E-Infrastructures
H2020-EINFRA-2014-2015

EINFRA-4-2014: Pan-European High Performance Computing Infrastructure and Services

PRACE-4IP

PRACE Fourth Implementation Phase Project

Grant Agreement Number: EINFRA-653838

D4.1
Interim PRACE Training Report

Final

Version: 1.2
Author(s): Ioannis Liabotis, GRNET
Date: 22.02.2016

Project and Deliverable Information Sheet

PRACE Project	**Project Ref. №: EINFRA-653838**	
	Project Title: PRACE Fourth Implementation Phase Project	
	Project Web Site: http://www.prace-project.eu	
	Deliverable ID: D4.1	
	Deliverable Nature: Report	
	Dissemination Level: PU	**Contractual Date of Delivery:** 29 / February / 2016
		Actual Date of Delivery: 29 / February / 2016
	EC Project Officer: Leonardo Flores Añover	

* - The dissemination level are indicated as follows: **PU** – Public, **CO** – Confidential, only for members of the consortium (including the Commission Services) **CL** – Classified, as referred to in Commission Decision 2991/844/EC.

Document Control Sheet

Document	**Title: Interim PRACE Training Report**	
	ID: D4.1	
	Version: 1.2	**Status:** ***Final***
	Available at: http://www.prace-project.eu	
	Software Tool: Microsoft Word 2010	
	File(s): D4.1.docx	
Authorship	**Written by:**	Ioannis Liabotis, GRNET
	Contributors:	Ioannis Liabotis (GRNET), Simon Wong (ICHEC), Katarzyna Pawlikowska (CSCS), Rolf Rabenseifner (HLRS)
	Reviewed by:	Ondřej Jakl, IT4I-VSB Veronica Teodor, FZJ
	Approved by:	MB/TB

Document Status Sheet

Version	Date	Status	Comments
0.1	15/December/2015	Draft	Initial TOC
0.2	20/January/2016	Draft	Initial Draft
0.3	01/February/2016	Draft	First Full version
1.0	08/February/2016	Draft	Final Draft
1.1	09/February/2016	Draft	Update
1.2	22/February/2016	Final Draft	Update based in Internal Review Comments

Document Keywords

Keywords:	PRACE, HPC, Research Infrastructure, training, face-to-face training, Seasonal Schools, PRACE Advanced Training Centres, PATC, MooC, International HPC Summer School, Centres of Excellence, CoE.

Table of Contents

List of Figures

List of Tables

References and Applicable Documents

[1] P. Manninen and S. Wong (2011). PRACE-1IP D3.2.3: PRACE Advanced Training Centres.

[2] M. Louhivuori, P. Manninen and S. Wong (2012). PRACE-2IP D4.2: Establishment of PRACE Advanced Training Centres.

[3] S. Wong, S. Eritokritou, M. Polydorou (2013). PRACE-2IP D4.3: Final Training Report.

[4] O. Jakl (2014). PRACE-3IP D4.2: Report on Training Events.

[5] M. Louhivuori, S. Eritokritou, O. Jakl, I. Liabotis and S. Wong (2015). PRACE-3IP D4.5: Final Report on Training Activities.

[6] D. Henty, S. Wong, M. Louhivuori and R. Rabenseifner (2013). PRACE-3IP D4.1: Continuity Plan for the PRACE Advanced Training Centres.

[7] S. Wong, I. Liabotis, M. Kern, N. Alexandrov, O. Jakl, R. Rabenseifner and S. Eritokritou (2015). PRACE-4IP D4.3: Assessment of PRACE Advanced Training Centres.

List of Acronyms and Abbreviations

aisbl	Association International Sans But Lucratif (legal form of the PRACE-RI)
BoD	Board of Directors
CoE	Centre of Excellence
CPU	Central Processing Unit
CUDA	Compute Unified Device Architecture (NVIDIA)
DFT	Density Functional Theory
DoA	Description of Action (formerly known as DoW)
EC	European Commission
e-CAM	e-infrastructure centre of excellence for software training and consultancy in simulation and modelling
ETP4HPC	The European Technology Platform for High Performance Computing
GPGPU	General Purpose Graphic Processing Unit
HPC	High Performance Computing; Computing at a high performance level at any given time; often used synonym with Supercomputing
MB	Management Board
MooC	Massively open online Course
MPI	Message Passing Interface
PATC	PRACE Advanced Training Centres
PRACE	Partnership for Advanced Computing in Europe; Project Acronym

List of Project Partner Acronyms

BADW-LRZ	Leibniz-Rechenzentrum der Bayerischen Akademie der Wissenschaften, Germany (3rd Party to GCS)
BILKENT	Bilkent University, Turkey (3rd Party to UYBHM)
BSC	Barcelona Supercomputing Center - Centro Nacional de Supercomputacion, Spain
CaSToRC	Computation-based Science and Technology Research Center, Cyprus
CCSAS	Computing Centre of the Slovak Academy of Sciences, Slovakia
CEA	Commissariat à l'Energie Atomique et aux Energies Alternatives, France (3rd Party to GENCI)
CESGA	Fundacion Publica Gallega Centro Tecnológico de Supercomputación de Galicia, Spain, (3rd Party to BSC)
CINECA	CINECA Consorzio Interuniversitario, Italy
CINES	Centre Informatique National de l'Enseignement Supérieur, France (3rd Party to GENCI)
CNRS	Centre National de la Recherche Scientifique, France (3 rd Party to GENCI)
CSC	CSC Scientific Computing Ltd., Finland
CSIC	Spanish Council for Scientific Research (3rd Party to BSC)
CYFRONET	Academic Computing Centre CYFRONET AGH, Poland (3rd Party to PNSC)
EPCC	EPCC at The University of Edinburgh, UK
ETHZurich (CSCS)	Eidgenössische Technische Hochschule Zürich – CSCS, Switzerland
FIS	FACULTY OF INFORMATION STUDIES, Slovenia (3rd Party to ULFME)
GCS	Gauss Centre for Supercomputing e.V.
GENCI	Grand Equipement National de Calcul Intensiv, France
GRNET	Greek Research and Technology Network, Greece
INRIA	Institut National de Recherche en Informatique et Automatique, France (3rd Party to GENCI)
IST	Instituto Superior Técnico, Portugal (3rd Party to UC-LCA)
IUCC	INTER UNIVERSITY COMPUTATION CENTRE, Israel
JKU	Institut fuer Graphische und Parallele Datenverarbeitung der Johannes Kepler Universitaet Linz, Austria
JUELICH	Forschungszentrum Juelich GmbH, Germany
KTH	Royal Institute of Technology, Sweden (3rd Party to SNIC)
LiU	Linkoping University, Sweden (3rd Party to SNIC)
NCSA	NATIONAL CENTRE FOR SUPERCOMPUTING APPLICATIONS, Bulgaria
NIIF	National Information Infrastructure Development Institute, Hungary
NTNU	The Norwegian University of Science and Technology, Norway (3rd Party to SIGMA)
NUI-Galway	National University of Ireland Galway, Ireland
PRACE	Partnership for Advanced Computing in Europe aisbl, Belgium
PSNC	Poznan Supercomputing and Networking Center, Poland
RISCSW	RISC Software GmbH

RZG	Max Planck Gesellschaft zur Förderung der Wissenschaften e.V., Germany (3rd Party to GCS)
SIGMA2	UNINETT Sigma2 AS, Norway
SNIC	Swedish National Infrastructure for Computing (within the Swedish Science Council), Sweden
STFC	Science and Technology Facilities Council, UK (3rd Party to EPSRC)
SURFsara	Dutch national high-performance computing and e-Science support center, part of the SURF cooperative, Netherlands
UC-LCA	Universidade de Coimbra, Labotatório de Computação Avançada, Portugal
UCPH	Københavns Universitet, Denmark
UHEM	Istanbul Technical University, Ayazaga Campus, Turkey
UiO	University of Oslo, Norway (3rd Party to SIGMA)
ULFME	UNIVERZA V LJUBLJANI, Slovenia
UmU	Umea University, Sweden (3rd Party to SNIC)
UnivEvora	Universidade de Évora, Portugal (3rd Party to UC-LCA)
UPC	Universitat Politècnica de Catalunya, Spain (3rd Party to BSC)
UPM/CeSViMa	Madrid Supercomputing and Visualization Center, Spain (3rd Party to BSC)
USTUTT-HLRS	Universitaet Stuttgart – HLRS, Germany (3rd Party to GCS)
VSB-TUO	VYSOKA SKOLA BANSKA - TECHNICKA UNIVERZITA OSTRAVA, Czech Republic
WCNS	Politechnika Wroclawska, Poland (3rd Party to PNSC)

Executive Summary

The Training Work Package (WP4) of the PRACE Fourth Implementation Phase (PRACE-4IP) project is responsible for the training activities of PRACE. Such training activities include the face-to-face training events, as well as a series of on line training offering such as the Massive open online Course (MooC), the training code repository (CodeVault), the training portal etc. This deliverable is a report of the face-to-face training events of PRACE-4IP during the initial 13 months of the project.

