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PRACE-5IP

PRACE Fifth Implementation Phase Project

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Interim PRACE Training Report
Final

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Table of Contents

List of Figures

List of Tables

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[22] HPCwire, www.hpcwire.com

[23] Scientific Computing World, www.scientific-computing.com

[24] PRACE Events portal, http://events.prace-ri.eu

[25] PRACE Training portal, http://www.training.prace-ri.eu

[26] DSpace, software for building open digital repositories, www.dspace.org

[27] Invenio Digital Library Framework, customised digital library, institutional repository, multimedia archive, or research data repository on the web. invenio-software.org

[28] EPrints, a free and open-source software package for building open access repositories, www.eprints.org

[29] CodeVault repository located at gitlab, https://gitlab.com/PRACE-4IP/CodeVault

[30] CodeVault located at PRACE's own infrastructure, https://repository.prace-ri.eu/git/

[31] EUDAT - Research Data Services, Expertise & Technology Solutions, https://www.eudat.eu/

List of Acronyms and Abbreviations

aisbl	Association International Sans But Lucratif (legal form of the PRACE-RI)
BLAST	Basic Local Alignment Search Tool
BoD	PRACE Board of Directors
CFD	Computational Fluid Dynamics
CMS	Content Management System

CoE	Center of Excellence
CPU	Central Processing Unit
CUDA	Compute Unified Device Architecture (NVIDIA)
EC	European Commission
FSI	Fluid-Structure Interaction
GM	General Manager
GPU	Graphic Processing Unit
HPC	High Performance Computing; Computing at a high performance level at any given time; often used synonym with Supercomputing
ISC	International Supercomputing Conference; European equivalent to the US based SCxx conference. Held annually in Germany.
MB	Management Board (highest decision making body of the project)
MOOC	Massive Open Online Course
MPI	Message Passing Interface
NGS	Next-Generation Sequencing
PA	Preparatory Access (to PRACE resources)
PATC	PRACE Advanced Training Centre
PGAS	Partitioned Global Address Space
PRACE	Partnership for Advanced Computing in Europe; Project Acronym
PRACE-PP	PRACE Preparatory Phase project
PTC	PRACE Training Centre
RMA	Remote Memory Access
RI	Research Infrastructure
RIKEN	A large research institute in Japan with 3,000 scientists on seven campuses across Japan, founded in 1917.
SME	Small and Medium Enterprise
SSC	Scientific Steering Committee
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
UEABS	Unified European Application Benchmark Suite

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 (3rd 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., Germany
GENCI	Grand Equipement National de Calcul Intensif, France
GRNET	Greek Research and Technology Network, Greece
ICHEC	Irish Centre for High-End Computing, hosted by NUI Galway
INRIA	Institut National de Recherche en Informatique et Automatique, France (3rd Party to GENCI)
IST	Instituto Superior Técnico, Portugal (3rd Party to UC-LCA)
IT4I	IT4Innovations, National supercomputing centre at VŠB-Technical University of Ostrava, Czech Republic
IUCC	Inter University Computation Centre, Israel
JUELICH	Forschungszentrum Juelich GmbH, Germany
KIFÜ (NIIFI)	Governmental Information Technology Development Agency, Hungary
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
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
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)
WCNS	Politechnika Wroclawska, Poland (3rd Party to PNSC)

Executive Summary

The Training Work Package (WP4) of the PRACE Fifth Implementation Phase (PRACE-5IP) project is responsible for the training activities of PRACE. In addition to the extensive programme of face-to-face training delivered by the PRACE Advanced Training Centres (PATCs) and PRACE Training Centres (PTCs), the training activities also include the On-demand training events, a series of online training offerings such as the Massive Open Online Courses (MOOCs), the training code repository (CodeVault) and the training portal. This deliverable is a report of all the PRACE-5IP training activities during the initial 15 months of the project.

PRACE-5IP continued the training activities of PRACE-4IP starting from February 2017. Between February 2017 and April 2018, the six PATCs delivered 103 courses, 290 course-days with 2,396 participants, while the four PTCs delivered 12 courses, 21 course-days with 351 participants. The feedback responses received have been overwhelmingly positive (8.5/10 average overall rating for PATC courses).

