (CINECA)
- Paola Alberigo (CINECA)

Venue

CINECA, this venue was chosen for its facilities: a classroom for 50 participants with network connectivity and microphone at each seat, equipped with a powerful projector and a system for streaming; access to the supercomputer PLX (an hybrid cluster GPU+CPU) for the training activities.

Budgeting

The expenses are based on 41 participants and 6 invited teachers. All participants had coffee breaks and lunches included as well as a social dinner on Thursday. The total expenses from the caterings and social event was 5441 euro. The speakers' travel expenses totalled 1952 euro. The amount of 3500 euro was allocated for grants provided to participants not funded by their institution and not coming from the Bologna area; their amount was 200 euro for Italian and 300 euro for non-Italian students. Finally, part of the budget was also used to advertise the event by printing and sending posters to universities and research institutes. The total amount of expenses is 10.892,42 EUR.

Program & content

Program committee

- Marzia Rivi (CINECA)
- Giovanni Erbacci (CINECA)
- Brian Wylie (JSC)
- Ivan Girotto (ICHEC)

Final program

See: *www.cineca.it/en/page/prace-winter-school-agenda*

List of trainers

Teacher	Affiliation	Topic
Giovanni Erbacci	CINECA, Italy	HPC architectures and parallel programming
Pascal Vezolle	IBM	IBM BlueGene/Q architecture
Carlo Cavazzoni	CINECA, Italy	Accelerator architectures (GPU,MIC)
Andrew Emerson	CINECA, Italy	Hybrid Cluster PLX
Mark Bull	EPCC, UK	OpenMP, OpenACC
Rolf Rabenseifner	HLRS, Germany	Hybrid programming MPI+OpenMP, MPI3
Brian Wylie	JSC, Germany	Debugging and profiling tools, Scalasca
Massimo Bernaschi	CNR, Italy	CUDA, hybrid programming MPI+CUDA
Mauro Bisson	CNR, Italy	CUDA, hybrid programming
Massimiliano Culpo	CINECA, Italy	Hybrid programming MPI+OpenMP
Filippo Spiga	ICHEC, Ireland	Hybrid programming MPI+OpenMP+CUDA

Designing the program

The main purpose of this event was to introduce participants to the emerging technologies and programming techniques on high performance computing. In particular, the school was focused on hybrid programming for the best exploitation of massively parallel architectures. Therefore, it was presented both some MPP architectures and some programming languages to be used together with MPI for the exploitation of such systems. In the schedule of this event, time was also dedicated to allow participants to do some practise on the CINECA hybrid cluster.

Description of the contents

Lectures were organized in three sections according to the following topics: architectures, programming languages and programming tools. The architectures presented were accelerators (Intel MIC, NVIDIA GPUs, FPGAs) and the new IBM system BlueGene/Q that will be provided by CINECA as PRACE Tier-0 system the next year. Then OpenMP and CUDA were introduced as well as their usage together with MPI. A brief introduction to OpenACC and the new features of MPI3 were also provided. Finally, an overview on profiling and debugging tools was presented with particular attention to Scalasca. Exercises were focused on MPI+OpenMP and MPI+CUDA programming.

Video presentations can be found at *http://streaming.cineca.it/winterschool/* and from the PRACE training portal.

Computer resources

Each student was given one month's access to CINECA's supercomputing system used for the exercise sessions, the largest public GPU cluster in Europe. It comprises 274 compute nodes, each containing 2 NVIDIA Tesla M2070 and 2 Intel(R) Xeon(R) Westmere six-core E5645 processors. Ethernet connectivity was available at every seat in addition to wireless access.

Participants & feedback

Number of participants by country

Country	Number of participants
Croatia	1
Czech Republic	2
France	2
Germany	4
Italy	19
Ireland	1
Norway	1
Poland	1
Romania	2
Serbia	2
Spain	3
Sweden	1
Switzerland	1
Total	**40**

Process for selecting the participants

The number of participants was limited to 40 students, selected according to their experience and qualifications. Knowledge of a high level programming language (C/C++ or FORTRAN) was required, as well as a working experience in parallel programming with MPI. The involvement in a computational project was also an added value.

Statistics 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 8.16 basing on answers from 25 participants. A separate survey using CINECA's own form was also carried out, with the following results, the scale being 1 – very poor, 2 – poor, 3 – insufficient, 4 – sufficient, 5 – fairly good, 6 – good, 7 – excellent; details of this evaluation are given below:

Question	Average	Number of answers
Task Achievement	5.65	31
Exercises	4.87	31
Facilities such as computer room, PC, etc..	5.9	31
Training materials	6.4	30
Usefulness of the topics for your daily activities	5.87	31
General evaluation	5.96	28

Analysis of the feedback

The feedback from the school supports the impression of a successful and well-organized school. Some comments are the following:

"Thank you very much for all support. I enjoyed a lot the school even if I was near to miss it due to the weather. I learned many things which are of real help in my research activity. I

enjoyed the most all the hand-on sessions and of course the slides were very well prepared. The presentations were also very good and clear."

"The very high level of the teacher positively impressed me. The school was a unique to deepen my expertise on such relevant matters. More attentions could be placed on the profiling techniques for hybrid parallel codes and in the practical way to assess the scalability of a given code, giving some suggestions to improve the code performance."