PRACE-4IP continued the training activities of PRACE-3IP starting from February 2015. Between February 2015 and January 2016 the six PRACE Advanced Training Centres (PATCs) delivered 76 courses, 213 course-days with 1723 participants. The feedback responses received have been overwhelmingly positive (8.4/10 average overall rating for PATC courses). Similarly, the PRACE seasonal schools in PRACE-4IP have been carefully selected via a well-designed selection process. The seasonal school scheduled for this reporting period, namely the PRACE Winter School 2015/2016 in Bratislava, Slovakia, attracted 36 attendees in total and obtained overall rating of 8.34/10. WP4 also started the collaboration with the Centres of Excellence (CoEs) where a number of on-demand events in collaboration with them are going to be organised. Finally, PRACE-4IP organised the 2015 International Summer School on HPC Challenges in Computational Sciences, 21-26 June 2015, in Toronto, Canada. All forms of face-to-face training are complementary, they contribute to the success of PRACE training activities, and should be continued in the future PRACE HPC training.

In accord with the PRACE-4IP goals most training events address also industrial users, and motivate them by showing the importance and benefits of HPC for the practice.

1 Introduction

One of the main aims of PRACE, since it has been initiated in 2008 by the PRACE Preparatory Phase project (PRACE-PP), has been to offer an educational programme suitable for the needs of the European students and researchers. An objective of PRACE-4IP, in particular, is to build up European human resources skilled in HPC and HPC applications. This can be achieved by, among others, organising highly visible events, enhancing the state of the art training provided by the PATCs, providing a better articulation with the offerings of the CoEs and the ETP4HPC, while improving online training developing at least one pilot MooC course. In more detail PRACE-4IP WP4 plans the creation of up to two MooCs. The first MooC is proposed to be entitled “Supercomputing” and being an introductory course, describe what supercomputers are, what they are used for and how to exploit their full computational potential. The second proposed MooC will aim to introduce individuals with limited programming knowledge to various High Performance Computing (HPC) facilities for big data analysis. In addition, PRACE-4IP WP4 strengthens its online training material provision, i.e. training presentations, video and other material included in the training portal, with the introduction of the PRACE CodeVault. The PRACE CodeVault is an open repository containing various high performance computing code samples for the HPC community. The CodeVault is an open platform that supports self-education of learning HPC programming skills where HPC users can share example code snippets, proof-of-concept codes and more. WP4 of PRACE-4IP implements this work.

In this document we describe the work done in the 1st year of the PRACE-4IP project, by the Training Work Package (WP4), particularly related to the face-to-face training events. Such events (existing or planned ones) are of the following types:

- PRACE Advanced Training Centres (PATC) Courses,
- PRACE Seasonal Schools,
- PRACE On-demand Events,
- International Summer School on HPC.

The majority of events during the reporting period, February 2015 to February 2016 where organised by the PATCs operating in well-established supercomputing facilities. The planning and selection of the PRACE Seasonal schools has been changed in comparison to the previous PRACE Implementation Phase projects during the period, and the Winter 2015/2016 Seasonal School that was organised in Bratislava, Slovakia was the 1st school that followed the new selection procedure. PRACE-4IP is in contact with the recently established Centres of Excellence in order to gather requirements, plan and organise on-demand training events in collaboration with them. Finally, WP4 co-organised the 2015 International Summer School on HPC Challenges in Computational Sciences in Toronto Canada and facilitated the selection of the 2016 International Summer School in Slovenia. A full list of courses provided by PRACE-4IP in the initial 13 months of the project is can be found in Annex B – The training requirements questionnaire towards the CoEs.

In this context this deliverable is organised as follows: Section 2 presents an overview of the PATC development and operation within the reporting period, Section 3 the relevant progress for Seasonal Schools, Section 4 the activities related to on-demand events, Section 5 the results of the activates related to the International Summer School on HPC and finally Section 6 provides the conclusions of the deliverable. Three Annexes are also made available including a list of all face-to-face training courses provided by PRACE during the reporting period, the questionnaire towards the CoEs, and the report from the Winter 2015/2016 Seasonal School.

2 PRACE Advanced Training Centres

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 developed programme of courses, designed and coordinated by PRACE with advice from external experts.

The main concepts of the PATCs, including their mission and objectives, were outlined in PRACE-1IP D3.2.3: PRACE Advanced Training Centres [1]. PRACE-2IP was responsible for implementation, the establishment of the PATCs [2] and their operation for the duration of the project, as described in PRACE-2IP D4.3: Final Training Report [3]. In summary, six PATCs were established in six partner countries (Finland, France, Germany, Italy, Spain and the UK). They have delivered some initial PATC courses and implemented a pilot PATC programme (of courses) over an approximately 18-month period. The activities of the PATCs then continued in the PRACE-3IP project (partially overlapping with the PRACE-2IP project in time), with ongoing course deliveries (as reported in [4] and [5]), as well as additional work to increase industry participation and to examine potential continuity plans for the PATCs [6].

In the PRACE-4IP project, significant effort has been allocated to evaluate the impact of the PATCs, take account of the lessons learnt so far and suggest ways to improve the network. This has been completed in the first year of the PRACE-4IP project, resulting in D4.3 Assessment of PRACE Advanced Training Centres [7]. Briefly, it carried out a Strengths,

Weaknesses, Opportunities and Threats (SWOT) analysis on existing PATC activities, and finally provided several recommendations. While the PATCs have been extremely successful in delivering a world-class programme of HPC-related courses to a large number of students and researchers, the level of participation from those based in non-PATC hosting countries has always been disproportionately low. Hence a major recommendation from the deliverable was to establish a framework where the PATC network can grow reasonably from its current formation. Other opportunities and recommendations are also discussed to facilitate increased flexibility in the implementation of the PATC programme, to carry out additional feedback/impact analysis, as well as to work with other communities for better dissemination and collaboration.

Furthermore, many of the PATCs are now involved in other WP4 activities such as developing Massive open online Courses (MooCs) and establishing a repository of example HPC codes called "CodeVault", which will be reported in other deliverables during the PRACE-4IP project. And additionally, some partners (e.g. ETH Zurich/CSCS) who were not the PATCs' core members so far, have started contributing to PATCs events, helping in their organisation and providing teachers.

2.1 Operation of the PATCs

The operation of the PATCs has remained relatively stable since many of the protocols and tools have developed and evolved from the PRACE-2IP and PRACE-3IP projects. The PATCs' activities are harmonised by the PATC Operational Management Board (OMB), which consists of representatives from each of the PATCs as well as a member of the PRACE-4IP project who is involved in the Training Work Package (WP4). Some of the key operational functions carried out by the PATC OMB during the PRACE-3IP project include planning of the annual PATC programmes (i.e. courses), as well as developing the centralised tools for course dissemination, registration, feedback collection. More details about these functions and processes can be found in [7].

2.2 PATC Courses from February 2015 to February 2016

In February 2015, PRACE-4IP officially took over the delivery of PATC courses from PRACE-3IP. This transition occurred in the middle of the academic year around which the annual PATC course programme is typically designed and scheduled. Hence while it is possible to derive the key statistics from PATC courses strictly within the first year of the PRACE-4IP project (76 courses, 213 course-days, 1,723 participants), this time period spans two PATC programmes (the 2014-15 and 2015-16 programmes). For the sake of consistency with previous deliverables, we shall examine the 2014-15 programme as a whole (inclusive of some PATC courses during the PRACE-3IP project) for further analysis and comparison with past programmes; the analysis of the yet incomplete 2015-16 PATC programme will be deferred until it has been fully implemented, although some statistics already collected are shown.