Similarly, the PRACE Seasonal Schools in PRACE-5IP have been carefully selected via a formal selection process. The Seasonal Schools scheduled for this reporting period, namely the Autumn School 2017 in Gdańsk, Poland and the Winter Seasonal School 2018 in Bratislava, Slovak Republic, attracted 39 attendees in total, and obtained high overall ratings.

In addition, WP4 continued the collaboration with the Centres of Excellence (CoEs) where a number of On-demand events were organised. Finally, WP4 co-organised the 2017 International Summer School on HPC Challenges in Computational Sciences in Boulder, Colorado, United States of America, from 25-30June 2017.

All forms of face-to-face and online training are complementary. They contribute to the success of the PRACE training programme, and should be continued in future PRACE HPC training activities. In accordance with the PRACE-5IP goals, the majority of training events also address industrial users, and motivate them by showing the importance and benefits of HPC for the practice.

1 Introduction

Training plays an important role in building a European base of highly-skilled, knowledgeable HPC users and application developers. This will be key to strategic initiatives such as EuroHPC, which aims to build a leading European ecosystem in terms of technology, applications and skills underpinned by exascale HPC infrastructure, by around 2022/2023. Efficient exploitation of exascale hardware will undoubtedly raise new challenges for application developers and users, who will also have influence over exascale technology development under EuroHPC. Hence developing human expertise is of paramount importance in the ecosystem. Europe is in a strong position in that regard and must sustain investments in HPC education and training programmes in order to remain competitive and to realise the aims of EuroHPC.

PRACE has been offering educational and training programmes for the needs of the European HPC community since 2008 when the PRACE Preparatory Phase project (PRACE-PP) began. One of

the objectives of the PRACE-5IP project is to provide training to support the needs of users and of the CoEs from different communities. This is achieved by organising high quality events, enhancing the state of the art training provided by the PATCs and PTCs, while improving online training by developing additional MOOC courses. During PRACE-5IP, up to three new online courses will be made available to the HPC community in addition to the two courses already developed under PRACE-4IP.

Furthermore, WP4 has elevated its online presence through its renewed storage and repository facility, the PRACE CodeVault, which is an open repository containing various HPC code samples for the community. The CodeVault is an open platform that supports self-education for learning HPC programming skills where HPC users can share example code snippets, proof-of-concept codes and more. While other PRACE-5IP WPs exploit the PRACE CodeVault facility for their corresponding needs, WP4 is responsible for the training material of CodeVault.

In this document, we describe the work carried out in the first year of the PRACE-5IP 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) and PRACE Training Centres (PTC) Courses,
- PRACE Seasonal Schools and On-demand Events,
- International HPC Summer School,
- PRACE Summer of HPC.

The majority of events during the reporting period, February 2017 to April 2018, were organised by the PATCs operating in well-established supercomputing facilities. As far as the Seasonal Schools organisation is concerned, the planning and selection continues to follow the new selection scheme that was initially introduced in the previous PRACE Implementation Phase project.

WP4 also co-organised the 2017 International Summer School on HPC Challenges in Computational Sciences in Boulder, Colorado, United States of America, from 25-30 June 2017, in collaboration with XSEDE (USA), RIKEN (JAPAN) and Compute Canada.

Finally, WP4 organised the PRACE Summer of HPC 2017 outreach and training programme for undergraduate students and early-stage post graduates.

This deliverable also presents the PRACE training strategy for supporting the needs of future HPC users, and a full list of courses provided in the initial 15 months of the project in the Annex.

The deliverable is organised as follows: Section 2 presents an overview of the PATC and PTC 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 activities related to the International HPC Summer School, Section 6 provides information on the 2017 PRACE Summer of HPC, Section 7 gives an update of the MOOC prepared by PRACE, Section 8 provides a report for the Training and Events portal of PRACE and Section 9 gives an update of the PRACE CodeVault. The PRACE training strategy, and conclusions are provided in Section 10 and 11. Several annexes are also made available including a list of all face-to-face training courses provided by PRACE during the reporting period, the reports from the Autumn 2017 and Spring

2018 Seasonal Schools that took place in Poland and Slovak Republic, respectively, and On-demand Events Templates and Reports.