"Very good mixing of advanced topics, proper venue with good audio and video facilities, high international mix of attendants".

Conclusions & lessons learned

Since CINECA is not well connected to the city centre, we could consider for the future events the organization of a shuttle service. Moreover, we should dedicate more space for exercises.

7.4 Preliminary report on the second Spring School

Maciej Cytowski

Name: PRACE Spring School 2012 - "School for Developers of Petascale Applications"

Dates: 16-18 May 2012

Location: Cracow, Poland

Organizers: PSNC/ICM, University of Warsaw, Warsaw, Poland; PSNC/ACC CYFRONET AGH, Cracow, Poland; VSB-TUO, Ostrava, Czech Republic

Organizational details

Local organizing committee

Name	Institution
Maciej Cytowski	PSNC/ICM, University of Warsaw
Maciej Szpindler	PSNC/ICM, University of Warsaw
Łukasz Dutka	PSNC/ACC CYFRONET AGH
David Horák	VSB-TUO
Ondřej Jakl	VSB-TUO

Venue

The PRACE Spring School 2012 took place at the AGH Institute of Computer Science, ul. Kawiory 21, 30-055 Cracow (*http://www.ki.agh.edu.pl/en*).

The building of Institute of Computer Science is a brand new building with a special facility prepared to host large conferences and workshops. The building has an impressive architecture, and all facilities are brand new. The venue offered three good lecture rooms with full multimedia equipment and air conditioning.

The venue is located close to the center of Cracow. Additionally there is a wide range of hotels with different standards available for participants.

Cracow international airport has direct connections to many European cities. One of the speakers decided to arrive only for his presentation due to other important duties. He was able to organize his travel during one working day.

There were already 2 other successful PRACE events organized at AGH in Cracow (PRACE Cracow Code Porting Workshop, PRACE WP3 F2F meeting).

Budgeting

Main part of budget was consumed with catering for coffee and lunches. The total cost of catering service for three days of the school and 80 persons (participants and organizers) was approximately 4930 Euro.

There were two evening social events on Day 1 and Day 2 of the school. The first event was organized in the Bohema restaurant located near the Main Market Square in Cracow. The total cost of this event was approximately 1975 Euro. The second event was organized in the Le Scandale restaurant in Kazimierz district in Cracow. The total cost of this event was 1831 Euro.

Travel and accommodation costs of PRACE Spring School 2012 speakers were covered by the school's budget. The total cost of those expenses was approximately 3550 Euro. In order to prepare the venue for the event and to ensure contiguous work of important local services

(e.g. network connection) the school's budget covered the venue supporting stuff. The total cost of this expense was approximately 1800 Euro. The total cost of video recordings together with on-line video transmission was approximately 3000 Euro. The total cost of supporting materials and equipment (e.g. printings) was approximately 200 Euro. The total cost of PRACE Spring School 2012 contest price was approximately 100 Euro.

Program & content

Program committee

Name and surname	Institution
Maciej Cytowski	PSNC/ICM, University of Warsaw
Maciej Szpindler	PSNC/ICM, University of Warsaw
Łukasz Dutka	PSNC/ACC CYFRONET AGH
Anna Němcová	VSB-TUO
David Horák	VSB-TUO
Ondřej Jakl	VSB-TUO

Designing the program

The program of the school was designed to cover three main topics:

- Access to PRACE resources and best practices on PRACE Tier-0 systems (**Day 1**),
- Parallel programming libraries and tools (**Day 2**),
- Performance analysis of parallel programs (**Day 3**).

The school was dedicated to students that develop parallel applications in different scientific disciplines. The school's focus was on parallel programming tools to speed up their work and to improve the scalability of their applications. PRACE Tier-0 systems where presented as high performance computing resources accessible to European scientists and software developers through scientific general calls and so-called preparatory access calls. Most importantly the idea of preparatory access calls of type A, B and C were presented to participants during the introductory lecture.

During the first day of the school participants received lectures on PRACE resources and services and most importantly on best practices for programming PRACE Tier-0 systems. Lectures on Jugene, Curie and Hermit were given by HPC specialists working and developing applications for those systems. At the end of the first day participants received instructions on how to login and work on the training HPC system.

The second day of the school was organized in three parallel sessions. The main idea was to finish Day 2 with each of the participants having his/her own parallel application ported onto the training HPC system. Based on the expertise of the organizers, the following research topics were proposed: finite element methods, particle methods and quantum physics. Each track was given an insight into novel parallel programming libraries, tools and techniques that can speed up the development process and increase the performance of applications.

The third day was planned and designed in close cooperation with the Virtual Institute for High Productivity Supercomputing (VI-HPS: *www.vi-hps.org*). The main purpose of this day was to present the performance analysis tools Scalasca and Vampir in few examples. The second part of the day was devoted to individual work on participants' codes. Participants could choose to analyze codes worked during Day 2 or codes they are developing in their own work.

Strong emphasis was put on giving participants an occasion to present their own work. They were welcome to bring and present their poster during the poster session organized at the end of Day 1.

In the introductory talk participants were encouraged to be active and to work hard on given exercises. We announced that there would be a PRACE Spring School 2012 contest for the three best developers of applications selected during three Day 2 tracks. Contest results and prizes were announced at the end of the school after the lunch break.

All participants received PRACE Spring School 2012 Certificates on the last day of the school.