2.2.1 *Key statistics on numbers of participants and courses*

Key statistics of PATC courses since their establishment is shown in Table 1. It can be seen that many of the key statistics are relatively consistent over the years, e.g. >1,500 participants annually, the feedback responses received have been overwhelmingly positive (8.4/10 average overall rating for PATC courses). There are also slight increases in the proportion of female participation and the number of those coming from non-academic institutions (e.g. industry).

While the level of participation from non-PATC hosting countries has increased somewhat in the 2014-15 programme compared to previous years, the geographical distribution of the participants will be analysed in the next subsection. The “non-host country” statistic is the percentage of participants who is affiliated with an institution outside of the country where the course was held. The “non-PATC” statistic is the percentage of participants who is affiliated with an institution that is not based in any of the PATC-hosting countries. For the average overall rating, maximum score of 10 means "excellent", whereas a zero score means a "waste of time". The 2015-16 programme consists of 72 courses totalling 198 course-days (shown in parentheses) that are being implemented at the time of this deliverable, the numbers reflect partial statistics collected.

	Start-up phase	**2012-13 programme**	**2013-14 programme**	**2014-15 programme**	**2015-16 programme**
Duration	Mar’12 - Jul’12	Aug’12 - Jul’13	Aug’13 - Jul’14	Aug’14 - Jul’15	Aug’15 – Jul’16
Number of courses	19	71	81	77	25 (72)
Total duration (days)	56	204	233	219	58 (198)
Number of participants	511	1,547	1,682	1,786	541
Number of participant-days	1,715	4,702	5,187	5,384	1,513
Female (%)	-	12.9%	14.4%	16.3%	19.6%
Non-academic (%)	-	9.9%	12.3%	15.6%	16.3%
Non-host country (%)	-	20.6%	25.4%	29.5%	14.6%
Non-PATC country (%)	-	13.8%	17.7%	19.9%	9.6%
Feedback response rate (%)	-	63%	64%	53%	-
Average overall rating (0-10)	-	8.5	8.4	8.4	-

Table 1: Key statistics of PATC courses since their establishment.

2.2.2 *Geographical distribution of the participants*

Following the trend from previous analyses of PATC programmes, the geographical distribution of course participants (i.e. the country where each work/study) tend to be highly skewed towards PATC countries, with a low level of participation from outside PATC countries. Shown in Figure 1 is the geographic distribution of PATC course participants within the 2014-15 programme. After normalising with national population sizes, the level of participation from PATC countries is in the order of six times that of non-PATC countries. Although it is to be noted that the situation has improved somewhat slightly over the last few years, with ~30% of participants in 2014-15 coming from non-PATC countries and representing a 10% increase from the 2012-13 PATC programme (Table 1). This has also been analysed in [7], leading to the recommendation that the PATC network should be expanded to increase geographic coverage of PATC participants. Such expansion could be achieved by the creation of PRACE Training Centres, in non-currently PATC hosting countries, sourcing PATC courses locally, collaborating with PATCs in delivering courses locally or by complementing the PATC programme with local courses.

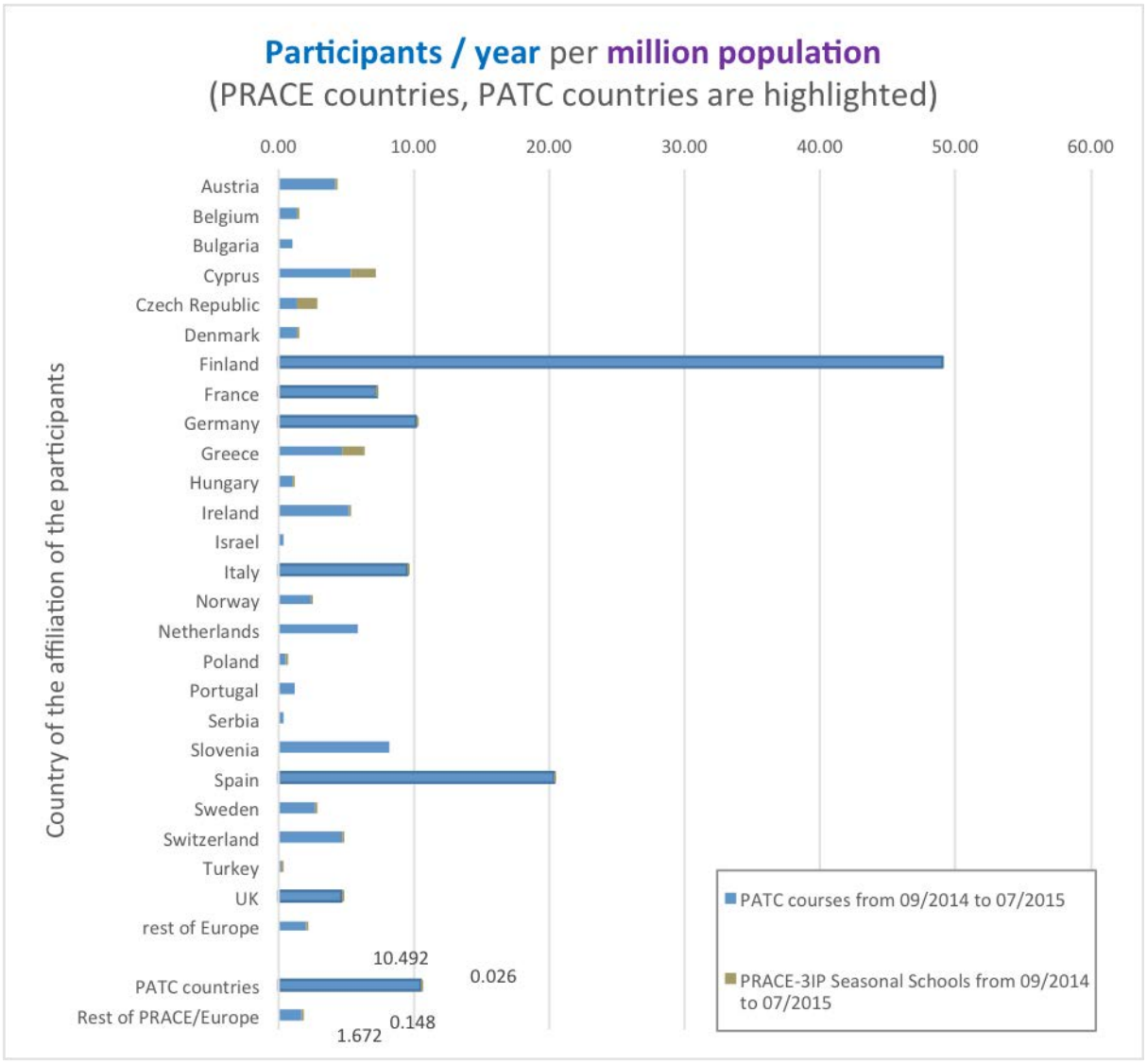


Figure 1: Geographic distribution of PATC course participants, normalised by national population sizes.

2.2.3 *Feedback from PATC course participants*

The feedback received from PATC course participants has generally been very positive. A key indicator is the average overall rating that the courses have accomplished, with the 2014-15 programme achieving an average score of 8.4/10 (Table 1). The feedback surveys also showed that participants are generally satisfied with the organisation of the courses, pace and the subject matter. However, the feedback response rate for the 2014-15 programme has been relatively poor and will need to be addressed in the 2015-16 programme, e.g. by encouraging students to complete the online feedback forms before they leave a course.

3 Seasonal Schools

The PRACE Seasonal Schools have been running since 2008 as part of the PRACE educational programme offering top-quality face-to-face training events organised around Europe, aiming to improve the skills necessary for the use of the PRACE ecosystem. The Seasonal School topics range from generic intermediate to advanced programming techniques

to more specialized topical schools that e.g. focus on a specific topic, such as big data, or offer discipline specific parallel tracks.