2 PRACE Advanced Training Centres and PRACE Training Centres

A network of six PRACE Advanced Training Centres (PATCs), represented by partners in Finland (CSC), France (Maison de la Simulation), Germany (GCS), Italy (CINECA), Spain (BSC) and the UK (EPCC), was established in 2012 to serve as European hubs of advanced, high-quality training for researchers working in the computational sciences. The PATCs have proven to be very successful, providing world-class courses for a large audience year-on-year. One of the major new development in the PRACE-5IP project is the establishment of four PRACE Training Centres (PTCs) to complement the activities of the PRACE Advanced Training Centres (PATCs). The selection and launch of the PTCs have already been described in PRACE-5IP deliverable D4.3 "Selection and Launch of the PTCs" [1], which also describes the pilot PTC 2017-18 programme, consisting of 18 courses (35 training days). Hence, this section reports on both the activities of the PATCs and PTCs in 2017-18.

2.1 The 2017-18 PATC Programme

The 2017-18 PATC programme was conceived and approved in June 2017. It includes a total of 82 courses (representing 209 training days) to be delivered by the six PATCs. Table 1 shows the key output and statistics from the six PATCs since their establishment in 2012. The implementation of the 2017-18 programme is ongoing at the time of this deliverable, with the successful implementation of ~75% of the courses (only one course had to be cancelled due to *force majeure*).

Relative to previous programmes, it can be seen that the PATCs continue to cater for a large European HPC audience in 2017-18 with 1,347 participants at 55 courses from August 2017 to April 2018. The feedback from these courses continue to be overwhelmingly positive; the PATC courses are consistently given an overall rating of 8.4 (out of 10, where higher scores indicate higher satisfaction or perceived quality) based on feedback received from participants. Other statistics such as the percentage of female, or non-academic participants have remained similar to the previous year. There seems to be a slight increase in the level of participation from non-host countries, i.e. participation at courses where the attendee is from an institution outside of the host's country, although this would need to be confirmed once the 2017-18 programme is completed. It can also be seen that ~11% of the participants so far have come from institutions that are neither hosting PATC nor PTC, in line with numbers from the past few years. Similar to past years, the geographic distribution of the participants appears to be highly skewed towards PATC-hosting countries. This will be discussed in more detail in the next subsection dealing with PTCs, which were established partly to help address this skewness in geographic distribution of participants.

Programme	Pilot	2012-13	2013-14	2014-15	2015-16	2016-17	2017-18 (partial)	
							PATCs	PTCs
Date from…	Mar-2012	Aug-2012	Aug-2013	Aug-2014	Aug-2015	Aug-2016	Aug-2017	Aug-2017
Date to…	Jul-2012	Jul-2013	Jul-2014	Jul-2015	Jul-2016	Jul-2017	Apr-2018	Apr-2018
Number of courses	19	71	81	77	73	78	55 (82)	12 (18)
Total duration (days)	56	204	233	219	203	215	158 (209)	21 (35)
Number of participants	511	1,547	1,682	1,786	1,567	1,658	1,347	351
Number of participant-days	1,715	4,702	5,187	5,384	4,601	4,881	3,976	2,635
Female (%)	-	12.9%	14.4%	16.3%	17.6%	19.3%	20.1%	22.4%
Non-academic (%)	-	9.9%	12.3%	15.6%	22.2%	19.4%	19.6%	15.5%
Non-host country (%)	-	20.6%	25.4%	29.5%	16.3%	16.2%	19.7%	23.4%
Non-PATC/PTC country (%)	-	13.8%	17.7%	19.9%	8.9%	11.9%	11.2%	9.4%
Feedback response rate (%)	-	63%	64%	53%	52%	65%	57%	40%
Average overall rating (0 – waste of time; 10 - excellent)	-	8.5	8.4	8.4	8.4	8.5	8.5	8.4

Table 1: Key statistics from the implementation of PATC programmes since 2012

The table above indicates the key statistics from the implementation of PATC programmes since 2012, with the 2017-18 PATC programme shown alongside the nascent PTC 2017-18 programme (the right-most two columns highlighted in grey). “Non-host country” indicates the proportion of participants affiliated with institutions from anywhere outside the country hosting the PATC course. “Non-PATC/PTC country” indicates the proportion of participants affiliated with institutions from non-PATC or non-PTC hosting countries.