Description of the contents

Welcome and PRACE introduction (30 min.) –important information about the PRACE project, general calls, preparatory access calls, training events and services in the PRACE project, brief introduction to main topics of the school

Best practices – JUGENE (tools, libraries, compilers, optimization) (90 min.) – introduction to the JUGENE architecture, most important information on how to develop efficient codes for the JUGENE system, description of tools, libraries, compilers and optimization techniques

Best practices – CURIE (tools, libraries, compilers, optimization) (90 min.) - introduction to the CURIE architecture, most important information on how to develop efficient codes for the CURIE system, description of tools, libraries, compilers and optimization techniques

Best practices – HERMIT (tools, libraries, compilers, optimization) (90 min.) - introduction to the HERMIT architecture, most important information on how to develop efficient codes for the HERMIT system, description of tools, libraries, compilers and optimization techniques

Introduction to Day 2 (15 min.) – first login to the training HPC system, first execution of codes on the training system

Track A – Finite element methods (6 h) – introduction to libraries for parallel FEM computations (PETSc, Trilinos), individual implementation of example efficient FEM codes, hands-on exercises on the training system, visualization of results with the use of VisNow software

Track B – Particle methods (6 h) – introduction to libraries for parallel random number generation (SPRNG) and load-balancing (Zoltan), individual implementation of an efficient parallel particles system code, hands-on exercises on the training system, visualization of results with the use of VisNow software

Track C – FFT in quantum physics (6 h) – introduction to libraries for parallel FFT computations (P3DFFT, FFTW), individual implementation of an efficient parallel quantum physics code, hands-on exercises on the training system, visualization of results with the use of VisNow software

Visualization (30 min.) – introduction to visual analysis, introduction of visualization tool VisNow (*http://visnow.icm.edu.pl*), reading and processing user's data with VisNow, presented during each track

Introduction to Day 3 (30 min.) – installation of front-end tools for performance analysis of parallel programs on participants' laptops, information about code examples and training system's setup

Introduction & overview of performance analysis tools (45 min.) – introduction to performance analysis tools available for parallel applications

Profile analysis with Scalasca (75 min.) – introduction to Scalasca, hands-on exercises on detailed profile analysis for parallel programs with Scalasca

Trace analysis with Vampir (90 min.) – introduction to Vampir, hands-on exercises on detailed trace analysis for parallel MPI programs with Vampir

Assisted analysis of participants' codes (90 min.) – all participants working together with lecturers on the performance analysis of codes developed during 2nd day of the school or their own codes

Computer resources

All participants were granted access to HPC system called Notos installed at ICM, University of Warsaw. Notos is an IBM Blue Gene/P system with 1024 nodes and 4096 cores (4GB RAM/node). All participants received their own login, password and home directory on the system.

Participants agreed to bring their own laptops. Laptops were mainly used as ssh terminals to login to supercomputer resources available for the school.

Participants & feedback

Number of participants by country

Country	Number of participants
Poland	32
Czech Republic	13
Serbia	4
Bulgaria	2
Germany	1
Israel	1
Republic of Macedonia	1
Total	54

Online video transmission participants: approx. 20 participants.

Distribution of student between Day 2 three tracks:

- Track A – Finite element methods: 26
- Track B – Particle methods: 16
- Track C – FFT in quantum physics: 12

Process for selecting the participants

All registered students were asked to briefly describe their motivation, scientific background and current HPC skills during the registration process. They were also asked to select one of the three Day 2 tracks that they want to participate in. Additionally each participant had the possibility to present his work during the poster session.

Initially after the registration deadline there were around 70 participants registered. We have selected a group of 55 students on the basis of their motivation, scientific background and current HPC skills. All selected participants were asked to confirm their final participation.

Additionally we have informed all other participants that they are on the waiting list.

Approximately 15 students subsequently notified us of their unavailability and we were thus able to accept all students from the waiting list. The final participant count was 54.

7.5 Preliminary report on the second Summer School

Tim Robinson

Name: Summer School on Code Optimisation for Multi-Core and Intel MIC Architectures

Dates: 21-23 June 2012

Location: CSCS, Lugano, CH

Organizer: CSCS

Organizational details

Local organizing committee

- Tim Robinson
- Neil Stringfellow
- Jeff Poznanovic

Venue

The PRACE Summer School 2012 was held at the new location of the Swiss National Supercomputing Centre (CSCS) in Cornaredo, Lugano. This venue was chosen because of its modern facilities (including the ability to record audio and slide presentations) and its close proximity to the city of Lugano. The conference room has a capacity of 30-40 participants.

Budgeting

The budget comprised the expenses for one remote speaker (flights, accommodation and transfers), lunches and coffee breaks, a casual dinner, and an evening dinner event, which was held at Grotto San Rocco. The venue for the workshop was available free of charge. Note: 1 CHF = 0.8 EUR.

Expense	Budgeted (CHF)
Speaker expenses	1600
Lunches	5000
Coffee breaks	1300
Materials	380
Dinner (Thurs)	2600
Dinner Event (Fri)	5160
Total	**16040**

Intel very generously funded the external speakers from Intel, TACC and NICS.

The school was planned to have a maximum of 33 students and there were 10 organizers/trainers making a total 43 participants.