Since 2012 Seasonal Schools have run in parallel with the PRACE Advanced Training Centres offering training opportunities mainly in countries where PATCs are not in operation. Among the aims of the Seasonal Schools particularly within the scope of the PRACE-4IP project is their extension focusing on new skills with a strong link to user communities.

3.1 PRACE-4IP Seasonal Schools Planning

In the past the selection of the host for each Seasonal School programme was done within the Training WP of the PRACE Implementation Projects that was financing the schools according to interests expressed by partners. Partners that wished to contribute to the project by hosting a Seasonal School allocated corresponding work effort to the work package and the location and order of the seasonal schools was then discussed and agreed among the participants to the Training WP. Criteria such as the location and past activities were taken into account with a preference given to new hosts and non-PATC countries. A declaration by the partner willing to host the school that they have the ability to host such school was provided as an assurance for the success of the school. At the end of PRACE-3IP it was evident that there is more interest in hosting Seasonal Schools than there are schools, and with many countries already having hosted a school the selection of hosts was not trivial anymore. Thus call for an open process to ensure fairness and transparency has been established.

3.2 Selection Procedure

Scope of Season School Selection Process

Similarly, to the PATC curriculum evaluation PRACE-4IP WP4 sought an independent fair and agreed selection process to assess the proposals of potential candidates for hosting the PRACE Seasonal Schools. The selection process took into account the following main criteria:

- Ability of a partner to host a Seasonal School.
- Location of the Seasonal School.
- Specific thematic area that will be covered by the candidate seasonal school.

Candidates submitted an application form with all relevant information in order to assist the selection panel make a decision for a final proposal to the PRACE-4IP project Management Board (MB) that needed to approve the selection and schedule.

The required information asked from applicants was:

- The training location (Country, city).
- The proffered season.
- The organising partner or partners.
- The thematic area to be covered by the particular seasonal school.
- A draft programme of the school including the number of days, sessions, any envisaged parallel tracks etc.
- Justification for the selection of the objectives and the thematic area of the school. i.e. particular needs of scientists in the area, links with communities, user survey data, previous school feedback etc.

- Description of their training activities for the last two years.
- Local trainers and their expertise in the thematic areas of the proposed seasonal school.
- Training venue and facilities.
- Hands on system to be available to students.
- Extra services such as live broadcast of the event, video recording etc.
- Proposed added value for the training programme.

Criteria of Selection

The following criteria are the generic guidelines that were given to the members of the selection panel in order to perform the selection of the Seasonal Schools hosting partners and therefore locations. The selection panel was encouraged to use such guidelines as well as the application information submitted by candidates to perform a final selection of Seasonal School hosting partners as well as propose the school's schedule. There was no weight associated with the criteria / guidelines presented below.

Seasonal School hosting countries were encouraged to collaborate with other partners that might already have expertise in such events' organisation in order to increase the quality of the schools.

- Location
  - The hosting country must be a PRACE member country.
  - The hosting country should not be a country that hosts PATCs.
  - Preference should be given to hosting countries that have not hosted or have a long time to host a seasonal school. This is under the condition that based on the rest of the application data it is clear that there is a potential for a high standard school to be organised.
  - The location of the hosting country and the organisation details should be such that it can attract students from other countries.
- Capability of the applicant or group of applicants to host the Seasonal School
  - Training experience in the last two years with proven track record of running large international training events.
  - Classroom(s) for 30-60 participants, with reliable network connectivity.
  - Lounges and other hospitable social areas for breaks and group sessions.
  - Extra services offered i.e. video recording.
  - Skilled trainers in the subjects to be covered that can add value to the lectures of the invited PRACE speakers.
  - Ability to do hands-on exercises.
- Training Content
  - Content to be of value and interest to a wide scientific community.
  - The application provides justification of the interest of communities to specific content.
  - Coverage of different topics not covered in other recent Seasonal Schools.

- Coverage of topics relevant to the geographic area and specific user needs.
- The proposed training courses should be well planned covering the objectives of the school.
- The programme committee should have links with PATCs i.e. one of the members to be related to a PATC partner.

Process and Timeline

The PRACE-4IP MB has agreed on the process and a selection committee. The selection committee comprises of five members of PRACE likely not to submit a Seasonal School proposal: two of the members proposed by the PRACE Board of Directors (BoD), One representing the PRACE-4IP MB and two other members proposed by PRACE-4IP WP4 with a preference of being from countries hosting PATCs. The selection panel suggested the hosting partners as well as the schedule for the schools. There is a possibility that the schedule of schools might change at a later stage in agreement among the partners that are affected by such changes and WP4.

Evaluation of the Process

The process has been developed at the beginning of the PRACE-4IP project and has been agreed by the Management Board of the PRACE-4IP consortium. This lead to some delay in opening the call for partners to provide their training plans. However, the outcome seems to be very satisfactory as it provides a very well planned Seasonal School programme that not only defines the location of the schools but also the thematic areas that each school covers. Since the process is now established such delays are not anticipated in the future. The number of proposals received by partners was higher than the six planned events, demonstrating the high interest of partners to organise and host Seasonal Schools. The final selection of schools leads to the need for ad hoc redistribution of effort within the WP4s activities. Finally, it is considered important that all countries have the opportunity to organise such Seasonal Schools, not only once, therefore the collaboration between less experienced and more experienced countries in organising such an event is highly recommended and it has actually been used in this first implementation of the selection process.

3.3 Selected Seasonal Schools Characteristics

The selection panel received applications from eleven countries. After reviewing all applications and taking into account the criteria of the evaluation as specified by the selection process, the selection panel created an ordered list of countries that should organise a PRACE-4IP Seasonal School. Appropriate arrangements for the organisation dates were performed at a later stage. The final plan for the PRACE-4IP Seasonal School schedule was proposed by the selection panel and accepted by the PRACE-4IP MB in July 2015.

Based on the declaration of candidates for their preferred days and the quality of proposals it was advised that the Autumn School 2015 will not be organised. This is due to the fact that the selection panel advised that no acceptable proposals for autumn 2015 were received. The 6 selected schools were scheduled to run from Winter 2015/16 to Spring 2017 according to the following schedule:

Winter 2015/2016: Slovakia

The mission of the Seasonal School is to get together experts and users in the field of Density Functional Theory (DFT) in order to pass along knowledge and experience in the theory itself, ways of parallel implementation of pertinent algorithms as well as efficient use of available DFT codes and program packages in HPC applications. DTF is the computational

method of choice for wide range of applications in physics, chemistry, material science and biology. It has wide community of developers, both in theory and programming, but much wider community of users for whom DFT is the workhorse in their daily routine. The focus of the Seasonal School has the potential to attract enough local and international participants as it addresses issues they may be facing everyday: which program package to choose for efficient parallel applications on certain problem (size) and available computational resources; how are the DFT algorithms implemented for distributed/shared memory parallel computers and other technologies (GPUs, Intel Xeon Phi, etc.); what limits the applicability and parallel scaling of the particular DFT method in all possible respects etc. Attendees that may need to strengthen their knowledge in general parallel algorithms will be provided introductory lectures on MPI/OpenMP and GPU/Intel Xeon Phi programming.

Spring 2016: Ireland

The mission of the school will be to cover methodologies and best practices in exploiting material science applications on HPC systems, in particular PRACE resources. Importantly, discussions are taking place to make this a collaborative event between PRACE and the upcoming European Centre of Excellence (CoE) in Material Science, e-CAM, led by an Irish university (UCD) but also involves many European centres including PRACE partners; it would represent a highly visible collaboration between PRACE and the CoEs. The programme of the school will contain a mix of scientific talks and hands-on training with material science applications on HPC platforms, targeting mainly postgraduate students and postdoctoral researchers. The planned dates for this event are 16-20 May, thus making it a 5 day seasonal school in collaboration with the e-CAM CoE.