2.2 The 2017-18 PTC Programme

The selection and establishment of four PTCs took place in early 2017. The PTCs, represented by partners in Greece (GRNET), the Czech Republic (IT4I), Ireland (ICHEC), the Netherlands (SURFsara), were selected based on the following evaluation criteria:

- Ability to carry out the requested number of training events,
- Consistency and track record of training activities,
- Availability, range and expertise of local trainers,
- Justification for a tentative training programme to be proposed by each PTC,
- Suitability of the hosting site for attracting students from local and surrounding regions.

Therefore, the first PTC programme was based on what the selected PTCs had already proposed in their respective proposals. The joint programme, including the proposed 18 courses from all four PTCs, was subsequently approved in June 2017. The courses on offer cover a range of topics, including domain-oriented applications (e.g. for the engineering, meteorology, molecular simulation communities), data management and processing, many-core programming, etc.

Table 1 shows some of the key statistics from the pilot PTC programme (from August 2017 to April 2018), which is still ongoing at the time of this deliverable. A total of 12 courses (out of the proposed 18) has been organised thus far, representing 18 out of the 35 target training days. This has attracted a total of 351 participants, representing 2,635 student training-days. Compared to the PATC statistics shown together (Table 1), the joint PTC programme is obviously smaller in scale,

on the order of a single PATC in terms of its course offering (e.g. training days). The other statistics analysed for the PTCs also mirror those from the PATCs, e.g. the level of female and non-academic participation, those from non-hosting or non-PATC countries (see Table 1).

With regards to the geographic distribution of participants, the PTCs have helped to address some of the skewness towards the original 6 PATC countries. Figure 1 shows the population-normalised distribution of PATC participants only in 2017-18, compared to the same numbers that includes both PATC and PTC courses. While most of the participants had been based in PATC-hosting countries previously, the PTCs (in combination with Season Schools and On-demand training events) have attracted participants in other countries to help address the skewness.

2.3 The Future of PATCs and PTCs

It can be seen from Table 1 and their respective programmes (see Annex 12.1), the nature of activities of the PATCs and PTCs can be very similar apart from the amount of courses provided and somewhat different focus (emphasis on more advanced courses for PATCs and the freedom to host more basic level courses for PTCs; but these are not strict, e.g. PTCs may offer advanced courses at times, PATCs may sometimes be compelled to provide more basic level courses to engage new communities). Hence in order to streamline the nomenclature of the PRACE training offering, both the PATCs and PTCs will simply be referred to as PRACE Training Centres (PTCs) in future. This rebranding shall be completed in the transition to the 2018-19 PTC programme that will be jointly coordinated among 10 partners (6 former PATCs and 4 former PTC hosting countries).