Program & content

Program committee

- Tim Robinson (CSCS)
- Neil Stringfellow (CSCS)
- Jeff Poznanovic (CSCS)
- David Henty (EPCC)
- Jim Jeffers (Intel)

Designing the program

Interest in the Intel MIC architecture had gathered serious momentum throughout Europe in early 2012, and many of our own users at CSCS had asked us whether we were investigating the MIC architecture. We felt therefore that hosting a PRACE Summer School that focussed on the Intel MIC would be an ideal opportunity to continue this momentum, and to provide European researchers with the opportunity of benefitting – through PRACE – from what would be the first (open) MIC-related training event held in Europe.

Many recent PRACE training events had been GPU-centric, and we considered that it would be interesting to offer training on efficiently using the MIC architecture in order to redress the balance among the various flavours of HPC accelerators. In particular, the GPU-based accelerator training events tended to concentrate a great deal on how to program the device using proprietary languages, whereas the more familiar programming models on the MIC would allow the course to concentrate more on how to deliver performance optimisations relevant to the real science applications of the attendees.

We had seen that Intel had allowed some sites to share information on their MIC successes at events such as at ISC11, and we contacted Intel to discuss the possibility delivering MIC training to the PRACE user community (and to thus extend their reach beyond the current NDA partners). Intel indicated to us that the time frame of late June worked well for them with regards to the availability of technical speakers (the workshop would be held immediately after ISC12 in Hamburg). In order to have as successful and interesting an event as possible, we suggested that in addition to trainers from Intel it would be beneficial to have speakers from other sites deliver their experiences and success stories porting their applications to the MIC. Speakers from TACC and NICS agreed to participate. Moreover, TACC indicated that they were willing to provide access to an eight-unit Knights Corner cluster that they were building in Austin, Texas.

We thus designed a three-day intensive course on programming and tuning techniques for modern multi- and many-core processors, with a particular focus on the Intel Many Integrated Core (MIC) architecture. Topics were designed at an advanced level and included structuring code to enable SIMD vectorization, efficient usage of the register, cache and memory hierarchy, use of multi-threading techniques to maximize resource utilization, data locality considerations on multi-socket NUMA nodes, and inter-node communication. Many of these optimisation strategies are generic and can be readily applied to other architectures such as Xeon (and other AMD, IBM etc. processors). The second two days of the course were devoted to MIC: Intel specialists introduced the Many Integrated Core architecture and programming environment, and delved into greater detail of the use of multi- and many-core programming techniques on the Intel MIC. Demonstrations and hands-on sessions were integrated throughout the course to illustrate the topics in greater depth, and user case studies highlighted real-world experiences on porting scientific codes to the Intel MIC architecture.

Description of the contents

This is a preliminary agenda.
Day 1: Review of multi-core architectures
Optimisation for multi- and many-core architectures including sessions on:

- Optimising for the memory, cache and register hierarchy
- Vectorisation and SIMD
- Multi-threading and inter-core optimization
- NUMA and UMA considerations.

- Practicals will be held on a number of architectures including Intel Xeon and AMD Opteron.

Day 2: Intel MIC - architecture, programming and execution models, use as a device or in native model

- MIC in a multi-node environment.
- Optimising applications for the MIC architecture.
- Compilers and performance tools.
- Practicals utilising remote and local Knights Corner servers

Day 3: Continuation of MIC optimisation strategies.
User experience presentations from people who have been able to show tuning and performance improvements on the MIC.

Computer resources

Access was provided to a 16-cabinet Cray XE6 on-site at CSCS for exercises related to generic multi- and many-core issues. Remote access was provided to an eight-unit Knights Corner cluster in Austin, Texas, for exercises specific to the MIC architecture. Wifi was provided free of charge to all participants (who were expected to bring their own laptops to the training event).

Participants & feedback

Number of participants by country

Country	Number of participants
Austria	2
Bulgaria	1
Germany	4
Italy	1
Netherlands	2
Serbia	1
Spain	4
Switzerland	14
United Kingdom	1
United States	2
Total	**32**

Process for selecting the participants

As this workshop was the first open Intel MIC training event in Europe we expected that applications would be significantly oversubscribed. For this reason, we asked applicants to answer several questions relating to their skills and motivations for attending the course:

a. Please describe your research project and your own contribution to it (1 paragraph).

b. Please describe why you wish to participate, what you expect to learn, and how you plan to apply what you learn (1 paragraph).

c. Please describe your abilities in the C, C++ and Fortran (and other) programming languages (1-2 sentences).

d. Please describe your experience in high-performance computing (1-2 sentences).

Final selection was based, therefore, not only on an applicant's proven proficiency in programming for high performance computing, but also that the applicant described clearly how the course material would be applied directly to his or her work in the very near future. We received approximately 70 applications for the ca. 30 places available.

7.6 Report on the EU-US Summer School

Hermann Lederer

Name: EU-US Summer School 2011

Dates: Aug 7-12, 2011

Location: South Lake Tahoe, California, US

Organizers: CSC, RZG (PRACE+DEISA), NCSA (XSEDE)

Organizational details

Local organizing committee

Scott Lathrop, NCSA (XSEDE)

Venue

Embassy Suites Lake Tahoe Hotel and Resort, Lake Tahoe, California. For 2011, a location in the US had to be selected, after the 2010 event in Europe. This was done in a few iterations together with TeraGrid/XSEDE after TeraGrid was making proposals. The venue was selected on attractiveness and hosting costs.