Autumn 2016: Austria

The goal of this Seasonal School is to make participants familiar with modern techniques and tools for the development of scalable applications on modern computer architectures (massively parallel systems as well as many-integrated-core architectures). The school will pursue an integrated approach where various topics are presented that complement each other. In order to make the programme attractive for participants with varying backgrounds, the programme will offer both, more basic topics (parallel programming with OpenMP and MPI, parallel I/O, profiling techniques and tools) and more advanced/specialized ones (Xeon Phi programming, advanced topics in parallel programming, Portable Extensible Toolkit for Scientific computing) from which the participants can individually select that portfolio that is most suitable for their background.

Winter 2016/2017: Israel

Recognizing that HPC resources and cloud-based infrastructures are the cornerstone to ambitious academic scientific research, the school will bridge the gap between them and leverage their power to enable top level research. The school’s mission is to raise awareness of the usability of PRACE HPC resources and cloud infrastructures, reaching researchers with varying levels of expertise, from multiple disciplines to provide a very thorough overview including fundamental HPC topics and to introduce topics of importance and interest to the computational science community.

Early Spring 2017 Sweden

Life Science research has become increasingly digital, and this development is accelerating rapidly. Biomolecular modelling techniques such as homology modelling, docking, and molecular simulation have advanced tremendously due to world leading European research, resulting in extreme demands for better computational performance and throughput as these tools are used in applied research and industrial development. This research has direct

influence on our daily life in areas such as health and medical applications, the development of new drugs, efficient drug delivery, biotechnology, environment, agriculture and food industry. Life Science is one of the largest and fastest growing communities in need of high-end computing, and it is a critically important industrial sector for Europe. The dedicated CoE for Biomolecular Research (BioExcel) has recently been established in Sweden, Stockholm where KTH is the coordinating partner. Thus the mission of this school will be to give a comprehensive curriculum on several widely used life science software on PRACE HPC systems. Discuss their scalability and performance issues and teach best practices on HPC systems that have been observed during PRACE research activities. Extensive hands-on sessions will cover more than half of the school period.

Mid Spring 2017: Cyprus

The mission of the Seasonal School will be to have two parallel sessions to cater for the training requirements of different persons in the PRACE community.

One of these sessions will be a HPC system's administrator track. This is something that PRACE has not yet offered in its Seasonal School training and will be beneficial to PRACE and other HPC sites. Given the large number of systems present and available to users through PRACE Project Calls and PRACE DECI calls, it is important for the system administrators of these sites to have up to date, state of the art education on the latest technologies and tools which could help in their duties and allow them to better help PRACE and their respective users who gain access to their systems. Furthermore, experienced administrators from PRACE will be able to share their expertise, network with each other, discuss, advise and share ideas.

The second session will be performed in collaboration with the regional (South Eastern Europe and Mediterranean) Virtual Research Environment that supports the fields of life sciences, climatology and cultural heritage. The focus will be not only on HPC compute but also data management and domain specific services deployed over different computational resources including HPC, cloud and grid. Parts of the second session will be relevant to PRACE communities as apart from HPC this will provide them with training on data management and more specifically training for data generation, processing, preparation of the data for the simulation step and data analysis.

3.4 Initial Feedback from Winter School 2015/1016

The mission of the Seasonal School was to get together experts and users in the field of Density Functional Theory (DFT) in order to pass along knowledge and experience in the theory itself, ways of parallel implementation of pertinent algorithms as well as efficient use of available DFT codes and program packages in HPC applications. DTF is the computational method of choice for wide range of applications in physics, chemistry, material science and biology. It has wide community of developers, both in theory and programming, but much wider community of users for whom DFT is the workhorse in their daily routine. The school focus in subjects such as: which program package to choose for efficient parallel applications on certain problem (size) and available computational resources; how are the DFT algorithms implemented for distributed/shared memory parallel computers and other technologies (GPUs, Intel Xeon Phi, etc.); what limits the applicability and parallel scaling of the particular DFT method in all possible respects etc.

The school was held in Bratislava, Slovakia between 25-28 January 2016. Trainers where invited from the US, Germany, Switzerland and Austria as well as local trainers from Slovakia. The total number of participants was 36, including 20 from Slovak Republic, 14

from Czech Republic, 1 from Slovenia, 1 from Greece. The overall score of this school was 8.34.

4 On-demand Events Planning

One of the aims of PRACE is to provide computational services to the different CoEs. The services will include compute time on PRACE supercomputers, training and access to competence. Part of the educational programme of the PRACE-4IP project is the collaboration with CoE and ETP4HPC and the organisation of a series of on-demand events. Six such events are envisaged to be organised during the PRACE-4IP project.

On-demand events could be events specifically organised for CoE communities in a supercomputing centre of PRACE, or some additional training days to events that are already being organised by CoEs.

To better understand the requirements for the different CoEs, PRACE-4IP WP4 and WP7 prepared a technical discussion with different members of the CoEs. As a guideline for the discussion both work packages prepared a questionnaire (see Annex B – The training requirements questionnaire towards the CoEs) while the actual discussion where conducted as a teleconference or a Skype meeting. Further to that the PRACE-4IP WP4 leader participated in the CoE-PRACE-EXDCI-ETP collaboration meeting where initial ideas of collaboration among the participants have been exchanged. The work package is also in contact with ETP4HPC regarding possibilities and need for collaboration in training activities.

The structure of the questionnaire from the training point of view was the following: The required level of training, the technologies and platforms that are of interest to the CoE, the specific codes that are of use and interest to the CoEs and the type of involvements that the CoE have with these codes, the algorithms of interest to the CoE, the programming tools, the preferred locations and the type of events (a dedicated event, or an event co-located with other CoE events).

We have received answers from the following CoEs: EoCoE, BioExcel, MaX, ESiWACE, e-CAM, POP, NoMaD and COEGSS.

The following remarks summarise the requirements of the CoEs in terms of training and more specifically the on-demand events:

- Most of the CoEs require advanced training however basic and intermediate training is also required by the majority of them. A couple of CoEs do not have yet clear requirements and would come back to the activity at a later stage regarding training. The activity via collaborating partners maintains contacts with those CoEs.
- All of the CoEs require training in a variety of technologies and platforms such as x86, Power, Xeon Phi, GPUs.
- Regarding application coding expertise, while several CoEs are interested in general training, development, usage of application codes, most of them require specialised training in optimization, debugging and performance analysis of such application codes.
- Regarding algorithms, CoEs are interested in a variety of them including Dense Linear Algebra, Spare Linear Algebra, FFTs, N-Body, Mesh. Special interest from CoEs is given to the data management aspects of using HPC systems.

- In terms of programming tools, the most popular needs among the CoEs are the following: MPI, OpenMP, OpenCL, CUDA, OpenACC, as well as OmpSs and thread building blocks.
- Several CoEs expressed their requirements in terms of the location for organising on-demand trainings events. Locations preferences are obviously based on the location of the centres and their partners.
- Finally, the CoEs agree that on-demand events can be organised either as independent training events or training days appended in some other CoE specific events.

Based on the above results and the particular needs of individual CoEs PRACE partners involved in the Training WP are at the moment of writing this deliverable, preparing proposals for the organisation of the on-demand events. Such proposals will be communicated to the CoEs and the exact contents and days of such events will be planned.

5 International Summer Schools

The International HPC Summer School on Challenges in Computational Sciences is a series of events started in 2010 and taking place annualy. Initiated by NSF's TeraGrid and EU's DEISA project, the first school was organised in Italy in 2010, and was then continued by NSF's XSEDE and EU's PRACE projects with locations alternating between North America and Europe. The objective of the Summer School is to familiarise the best students of the respective continents or countries in computational sciences with a strong bond to supercomputing with all major state of the art aspects related to HPC for a broad range of scientific disciplines, catalyse the formation of networks, provide mentoring through faculty members and supercomputing experts from renowned HPC centres, and to facilitate international exchange and open further carrier options.

5.1 International Summer School 2015

The international HPC Summer School of 2015 was held between 21-26 June 2015, in Toronto, Canada. The main topics covered in this six-days event were the following:

- HPC challenges by discipline (e.g, earth, life and materials sciences, physics).
- HPC Programming Proficiencies.
- Performance analysis and profiling.
- Algorithmic approaches and numerical libraries.
- Data-intensive computing.
- Scientific visualisation.
- Canadian, EU, Japanese and U.S. HPC-infrastructures.