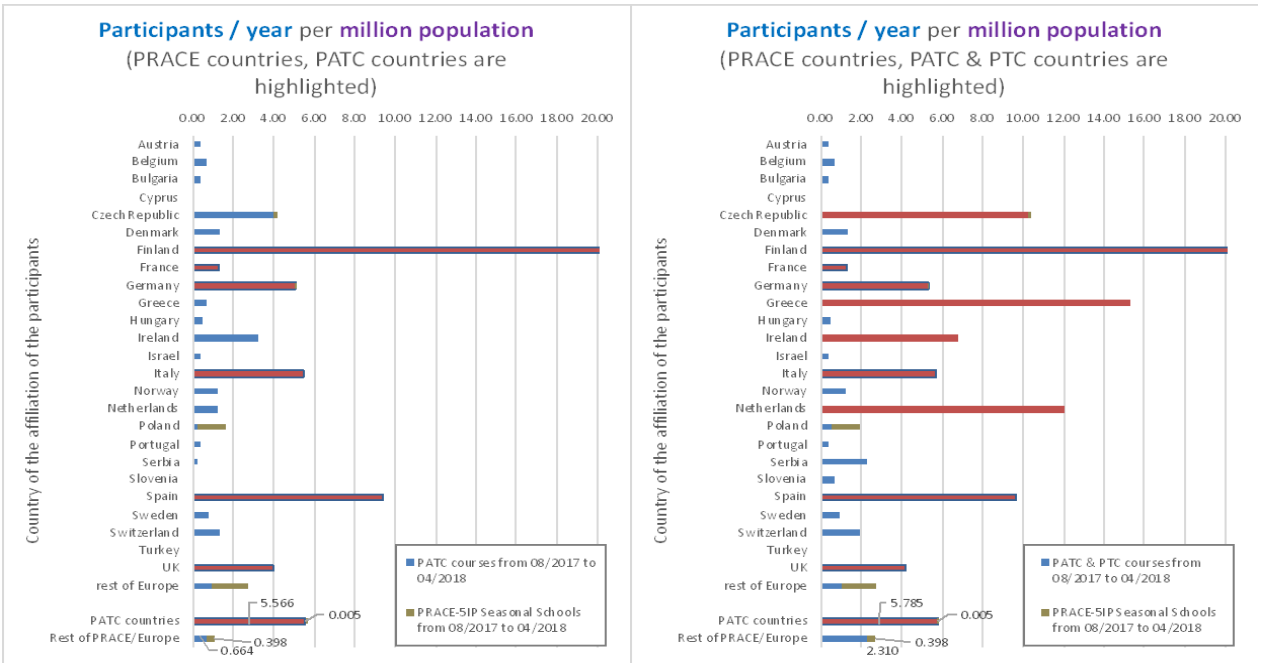

Figure 1: Geographic distribution of participants at 2017-18 PATC courses only, compared to that of participants at both 2017-18 PATC and PTC courses. The level of participation is normalised by the population of each country.

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 specialised 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. With the introduction of the PTCs in PRACE-5IP, the Seasonal School also run in parallel to the PTCs. To maximize PRACE training coverage around Europe, PATC or PTC hosting countries are not eligible to apply for hosting Seasonal Schools.

3.1 Selection Process

In the PRACE Implementation Phase Projects that preceded the fourth, there was big demand for hosting Seasonal Schools than there were available slots. This resulted in the establishment of a selection process for hosting Seasonal Schools [2] in PRACE-4IP to ensure fairness and transparency. The same process took place in PRACE-5IP in order to select the hosting countries for the six available Seasonal School slots. However, what was not expected is that, since PATC or PTC hosting countries could not apply for Seasonal Schools, the set of remaining countries was not large enough to create the demand noticed in previous years. Therefore, when the Call for Seasonal Schools ended in June 2017, the committee received on only two applications. This resulted in internal discussions from whom the final decision was to open a second Call for Seasonal Schools. In the second Call, four countries applied, resulting in the six countries to host the Seasonal Schools for PRACE-5IP.

The MB approved the selection of the first two Seasonal Schools in July 2017 and the selection of the four remaining Schools in April 2018. Table 2 summarises the Seasonal Schools dates, location and main subject. More details on the events are available in the relevant section of the PRACE agenda system accessed via [3].

School	Location	Date	Main Subject	Overview
Autumn 2017	Poland	20-24 November 2017	Computational Fluid-Structure Interaction	Sec. 3.2.1
Spring 2018	Slovakia	23-26 April 2018[1]	PRACE Seasonal School on Bioinformatics	Sec. 3.2.2
Autumn 2018	Slovenia	24-26 September 208	HPC for engineering and Life sciences	Sec. 3.2.3
Winter 2018	Bulgaria	December 2018	School on Computational Chemistry, Biochemistry and Materials Science – Methods and Tools	Sec. 3.2.4
Winter 2019	Belgium	February 2019	Introduction to Machine Learning for scientist	Sec. 3.2.5
Spring 2019	Sweden	May 2019	HPC in the Life Sciences	Sec. 3.2.6

Table 2: PRACE-5IP Seasonal School schedule

[1] Postponed from Winter 2017 to Spring 2018 (April), due to organisational issues.

3.2 Overview of accepted Seasonal Schools

In this section, we provide a summary of the contents of all accepted Seasonal Schools.

3.2.1 Poland, Computational Fluid-Structure Interaction (Autumn 2017, past event)

Large number of the mechanical, aerospace, civil and hydro engineering machines are operating in a complex environment. Floating offshore wind turbine or the helicopter in flight are only a reference examples of the problem. Operational loads and resulting structural response of the investigated object are coming from aerodynamic, hydrodynamic and thermal forces. Traditionally those mechanical systems are being studied w.r.t the different scientific disciplines: solid mechanics, flow mechanics, material sciences and computer methods only to name major domains. It leads to the approximate and often imprecise results of numerical simulations. Multi-physics approach is required to adequately address the complexity of the real-life operation of the mechanical systems.