Budgeting

Hosting costs were covered by NSF, travel costs for EU participants by PRACE – 30,000 euro in total.

Program & content

Program committee (EU side)

- Pekka Manninen (CSC)
- Ari Turunen (CSC)
- Nix Mc Donnel (ICHEC)
- Simon Wong (ICHEC)
- Hermann Lederer (RZG)

Final program & trainers

Sunday, Aug. 7

6:00 p.m. Welcome reception

Monday, Aug. 8

7:30 a.m. Full breakfast and registration
8:30 a.m. HPC Challenges and Technology: PRACE Overview (Lennart Johnsson, University of Houston), XD Overview –(John Towns, NCSA)
9:00 a.m. Introduction of participants
10:30 a.m. Break
11:00 a.m. Exascale Software Project (David Keyes, Columbia University and KAUST)
Noon Lunch and team building
1:30 p.m. Programming: Overview on Mixed MPI/OpenMP Programming, UPC, CAF, StarSs Model (Alejandro Duran, Polytechnical University of Catalunya, Barcelona; David Henty, EPCC, University of Edinburgh, UK)
6:00 p.m. Poster session and buffet dinner

Tuesday, Aug. 9

7:30 a.m.	Full breakfast
8:30 a.m.	Challenges by Scientific Disciplines I *Parallel track 1:* Materials Science (Thomas Schulthess, ETH Zurich & CSCS, Switzerland) *Parallel track 2:* Plasma Physics (Frank Jenko, Max Planck Institute for Plasma Physics, Garching)
9:30 a.m.	Challenges by Scientific Disciplines II *Parallel track 1:* Life Sciences — Amber (Thomas Cheatham, Univ. Utah) *Parallel track 2:* CFD/Engineering (Ulrich Rist, University of Stuttgart)
10:30 a.m.	Break
11:00 a.m.	Challenges by Scientific Disciplines III *Parallel track 1:* Cosmology (Britton Smith, Michigan State University) *Parallel track 2:* Metagenomics — Earthmicrobiome Project (Folker Meyer, University of Chicago)
Noon	Lunch and team building
1:30 p.m.	Performance Analysis & Profiling: PAPI, IPM, PerfSuite, TAU (Philip Blood, PSC, Pittsburgh, US; Bernd Mohr, FZJ, Juelich, Germany)
5:00 p.m.	Dinner on your own

Wednesday, Aug. 10

7:30 a.m.	Full breakfast
8:30 a.m.	Challenges by Scientific Disciplines IV Parallel track 1: Life Sciences — GROMACS (Erik Lindahl, University of Stockholm) Parallel track 2: Engineering — A Software Environment for Efficient Flow Simulations (Hans-Joachim Bungartz, Technical University of Munich)
9:30 a.m.	Numerical Algorithms & Parallel I/O Parallel track 1: Numerical Algorithms — Scalable fast algorithms for Coulomb interactions (Olaf Lenz, University of Stuttgart) Parallel track 2: Parallel I/O (Lonnie Crosby, National Institute of Computational Sciences)
10:30 a.m.	Break
11:00 a.m.	Open community-building time
Noon	Lunch and team building
1:30 p.m.	Parallel Programming: GPU/CUDA programming (hands-on) (Wen-Mei Hwu, NCSA)
5:00 p.m.	Dinner on your own

Thursday, Aug. 11

7:30 a.m.	Full breakfast
8:30 a.m.	Challenges by Scientific Disciplines V *Parallel track 1:* Numerical Libraries (Tony Drummond, LBNL, Berkeley, US) *Parallel track 2:* Workflow Tools (Scott Callaghan, Southern California Earthquake Center, USC)
9:30 a.m.	Data Intensive Computing (John R Johnson, Pacific Northwest Laboratory)
Noon	Lunch and team building
1:30 p.m.	Scientific Visualization (Amy Szczepański, University of Tennessee/NICS)
4:30 p.m.	Wrap-up session
5:00 p.m.	Dinner on your own

Designing the program

The goal was to expand the knowledge of the attendees about high performance computing (HPC) and it applications in multiple fields of science and engineering. The goal was also to foster new collegial friendships and partnerships (nationally and internationally) among the presenters and attendees.

Participants & feedback

Number of participants by country

35 from students from US, 25 students from Europe, 25 presenters.

Process for selecting the participants

An open worldwide call was done, resulting in 2346 student applications. 35 US students were selected by an US selection committee, 25 European students were selected by an European selection committee. The European selection committee consisted of six scientists from Finland (CSC), France (CEA), Italy (CINECA), Germany (RZG), UK (EPCC) and Spain (BSC)

Analysis of the feedback

In order to assess the value and impact of the summer school and to help plan for future events, a survey of the attendees was conducted at the conclusion of the summer school. A separate survey was conducted with the presenters and support staff to capture their perspectives on the quality of the summer school and how it could be improved in future events. We received survey responses from 52 of 58 (90%) participants, and 18 of 26 (69%) presenters and support staff.

Partipants were asked about their goals for attending and the extent to which the summer school met those goals. Overwhelmingly the responses indicated that the summer school met their goals, and some said the event exceeded their expectations.