5.2 Planning for the International Summer School 2016

This year’s International HPC Summer School will be organised in Europe. A proposal from Slovenia has been received and after being evaluated by all the organising members it was accepted. The seventh International HPC Summer School in 2016 is going to take place in Ljubljana, the capital of Slovenia and European Green Capital 2016, from 26 June - 1 July. The five-days, expense-paid event will bring together 80 excellent students from many parts

of the world, to participate for one week in an exciting programme coupled with dedicated mentoring and networking.

6 Conclusions

Continuing the training activities of PRACE-3IP starting from February 2015, PRACE-4IP is extending the PRACE training offerings with the introduction of the Massive open online Courses (MooCs) and the CodeVault, a core repository for training codes open to all students worldwide. Further to that PRACE maintains the training portal that is a repository of a lot of training material from the face-to-face training events, including presentations, hands-on material as well as videos from the events. Despite all these online training offerings, face-to-face training holds a very strong position in PRACE training events. Both PATCs, Seasonal Schools and the International HPC Summer School attracted hundreds of students to travel across great distances with the goal to take part in courses of international scope, in which they can not only learn a lot, but also present their own work, consult it with experts, find new collaborators, try their codes on new machines, and so on. The face-to-face PRACE training offering will be strengthened with the on-demand events in collaboration with the CoEs. The collaboration with the CoEs is already being materialised by means of organising particular Summer Schools events. We strongly believe that the excellent reputation of PRACE training events must imply the commitment to further develop and improve this service.

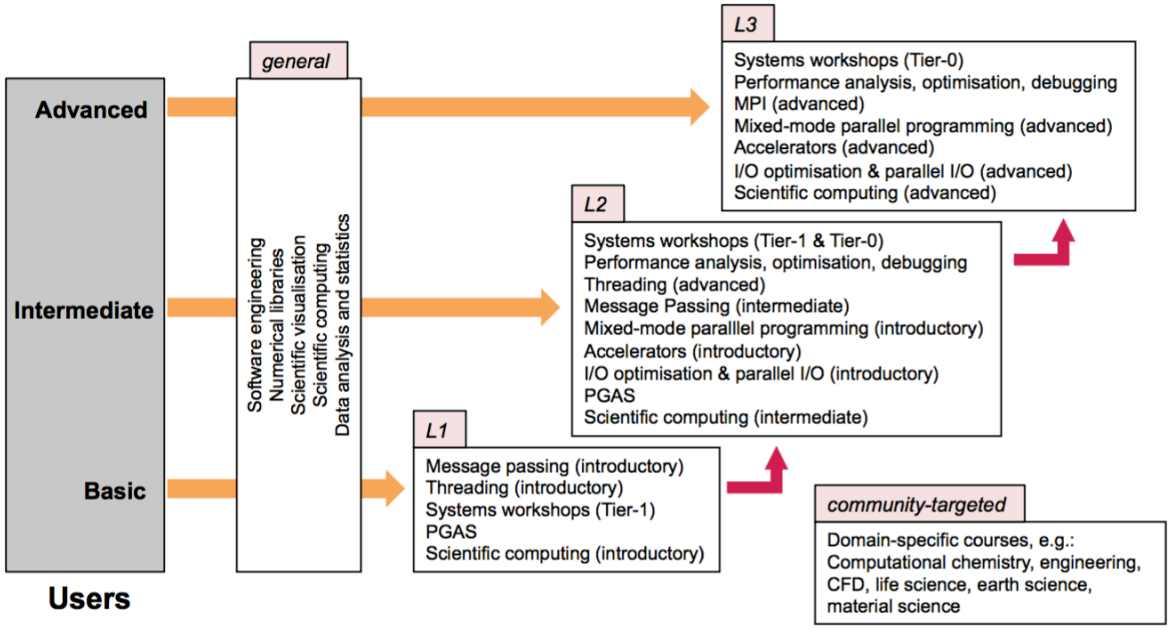
7 Annex A – Training Courses offered by PRACE February 2015 - January 2016

Type	Title	Host	Location	Start Day	# of Days
PATC	Advanced visualization with Paraview	MdS	Saclay, FR	2016-01-27	2
Seas Sc	PRACE Winter School 2016	CCSAS	Bratislava, SK	2016-01-25	4
PATC	Python in High-Performance Computing	CSC	Espoo, FI	2016-01-25	3
PATC	Ab initio Periodic Codes - Joint MCC-UKCP-EPCC Workshop	EPCC	Daresbury, UK	2016-01-19	4
PATC	Introduction to hybrid programming in HPC	GCS	Garching, DE	2016-01-14	1
PATC	Introduction to OpenMP and MPI	EPCC	Edinburgh, UK	2015-12-16	1
PATC	Shared-Memory Programming with OpenMP	EPCC	Edinburgh, UK	2015-12-15	2
PATC	Introduction to simulation environment for Earth Sciences	BSC	Barcelona, ES	2015-12-15	2
PATC	Software Carpentry	EPCC	Edinburgh, UK	2015-12-14	2
PATC	Efficient Parallel IO on ARCHER	EPCC	Edinburgh, UK	2015-12-10	2
PATC	Node-Level Performance Engineering	GCS	Garching, DE	2015-12-10	2
PATC	Introduction to Accelerators	CSC	Espoo, FI	2015-12-08	3
PATC	Programming on GPUs	MdS	Saclay, FR	2015-12-07	3
PATC	Python for computational science	CINECA	Bologna, IT	2015-12-01	3
PATC	Debugging & Optimization	MdS	Montpellier, FR	2015-11-30	5
PATC	Practical Software Development	EPCC	Edinburgh, UK	2015-11-24	2
PATC	Parallel Programming Workshop	BSC	Barcelona, ES	2015-11-23	5
PATC	High Performance Molecular Dynamics	CINECA	Bologna, IT	2015-11-18	3
PATC	Data Carpentry	EPCC	Edinburgh, UK	2015-10-29	2
PATC	Advanced MPI	EPCC	Edinburgh, UK	2015-10-28	2
PATC	Debugging and Optimization of Scientific Applications	CINECA	Bologna, IT	2015-10-26	3
PATC	Introduction to Parallel Programming	CSC	Espoo, FI	2015-10-20	3
PATC	Parallel Programming with MPI and OpenMP and Advanced Parallel Programming	GCS	Stuttgart, DE	2015-09-28	5
PATC	Industrial Workshop on COMSOL and OpenFOAM	CSC	Stockholm, SE	2015-09-23	3
PATC	Introduction to Fortran Programming	CSC	Espoo, FI	2015-09-22	3
PATC	Advanced Fortran Topics	GCS	Garching, DE	2015-09-17	2
PATC	Message-Passing Programming with MPI	EPCC	Edinburgh, UK	2015-07-15	3
PATC	Hands-on Introduction to HPC	EPCC	Edinburgh, UK	2015-07-13	2
PATC	Programming and Tuning Massively Parallel Systems (PUMPS)	BSC	Barcelona, ES	2015-07-06	5
PATC	Node-level Performance Engineering	GCS	Stuttgart, DE	2015-07-06	2
PATC	Advanced OpenMP	EPCC	Manchester UK	2015-07-02	2
PATC	Introduction to Molecular Dynamics on ARCHER	EPCC	Strathclyde, UK	2015-06-29	3
PATC	Programming paradigms for new hybrid architectures	CINECA	Bologna, IT	2015-06-29	3
PATC	Performance Analysis Workshop	EPCC	Durham, UK	2015-06-25	2
Int Sum Sc	International HPC Summer School 2015	PRACE	Toronto, CA	2015-06-22	5
PATC	Workshop HPC Methods for Engineering	CINECA	Milan, IT	2015-06-17	3
PATC	Hybrid MPI/OpenMP programming	MdS	Saclay, FR	2015-06-15	4
PATC	Atomic and molecular calculation software on massively parallel machines: present and future	MdS	Bruyères-le-Châtel, FR	2015-06-10	2
PATC	School on Scientific Data Analytics and Visualization	CINECA	Milan, IT	2015-06-08	5
PATC	Runtime systems for heterogeneous platform programming	MdS	Bordeaux, FR	2015-06-04	2
PATC	Introduction to CUDA Programming	BSC	Barcelona, ES	2015-06-02	4
PATC	Uncertainty quantification	MdS	Saclay, FR	2015-05-26	3
PATC	A Hands on introduction to HPC for Women in HPC in collaboration with PRACEDays15	EPCC	Dublin, IE	2015-05-25	2