Seasonal School on Computational Fluid-Structure Interaction (FSI) tries to close the isolated domain analysis gap. The FSI School offers an integrated multidisciplinary training covering the comprehensive spectrum of the mathematical theorems, fluid and solid dynamics, numerical modelling techniques and all this within the framework of the HPC resources and tools able to tackle the challenging problems of the coupled multi-physics problems. Lectures will be followed with the laboratory exercises run on the CI TASK cluster. The course is addressed to wide audience ranging from PhD students to more senior researchers active in the science and industrial R&D departments.

3.2.2 Slovakia, PRACE Seasonal School on Bioinformatics (Spring 2018, past event)

Bioinformatics is growing in popularity rapidly over the past years due to lots of reasons, such as availability of high-throughput sequencing techniques, high-quality (open access) databases, as well as the availability of ready-to-use machine learning frameworks and libraries. The extent of applicability of the bioinformatics algorithms and programs is, however, often limited by computer resources that researchers have at hand. The goal of the Seasonal School is to evangelise HPC as the tool they can use to overcome this barrier limiting their research.

There are a lot of tools available, that researchers working in this field can use, but most of them were developed for desktop applications. In this workshop, we will present tools / frameworks that are designed towards parallel computer architectures, thus suitable for running them on computer clusters or supercomputers. Participants will not only learn about dedicated bioinformatics software, such as BLAST (Basic Local Alignment Search Tool), but also on generally applicable tools, such as the R programming language or the Apache Spark framework, suitable for parallel (pre)processing of Big Data.

The workshop is composed of introductory sessions on bioinformatics and NGS (Next-Generation Sequencing), lectures and hands-on sessions on using R in parallel, a short course on analysis of large data sets with Apache Spark (primarily using Python) and finally the lecture on BLAST and how to convert BLAST tasks in parallel jobs.

3.2.3 Slovenia, HPC for engineering and Life sciences (Autumn 2018, future event)

The aim of the Seasonal School is to increase the competencies of Slovenian academic and industrial researchers. A national HPC consortium founded in 2016 has set a strategic goal of giving training for industry personnel (trainees and interns) and university students and researchers. The call for PRACE Seasonal events is a good stimulus for progress in this direction. The proposed event will have regional impact in the neighbouring countries like Austria, Croatia, Serbia, Bosnia and Herzegovina from where participants might also come, along with the rest of Europe. This event is expected to increase the number of HPC users in the region, also among small and medium size enterprises (SMEs), which is seen by the organiser as particularly important target group.

3.2.4 Bulgaria, School on Computational Chemistry, Biochemistry and Materials Science – Methods and Tools (Winter 2018, future event)

Bulgaria's proposal aims at demonstrating and exposing the use of Computational (incl. HPC) methods and tools in the fields of Chemistry, Biochemistry and Materials Science, areas in which the academic community in Bulgaria has shown visible progress that is globally recognised. With contributions from the UK's Hartree Centre and the STFC Scientific Computing Department, we want to show that knowledge exchange between scientists with different academic experience and between academia and industry is the facilitation process for setting collaborative projects in which academic and industrial interests, experiments, HPC modelling and application development meet to boost one another. The School aims to discuss the methodologies, numerical methods and their implementation used by state-of-the-art codes in an HPC environment. We shall present a number of examples where the use of HPC modelling has been essential in solving scientific problems at atomic and molecular level. We shall also provide basic introduction and training in some of the HPC applications developed at Daresbury Laboratory, relevant to collaborative projects of both academic and industrial nature.

3.2.5 Belgium, Introduction to Machine Learning for scientist (Winter 2019, future event)

Machine learning is increasingly being used as a tool to explore, understand, and analyse the data that is generated in a wide variety of scientific domains. Classic approaches to data processing start to break down under the avalanche of data produced by modern measurement and diagnostic techniques. In the first part of this School, researchers at the cutting edge of their domain will get an overview and a solid understanding of machine learning algorithms, and how they can be used to solve various research questions. The second part will build on this knowledge, and bring applications to the next level by introducing the technology to perform machine learning analysis at scale, needed for HPC data output for instance.

3.2.6 Sweden, HPC in the Life Sciences (Spring 2019.future event)

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 been established in Sweden, Stockholm where KTH is the coordinating partner.