When asked for their overall assessment, more than 90% of the participants rated the summer school as excellent or very good. Fully, 100% of the responded presenters and support staff all rated the summer school as excellent or very good.

7.7 Report on the second Scientific Workshop

Krassimir Georgiev

Name: PRACE Workshop on HPC Approaches on Life Sciences and Chemistry

Dates: February 17 – 18, 2012

Location: Sofia, Bulgaria

Organizer: NCSA

Organizational details

Local organizing committee

- Krassimir Georgiev, NCSA
- Georgi Prangov, NCSA

Venue

Dedeman Sofia Hotel Princes. This hotel was selected because of the best conditions for the two working days, equipment, etc. for the best price.

Program & content

Program committee

- Stoyan Markov, NCSA
- Svetozar Margenov, NCSA
- Krassimir Georgiev, NCSA
- Leandar Litov, NCSA

List of trainers

- Florian Berberich (JSC, Germany)
- Ivan Girotto (ICHEC, Ireland)
- Vit Vondrak (VSB, Czech Republic)
- Zdenec Dostal (VSB, Czech Republic)
- Vassil Aleksandrov (BSC, Spain)
- Murat Manguoglu (METU, Turkey)
- Danica Stojilkovic (IPB, Serbia),
- Christopher Johnson (EPCC, UK)
- Svetozar Margenov (NCSA, Bulgaria)
- Emanouil Atanassov (IICT-BAS, Bulgaria)
- Peicho Petkov (NCSA, Bulgaria)
- Georgi Vayssilov (IICT-BAS, Bulgaria)
- Plamenka Borovska (IICT-BAS, Bulgaria)

Participants & feedback

Number of participants by country

Country	Number of participants
Bulgaria	46
Germany	1
Sweden	1
UK	1
Ireland	1
Turkey	1
Slovenia	1
Czech Republic	2
Spain	1
Total	**55**

Process for selecting the participants

The participants were selected based on a questionnaire published on both the PRACE web site and the web site of NCSA (Bulgaria). Most of the participants had preliminary experience with parallel computers and only a few were beginners. Several undergraduate students from three Bulgarian universities (Sofia University, Technical University of Sofia and Medical University of Sofia) attended the two days lectures and discussions.

Analysis of the feedback

No feedback survey for this event has been carried out. The main reason is that we consider such types of surveys to be more appropriate for training events or seasonal schools but not so helpful for general seminars and workshops.

Nevertheless, there was a special discussion in the end of the Workshop where participants had the possibility to express their opinion of the Workshop: The information regarding the Workshop, the registration processes, the venue and catering, the quality of the lectures, and the relevance of the topic were all considered as being of high quality.

Conclusions & lessons learned

The Workshop attracted participants from a total 9 countries, but in terms of the numbers of participants from each country, it was heavily weighted towards Bulgaria.

7.8 Report on the HP-SEE/LinkSceem-2/PRACE Summer Training

Ioannis Liabotis

Name: Joint HP-SEE/LinkSceem-2/PRACE Athens Summer Training

Dates: 13th to the 15th of July 2011 (3 full days)

Location: Athens, Greece

Organizers: HP-SEE (http://www.hp-see.eu), LinkSceem (http://www.linksceem.eu/ls2/) and PRACE-1IP projects (GRNET)

Organizational details

Local organizing committee

Name	Organization
Ioannis Liabotis	GRNET, Greece
Dimitra Kotsokali	GRNET, Greece
Fotis Georgatos	CaSToRC, Cyprus
Christos Nicolaou	CaSToRC, Cyprus
Danica Stojiljkovic	IPB, Serbia
Antun Balaz	IPB, Serbia

Venue

Training Center of the Hellenic Telecommunications Organization (OTE Academy) in Athens, Greece. The location was selected due to its good facilities being a dedicated training center that hosts large industrial and academic training events. The same venue had previously hosted the 2nd PRACE seasonal school during the PRACE Preparatory Phase project.

Budgeting

The running costs of the event were covered by the HP-SEE and LinkSCEEM projects. Limited PRACE-1IP resources – in the form of PRACE-1IP person months – were used to cover parts of the organizational work for the event.

Program & content

Program committee

Name	Organization
Ioannis Liabotis	GRNET, Greece
Paschalis Korosoglou	GRNET, Greece
Todor Gurov	IICT, Bulgaria
Pekka Manninen	CSC, Finland
Fotis Georgatos	CaSToRC, Cyprus
Christos Nicolaou	CaSToRC, Cyprus
Danica Stojiljkovic	IPB, Serbia
Dusan Vudragovic	IPB, Serbia
Antun Balaz	IPB, Serbia