PATC	Single-sided PGAS Communications Libraries	EPCC	Bristol, UK	2015-05-20	2
PATC	18th VI-HPS Tuning Workshop	MdS	Grenoble, FR	2015-05-18	5
PATC	Systems Workshop: Programming ARM based prototypes	BSC	Barcelona, ES	2015-05-15	1
PATC	Heterogeneous Programming on GPUs with MPI + OmpSs	BSC	Barcelona, ES	2015-05-13	2
PATC	Introduction to Parallel Computing with MPI and OpenMP	CINECA	Milan, IT	2015-05-11	3
PATC	Performance Analysis and Tools	BSC	Barcelona, ES	2015-05-11	2
PATC	Intel MIC&GPU Programming Workshop	GCS	Garching, DE	2015-04-27	3
PATC	Introduction to Unified Parallel C (UPC) and Co-array Fortran (CAF)	GCS	Stuttgart, DE	2015-04-23	2
PATC	Hands-on Porting and Optimisation Workshop	EPCC	Edinburgh, UK	2015-04-20	1
PATC	GPU Programming with CUDA	GCS	Juelich, DE	2015-04-20	3
PATC	Debugging and Optimization of Scientific Applications	CINECA	Rome, IT	2015-04-20	3
PATC	ARCHER Software Carpentry Workshop	EPCC	London, UK	2015-04-16	2
PATC	OpenACC Programming for Parallel Accelerated Supercomputers	GCS	Stuttgart, DE	2015-04-16	2
PATC	Systems Workshop: Programming MareNostrum III	BSC	Barcelona, ES	2015-04-16	2
PATC	Introduction to Fortran programming	CSC	Espoo, FI	2015-04-14	3
PATC	Advanced Topics in High Performance Computing	GCS	Garching, DE	2015-04-07	4
PATC	Parallel linear algebra	MdS	Montpellier, FR	2015-04-07	4
PATC	Advanced Usage on CURIE Tier-0 Supercomputer: Best practices and code optimization	MdS	Bruyères-le-Châtel, FR	2015-03-31	3
PATC	Workshop HPC enabling of OpenFOAM for CFD applications	CINECA	Bologna, IT	2015-03-25	3
PATC	Parallel I/O and Portable Data Formats	GCS	Juelich, DE	2015-03-16	3
PATC	Simulation Environments for Life Sciences	BSC	Barcelona, ES	2015-03-12	2
PATC	HPC numerical and domain specific Libraries	CINECA	Bologna, IT	2015-03-11	3
PATC	Spring School in Computational Chemistry 2015	CSC	Espoo, FI	2015-03-10	4
PATC	Fortran for Scientific Computing	GCS	Stuttgart, DE	2015-03-09	5
PATC	Parallel filesystems and parallel IO libraries	MdS	Saclay, FR	2015-03-05	2
PATC	Cray XC40 Optimization, and Parallel I/O Courses	GCS	Stuttgart, DE	2015-03-02	4
PATC	Industrial Services of the National HPC Centre Stuttgart	GCS	Stuttgart, DE	2015-02-25	1
PATC	Advanced Threading and Optimization	CSC	Espoo, FI	2015-02-24	3
PATC	17TH VI-HPS Tuning Workshop	GCS	Stuttgart, DE	2015-02-23	5
PATC	Introduction to scientific programming using GPGPU and CUDA	CINECA	Rome, IT	2015-02-19	2
PATC	Programming Distributed Computing Platforms with COMPSs	BSC	Barcelona, ES	2015-02-19	1
PATC	Petaflop System Administration; Marenostrum III	BSC	Barcelona, ES	2015-02-11	2
PATC	11th Advanced School on Parallel Computing	CINECA	Bologna, IT	2015-02-09	5
PATC	HPC-based simulations, Engineering and Environment	BSC	Barcelona, ES	2015-02-03	3
PATC	Third JUQUEEN Porting and Tuning Workshop	GCS	Juelich, DE	2015-02-02	3

8 Annex B – The training requirements questionnaire towards the CoEs

Introduction - PRACE Curriculum



Outline of the HPC curriculum with topics that are aimed at participants with different levels of HPC experience. The PATC curriculum achieves a wide coverage of these topics while Seasonal Schools also cover a wide range of such topics.

Training needs for the organisation of ad hoc training events targeting the needs of CoEs – questionnaire

1. Level of training - In general, at what level would your community require HPC training
    a. Basic
    b. Intermediate
    c. Advanced

2. Technologies and platforms - In what type of technologies and platforms you need training and at what level for each one of them?
    a. x86
    b. Power
    c. Xeon Phi
    d. NVIDIA GPGPU
    e. AMD GPGPU/APU
    f. Other

3. Codes - Would you like specific training for application codes you are using or developing? Where would you give more emphasis and what level of training do you require? (Please specify the code names for each category)
    a. General
    b. Development

c. Usage
d. Optimization
e. Debugging
f. Performance analysis
g. Other

4. Algorithms - What types of algorithms do you usually use or develop to solve your scientific problems and what level of training would you require for each one of them?
    a. Dense Linear Algebra
    b. Sparse Linear Algebra
    c. FFTs
    d. N-Body
    e. Mesh
    f. Data management
    g. Other

5. Programming tools - What programming tools do you use and what level of training would you require for each one of them?
    a. MPI
    b. Fortran CoArrays
    c. Unified Parallel C (UPC)
    d. Chapel Global
    e. Arrays Toolkit
    f. X10
    g. OpenMP
    h. OpenCL
    i. CUDA
    j. OpenACC
    k. OmpSs
    l. Thread Building Blocks (TBB)
    m. Cilk Plus
    n. Spark
    o. Other

6. Programming Languages - What programming languages do you use and what level of training would you require for each one of them?
    a. C
    b. C++
    c. Fortran
    d. Python
    e. Java

f. R
g. Other

7. Industry – Relationship with industry and commercial software
    a. Do you have industrial partners that require specialized training? i.e. at different levels of training different subjects than the core scientific communities of your CoE?
    b. Do you use commercial software and what type and level of training would you require for such software?

8. Location - Is there a preferred location where you would like to have a training

9. Organisation
    a. Would you prefer if some PRACE trainers experienced in the subjects you are interested in visit your training events in order to offer specialised courses?
    b. Would you prefer a dedicated training event at a location that you specify (and is convenient for PRACE trainers)?

Other requirements – please specify any other requirements or views you might have on your training needs.

9 Annex C PRACE Winter School 2016 - Event Report

1. Basic information about the event

1.1. Name

PRACE Winter School 2016: Density functional theory from the perspective of HPC

1.2. Dates

25.1.2016 - 28.1.2016

1.3. Location

Bratislava, Slovakia

1.4. Organizing sites

Computing Center of Slovak Academy of Sciences (CC SAS)

IT4Innovations National Supercomputing Center, Czech republic (IT4I)

1.5. Mission

The mission of the seasonal school is to get together experts and users in the field of Density Functional Theory (DFT) in order to pass along knowledge and experience in the theory itself, ways of parallel implementation of pertinent algorithms as well as efficient use of available DFT codes and program packages in HPC applications. DTF is the computational method of choice for wide range of applications in physics, chemistry, material science and biology. It has wide community of developers, both in theory and programming, but much wider community of users for whom DFT is the workhorse in their daily routine. From our perspective, the focus of the seasonal school has the potential to attract enough local and international participants as it addresses issues they may be facing everyday: which program package to choose for efficient parallel applications on certain problem (size) and available computational resources; how are the DFT algorithms implemented for distributed/shared memory parallel computers and other technologies (GPUs, Intel Xeon Phi, etc.); what limits the applicability and parallel scaling of the particular DFT method in all possible respects etc. Attendees that may need to strengthen their knowledge in general parallel algorithms will be provided introductory lectures on MPI/OpenMP and GPU/Intel Xeon Phi programming.