As mentioned in HPC wire [4], Life science research has long been compute-intensive but requirements have largely been satisfied with traditional workstations and simple clusters. That is changing: “Roughly 25 percent of life scientists, and this includes bench-level scientists, will require HPC capabilities in 2015, few of whom have ever used a command line,” said Ari Berman, GM of Government Services, the BioTeam consulting firm.

However, HPC in life science has special challenges: Since the size of the systems studied is typically limited, many programs have significant challenges to scale to very large computing systems, while there are also many challenges with achieving sampling on relevant time scales.

The mission of this School is to take one step beyond the traditional introductory tutorials and focus on advanced techniques that make it possible to reach longer time scales, use algorithms that make it possible to directly sample complex processes, and not least use large scale HPC resources more efficiently. We will have authors from a number of world-leading packages simply to make it clear that this is not primarily a matter of a specific piece of software, but general techniques.

The participants must have prior experience from one or more molecular dynamics simulation packages that they have used for their concrete research problem before. We might try to establish online resources to make it possible to learn that remotely before the workshop, but the workshop itself will assume prior knowledge.

At the workshop, we will discuss challenges with scalability and performance, and teach best practices on HPC systems (including using GPU acceleration) that have been observed during PRACE research activities. Several of these software packages are among the UEABS of PRACE.

We will show participants how to use a number advanced techniques such as free energy calculation, replica exchange, pathway sampling, metadynamics and Markov State Models that all rely on ensemble simulation algorithms to achieve much better scaling and sampling compared to traditional simulations.

Extensive hands-on sessions will cover more than half of the school period. Those will take place in the well-equipped laboratories of KTH where computers are already connected to the PRACE Tier-1 system Beskow at KTH-PDC. Beskow is one of the largest Tier-1 system within the Nordic countries.

Considering the established tight connection between PDC and industry, we expect also a number of industrial attendees.

The school will be organised in collaboration between SNIC/KTH and BioExcel.

3.3 Results of PRACE-5IP Y1 Seasonal Schools

During Y1 of the Project, only two Seasonal Schools have taken place; the Autumn 2017 School in Poland and the Winter 2017 School in Slovakia.

3.3.1 Autumn 2017 Seasonal School, Poland

The Autumn 2017 Seasonal School, named "PRACE Seasonal School on Computational Fluid-Structure Interaction", took place in Gdańsk University of Technology, Poland from 20.11.2017 to 24.11.2017. The programme included:

- Introduction to High Performance Computing
- Introduction to the CFD methods
- Introduction to Finite Element Model
- Introduction to the Fluid-Structure Interaction

All attendees were provided access to Tryton Supercomputer [5] for the course duration.

There were 32 participants to the Seasonal School, all from Poland. Most participants declared that they were satisfied the course level and contents. The organisers declared that the organisation of the Seasonal School was a valuable experience, easier than previously thought would be. The official report of the Seasonal School can be found in Annex 12.2.

3.3.2 Winter 2017 Seasonal School, Slovakia

The Slovakia Seasonal School

The Winter Seasonal School, named "PRACE Seasonal School on Bioinformatics", was finally organised in Spring 2018, due to organisational reasons. It took place in the Computing Centre of the Slovak Academy of Sciences in Bratislava, Slovak Republic from 23.04.2018 to 24.06.2018.

The programme included:

- Introduction to bioinformatics
- Parallel programming with R
- Analysing large datasets with Spark
- Running BLAST in Clusters.

There were 34 participants to the Seasonal School, most from Slovakia, one from Czech Republic and one from Germany. From the received evaluations, it can be extracted that the topic was relevant to the participants' research and inspiring. However, a rather significant number declared that the information provided was not good and had problems comprehending the lectures and the pace of teaching. The official report of the Seasonal School can be found in Annex 12.3.

4 On-demand Events

The On-demand events that are organised in the context of PRACE-5IP project are trainings specifically organised with the collaboration of research communities that have special needs for training and the expertise of PRACE trainers. Such targeted communities are mainly the Centres of Excellence (CoEs). PRACE-5IP continued the effort from previous PRACE Implementation Phases projects to collaborate with the CoEs in many different areas, including training. On-demand events can be organised by any PRACE-5IP partner institution. The trainings need to be given in English to accommodate the international participants.