Final program

Date	Module Title	Trainers/Affiliation
13th of July 2011 Morning	LinkSCEEM-2 session	Members of the LinkSceem project and user communities
13th of July 2011 Afternoon	Message Passing Interface (MPI)	Paschalis Korosoglou (A UTH, Greece)
13th of July 2011 Afternoon	Shared Memory Parallelism (OpenMP)	Paschalis Korosoglou (A UTH, Greece)
13th of July 2011 Afternoon	Hybrid (MPI + OpenMP) programming	Antun Balaz (IPB, Serbia)
13th of July 2011 Afternoon	Evaluation and Benchmarking of highly scalable parallel numerical libraries	Christos Theodosiou (AU TH, Greece)
13th of July 2011 Afternoon	Introduction to the IBM Blue Gene	Emanouil Atanassov (IIC T, Bulgaria)
14th of July 2011 Morning	MPI, OpenMP,Hybrid (MPI + OpenMP) programming hands-on	Paschalis Korosoglou (A UTH, Greece), Antun Balaz (IPB, Serbia), Christos Theodosiou (AU TH, Greece)
14th of July 2011 Afternoon	CUDA Programming	Massimo Bernaschi (CNR , Italy)
14th of July 2011 Afternoon	CUDA Programming, hands-on	Massimo Bernaschi (CNR , Italy)
15th of July 2011 Morning	WS-PGRADE/gUSE	Miklos Kozlovszky (SZT AKI, Hungary)
15th of July 2011 Morning	Profiling	Alan O'Cais (JSC, Germany) , Christian Roessel (JSC, Germany)
15th of July 2011 Morning	Profiling hands-on	Alan O'Cais (JSC, Germany) , Christian Roessel (JSC, Germany)
15th of July 2011 Afternoon	Optimisation and Benchmarking	Christopher Dahnken (IN TEL, Germany)
15th of July 2011 Afternoon	Optimisation and Benchmarking hands-on	Christopher Dahnken (IN TEL, Germany)

Designing the program

The training covered a series of advanced training modules in the following subjects:

- MPI, OpenMP, Hybrid Programming
- CUDA Programming
- HPC Portals and Workflow Management systems
- Profiling
- Optimization and Benchmarking

The first half day of the training event was dedicated to presentations of the LinkSCEEM-2 projects and its user communities. Although this session was organized by LinkSCEEM all participants attended and had the opportunity to gain some insight into the LinkSCEEM-2 project as well as the scientific applications supported by the project. The main training programme started in the afternoon of the first day.

Description of the contents

The full programme as well as the training material is available at: *http://indico.ipb.ac.rs/conferenceDisplay.py?confId=163*

Computer resources

- BlueGene/P Supercomputer in Bulgaria
- PARADOX x86 HPC Cluster in Serbia
- GPU nodes in HPC cluster in Bulgaria

Participants & feedback

Number of participants by country

Country	Number of Participants
Albania	3
Armenia	1
Bulgaria	2
Cyprus	3
Egypt	4
FYR of Macedonia	4
Georgia	1
Greece	22
Hungary	1
Israel	1
Moldova	3
Montenegro	2
Romania	2
Serbia	5
Syria	1
Total	**55**

Process for selecting the participants

The maximum number of participants that the training venue could accommodate was 60. It was decided that the selection committee should select 20 participants from LinkSCEEM and 40 from HP-SEE and PRACE. The selection would be based on the qualifications of applicants in terms of experience while making sure that the training would accept participants from all the countries that had partners participating in the HP-SEE and LinkSCEEM-2 projects. Two separate registration forms were created. The first was dedicated to participants affiliated to the LinkSCEEM-2 project, who could also apply for partial funding for attending the training event. The second was a generic form available to applicants from all over the world.

After the deadline for registration to the training event, the number of applicants was 165 - 46 of whom requesting funding while being affiliated with the LinkSCEEM-2 and 119 for the

general registration. After evaluation by the selection committee, 60 participants were selected; the training was ultimately attended by 55 persons.

Statistics of the feedback survey

As with all HP-SEE, LinkSCEEM-2, and PRACE trainings, an on-line evaluation form was provided to the trainees at the end of the school. The trainees could answer the survey anonymously. The set of questions provided to the trainees were a combination of the HP-SEE and PRACE training evaluation questionnaires. A total of 38 full responses were received from the 55 trainees that participated in the training event.

Overall, from the answers of the participants we can conclude that the joint HP-SEE, LinkSCEEM-2, and PRACE HPC training was a very successful event that facilitated the extension of participants' skills in popular areas of HPC programming, and that the duration of the event could be extended by one or two days. The overall rating of the training was 8.31 out of 10.

Conclusions & lessons learned

The event organized jointly by the three projects was successful and the trainees gained valuable insight into current HPC technologies that they can take back to their labs and apply to their HPC applications. The event proved a successful collaboration of three separate but related projects.

7.9 Report on two local HPC courses in Bulgaria

Plamenka Borovska

Name: "Parallel Programming with MPI on the BlueGene Supercomputer and High-Performance Computer Clusters" & "Applied Software for Programming the Bulgarian Supercomputer"

Dates: 6-7, 11-12, 20-21 April 2012 & 18-20, 25-27 May 2012

Location: Gabrovo & Sofia Bulgaria

Organizer: NCSA

Content

The main purpose of these training courses was to introduce participants to the high-performance computer systems and programming techniques on high-performance computer clusters and supercomputers. In particular, the training events were focused on parallel programming for IBM BlueGene architecture and high-performance computer clusters. Therefore it was presented both the architectural aspects of BlueGene architectures and parallel programming techniques with MPI and OpenMP for the exploitation of high-performance computer systems. In the schedule of the events, time was also dedicated to allow participants to do some practise on the heterogenious computer cluster and IBM Blade Center located at the High-Performance and GRID Computing Labs, Technical University of Sofia and to do some practise on the Bulgarian Supercomputer BlueGene.