1.6. Event URL

https://events.prace-ri.eu/event/440

2. Organizational details

2.1. Local organizing committee

Name	Organization
Michal Pitoňák	CC SAS
Lukáš Demovič	CC SAS
Jozef Noga	CC SAS
Tomáš Lacko	CC SAS
Ondřej Jakl	IT4I

2.2. Venue (name, its description and why it was selected; fluid text: analysis how good the selection was for the event)

PRACE Winter School 2016 was held in Bratislava, the capital of Slovakia, in the campus of the Slovak Academy of Sciences, with good accessibility via public transport and not far from several accommodation opportunities (hotels, hostels, dormitories). Training was held in a conference room of the Center for Quantum Technologies (QUTE) of the Institute of Physics of Slovak Academy of Sciences with the capacity of more than 50 people. Wireless connection was provided, each participant had his own desk. Coffee breaks were served in the corridor leading to the conference room as well as in a small kitchen next doors. According to the evaluation the school *obtained an overall rating of 8.34*.

3. Program & content

3.1. Program committee (table)

Jozef Noga	CC SAS
Michal Pitoňák	CC SAS
Lukáš Demovič	CC SAS
Ondřej Jakl	IT4I

3.2. Designing the program (fluid text: reasoning and goals-setting behind the program)

The program was concentrated on the Density Functional Theory (DFT) and particularly it's implementation on modern parallel computer architectures. DFT is the most commonly used computational method in chemistry and material science thus having a broad community of users. Our goal was to give deeper insight into implementation of the DFT methods and show ways how DFT is programmed on distributed/shared memory parallel computers and accelerators (MIC/GPU). DFT users can thus get a feeling on limitations of scaling their distributed calculations, choose proper architecture for their production jobs as well as get more familiar with parallel programming explained on theory they understand.

3.3. Description of the contents (brief commentary of each lecture and lab/exercise)

- Introduction to DFT I./II.: General overview of the density functional theory.
- Introduction to MPI: Brief overview of parallel computing and parallel computer architectures. Introduction to Message Passing Interface (MPI) for distributed memory parallelism, basis MPI commands (point-to-point and collective operations, etc.). During the hands-on session participants were given access to Aurel supercomputer to solve simple MPI exercises.
- Introduction to GPU and MIC: Overview of GPU/MIC architecture and programming models. During the hands-on session participants were given access to Salmon and Anselm supercomputers at IT4I to solve several exercises.
- DFT with Petachem: Extensive overview of DFT implementation on GPUs in Petachem. Real-life examples of extensive applications on biologically relevant molecules on GPUs. During the hands-on session participants prepared inputs and carried out a quantum-chemical simulation using Petachem on Anselm supercomputer.
- DFT with Turbomole: Extensive overview of shared and distributed-memory parallelization and other fast DFT algorithms implemented in Turbomole. During the hands-on session participants were familiarized with Turbomole GUI which serves for input preparation, job management and results visualization.
- DFT with CPMD: Overview of theory and implementation of plane-wave DFT for dynamic simulations. During the hands-on session participants carried out their own simulation on Aurel supercomputer.

- DFT with VASP: Lecture was focused on the theory, implementation and applications of DFT in material science. Hands-on session carried participants through the process of input preparation, calculation execution and results evaluation using the VASP program package.

4. List of Trainers

Fang Liu	Fang Liu is a Ph.D. candidate at Stanford University working with Professor Todd Martínez on GPU-accelerated quantum chemistry. She has worked on topics ranging from absorption spectrum simulation, GPU-accelerated DFT implementation, to polarizable continuum models. A few of her current research interests include restricted ensemble-averaged Kohn Sham methods, non-equilibrium solvation effects, and fragment-based electronic structure methods. ffangliu@stanford.edu
Marek Sierka	Professor Sierka's research group is a part of the Otto Schott Institute of Materials Research (OSIM) at the Faculty of Physics and Astronomy of the Friedrich-Schiller-Universität, Jena. His research activities focus on the development and applications of atomistic and quantum mechanical computational methods for investigating structure, properties and reactivity of complex materials. The hallmark of our research programme is close collaboration with experimental groups working in various disciplines of chemistry, physics and materials science. marek.sierka@uni-jena.de
Uwe Huniar	Prior to joining COSMOlogic in 2005, Uwe worked in the Ahlrichs group at the University of Karlsruhe where TURBOMOLE was created and developed for years. He is an expert for the TURBOMOLE program and maintains the source code. He is responsible for the TURBOMOLE support and also involved in the development of micelle applications with COSMO-RS and the COSMO*mic* tool. huniar@cosmologic.de
Dr. Ivano Tavernelli	In the field of quantum-classical dynamics developed and implemented in the CPMD software package novel theoretical frameworks able to combine electronic structure techniques based on density (DFT and TDDFT) with the calculation of nonadiabatic quantum and classical trajectories. His research interests in this field comprise adiabatic and nonadiabatic molecular dynamics (Ehrenfest dynamics, trajectory surface hopping, and Bohmian dynamics) for the study of photochemical and photo-physical processes in molecules, condensed phase, and biological systems. More recently extended his research activities in the field of material design, focusing on the combination of ab-initio and machine learning techniques together with big-data analysis for the design of new materials with improved properties. ita@zurich.ibm.com
Martijn Marsman	Dr. Marsman from the Department of Material Physics at Vienna University and is one of the main developers of the VASP program package. martijn.marsman@univie.ac.at
Prof. Vladimir Malkin	The group of Vladimir and Olga Malkin mostly concentrates its work on development of new quantum chemical methods for calculation of electronic structure and properties of molecules. Traditionally the central topic was the calculation of parameters of NMR and EPR spectroscopy by using density functional theory (DFT) method. Due to the fact that relativistic effects (first of all,

	spin-orbit coupling) affects these spectroscopic parameters much earlier than many other properties of molecules, it was natural that last years the group pays much attention to relativistic methods to calculate electronic structure. Lately the major interest starts to shift towards more fundamental topics: improvement efficiency of the existing QC methods, development of a new quantum chemical method based on density matrix theory, solving a time-dependent Dirac-Coulomb equation, going beyond Born-Oppenheimer approximation. vladimir.malkin@savba.sk
Dr. Lubomír Říha	Dr. Říha works at IT4Innovations National Supercomputing Center, VŠB - Technical University of Ostrava and focuses on a new hybrid domain decomposition method combining the FETI and FETI-DP methods that deliver better parallel scalability on a very large number of processors. He works on its C++ implementation using the Intel MKL library, and on the parallelization of the local coarse problems using Intel Xeon Phi accelerators. lubomir.riha@vsb.cz
Ing. Michal Merta	Is a researcher at IT4Innovations National Supercomputing Center, VŠB - Technical University of Ostrava. His professional interests are oriented towards dynamical contact problems, fast boundary element method and parallel computing. michal.merta@vsb.cz

3.6 Computer resources (listing: supercomputer accesses as well as local IT infra available for the attendees; fluid text: comment if they were sufficient for the event)

Aurel Supercomputer (IBM P775) supercomputer at CC SAS; Anselm (Bull) and Salomon (SGI) supercomputers with GPU and MIC accelerators at IT4I. Participants obtained temporary accounts, accessible from the laptops of their own via wireless connection, which allowed them to work on all the aforementioned resources during the event in sufficient extent.

5. Participants & feedback

5.1. Number of participants by country (table, full list of participants as an appendix)

Slovak Republic	20
Czech Republic	14
Slovenia	1
Greece	1

5.2. Analysis of the feedback (fluid text: analyze the feedback in general and all specific very good or bad comments)

Based on the survey results, we believe that participants mostly enjoyed the event in general. We also believe that we attracted just the right auditorium for the lectures speakers provided. We admit there were a few disturbing moments, such as unstable wifi connection at the beginning, but we enforced it just in time the hands-on sessions started. According to the evaluation the school *obtained an overall rating of 8.34.*

6. Awareness activities, outreach

The collaboration with IT4I including wide dissemination in the Czech Republic helped a lot in attracting many Czech participants, almost 40%. This is in striking contrary with no participants from Hungary and Austria,

countries that are even closer to Bratislava, which was an ideal venue from the point of view of being located near the border of four PRACE partners.