Parallel Programming with MPI on the BlueGene Supercomputer and High-Performance Computer Clusters:

Instructor	Affiliation	Topic
Plamenka Borovska	NCSA, TU-Sofia	HPC Systems and Architectures
Plamenka Borovska	NCSA, TU-Sofia	Parallel Programming with MPI
Desislava Ivanova	TU-Sofia	PRACE Infrastructure
Desislava Ivanova	TU-Sofia	IBM BlueGene Arhitecture
Milena Lazarova	TU-Sofia	Parallel Programming with MPI – hands on (I part)
Iva Nikolova	TU-Sofia	Parallel Methods for Matrix Multiplication
Veska Gancheva	TU-Sofia	Parallel Programming with MPI – hands on (II part)
Simeon Tsvetanov	TU-Sofia	Parallel Programming with MPI – hands on (III part)

Applied Software for Programming the Bulgarian Supercomputer

Course Instructor: Valentin Pavlov, NCSA. The course covered the topics:

- Introduction to Linux - kernel, shell, basic commands
- Introduction to GNU and IBM compilers for C / C + + / FORTRAN
- Compiling software - autoconf / automake, Cmake
- Introduction to MPI and OpenMP
- IBM Blue Gene / P hardware and software - DB2, mmcs_db_server, navigator, CIOD, CNK, mpirun, LoadLeveler
- IBM Blue Gene / P hardware and software (II part)

7.10 Lecture series: Supercomputer applications in natural sciences

Irini Doytchinova

The course was addressed to undergraduate students, PhD students and young scientists, studying or working in the field of natural sciences. The main goal of the course was to introduce to the participants the main supercomputer algorithms and tools used in the natural sciences.

Module	Lecturer(s)
Introduction to HPC on IBM Blue Gene/P Lecture General introduction to the field of High-performance computing; description of IBM Blue Gene/P's hardware and system software; guide for job preparation and submission and monitoring Practical Preparation of sample job control files and their submission, working with the LoadLeveler queue	Dr. Valentin Pavlov
Modeling of ligand – macromolecule interactions – part I Practical Introduction to web accessible databases with protein structures – PDB, SwissProt, UniProt. Basic skills of viewing, measuring and modifying 3D protein structures using VMD and PyMOL as well as molecuar dynamics trajectories visualization.	Prof. Leander Litor Dr. Peicho Petkov
Modeling of ligand – macromolecule interactions – part II Practical Introduction to GROMACS software package: assigning force field, simulation volume definition, addition of solvent and ions, system energy minimization.	Prof. Leander Litor Dr. Peicho Petkov
Modeling of ligand – macromolecule interactions – part III Practical Equilibration of protein in explicit solvent molecular dynamics simulation, MD production run set up and basic MD trajectory analysis.	Prof. Leander Litor Dr. Peicho Petkov
Practical applications of quantum chemical methods Lecture Basics of the quantum chemical methods. Density functional theory. DFT functionals. Basis sets. Practical Input file for quantum chemical calculations. Structure of the files. Analysis of the data. Gaussian 09 code.	Prof. Geogi Vayssilov Dr. Petko Petkov
Specific problems in modeling of chemical systems Lecture Evaluation of the solvent effects. Hybrid QMMM methods. Geometry optimization. Practical Input files for geometry optimization. Analysis of the results. Determination of local minima. Gaussian 09 code.	Prof. Geogi Vayssilov Dr. Petko Petkov
Simulations of spectral and electronic characteristics Lecture Simulation of infrared, UV and visible spectra. Estimation of	Prof. Geogi Vayssilov

atomic charges. Analysis of the electron density distribution. Practical Input files and analysis of the results for ab initio MD simulations. CP2K code.	Dr. Petko Petkov
Genomics and Proteomics Lecture Introduction to Genomics and Proteomics: structure, function and organization of the prokaryotic and eukaryotic genomes and proteoms; DNA and protein databases. Practical DNA, RNA and protein basic and derivative databases: organization and exploration. Biology data file formats. Comparative genomics: multiple sequence alignments.	Prof. Ivan Ivanov Dr. Kiril Kirilov
Sequence alignment Lecture Sequence alignment Practical Sequence alignment - software tools	Prof. Plamenka Borovska Dr. Veska Gancheva
Molecular interactions in proteins Lecture Non-covalent interactions, electrostatic interactions, computational approaches appropriate for supercomputing.	Prof. Andrey Karshikov
Drug design – part I Lecture Introduction to drug design and development. Methods for drug discovery. Thermodynamics of the interaction drug – macromolecule. Practical Machine learning methods for allergenicity prediction. Software WEKA.	Prof. Irini Doytchinova Dr. Ivan Dimitrov
Drug design – part II Lecture Ligand-based drug design. Main rules for data collection, analysis and design of new structures. Algorithms and tools. Practicals Molecular modeling of ligand-macromolecule complexes. Molecular docking of peptides on MHC protein by software GOLD. Quantitative structure – activity relationship (QSAR) analysis of compounds binding to 5-HT receptors by software MDL QSAR.	Prof. Irini Doytchinova Dr. Mariyana Atanasova Iva Valkova
Drug design – part III Lecture Structure-based drug design. Main rules for data collection, analysis and design of new structures. Algorithms and tools. Practical Molecular docking of peptides on MHC protein by software AutoDock.	Prof. Irini Doytchinova Atanas Patronov