4.1 Selection Process for the On-demand events

The process for the selection of the On-demand events is as lightweight as possible, ensuring at the same time the transparency of the process and the quality of the events. The Call for the organisation of On-demand events is continuously open. Eligible partners send their application form filled in to the On-demand events evaluation committee. The application form template is shown in Annex 12.4.

The committee is responsible to respond within 20 calendar days with their position/recommendation regarding the organisation of the event, including any possible recommendations for the improvement of the event. The selection committee is comprised of five members: BoD representative, MB representative and three WP4 representatives. T4.1 leader coordinates and facilitates the process, without any power to influence the final decision.

Since the process for the selection of the On-demand events is lightweight, there is no need for MB approval after each decision of the committee. The PMO is the responsible for taking the final decision for the organisation of the On-demand events, following the selection committee's position/recommendation. In case a committee member is from a PRACE partner involved in the proposal, the member will not participate in making the recommendation. The final decision should not come in more than 30 calendar days after the day of submission of the application.

4.2 Selection Criteria for the On-demand events

The following selection criteria apply to the selection of the On-demand events:

1. Importance of the community / organisation that requests the On-demand event (i.e. CoE, scientific or industrial community etc.) and relevance to the aims and objectives of PRACE and its training programme.
2. Capability of the applicant or group of applicants to host the On-demand event.
3. Clarity of the proposed programme and relevance to the aims and objectives of the event.

4.3 On-demand Events organised in Y1

Table 3 presents the On-demand events schedule for the first year of PRACE-5IP.

Location	Date	Main Subject
Espoo, Finland	7-9 June 2017	E-CAM Workshop on Particle-Based Models and HPC
Barcelona, Spain	21 November 2017	Energy-aware application development for heterogeneous computing
Umeå, Sweden	25-26 April 2018	Programming and optimizing the Knights Landing

Table 3: PRACE-5IP On-demand Events schedule

The reader can find the corresponding reports for each of the organised On-demand event in Annex 12.5.

4.4 Results of PRACE-5IP Y1 On-demand Events

The On-demand event named "E-CAM Workshop on Particle-Based Models and HPC" took place in the IT-center for science of CSC in Aalto University, Espoo, Finland, from 07.06.2017 to 09.06.2018. It attracted 21 participants, 17 from Finland, one from Estonia, Holland, Hungary and Germany, respectively. The non-statistically representative sample of evaluations gave an excellent grade to the event. The official report of the particular On-demand event can be found in Annex 12.5.1.

The event named "Energy-aware application development for heterogeneous computing" took place in the Barcelona Supercomputing Center in Barcelona, Spain, on November 21st, 2017. The organisers aimed to present the TANGO toolbox, which provides a set of tools to simplify and optimize the usage of distributed heterogeneous computing environments. It attracted 15 participants overall, 13 from Spain and one from Brazil and Iran, respectively. The official report of the particular On-demand event can be found in Annex 12.5.2.

The event named "PRACE Workshop on Programming and Optimizing the Intel Knights Landing Manycore Processor" took place in HPC2N, Umeå University, Sweden, from 24.04.2018 to 25.04.2018. It attracted 18 participants from various countries, including 10 participants from Sweden. The course focused on how to best use and efficiently program and optimize the Intel Manycore Processor codenamed "Knights Landing (KNL)". Since the event finished only a few days before the deadline for the input collection for this deliverable, there was no adequate time to collect and process evaluations from the participants. However, the organisers declare that the overall experience was positive. The official report of the particular On-demand event can be found in Annex 12.5.3.

5 International Summer School

The PRACE-5IP project has provided support to organise the eighth International HPC Summer School, which was held in Boulder, Colorado, USA on 25-30 June 2017. It has been an ongoing and very successful collaboration between PRACE, the U.S. National Science Foundation's eXtreme Science and Engineering Discovery Environment (XSEDE) project, Canada's Compute Canada and RIKEN Advanced Institute for Computational Sciences (RIKEN AICS).

The school was announced in December 2016 and had generated huge interest where 351 candidates applied for total of 80 places, attracting some of the most talented graduate students and postdoctoral scholars from institutions in Canada, Europe, Japan and the United States. Leading computational scientists and HPC technologists worldwide were also invited to offer instructions on a variety of topics and also provide advanced mentoring.

The 80 places were divided among the four partners as follows: 30 seats for European participants supported by PRACE, 30 seats for U.S. participants supported by XSEDE, 10 seats for Japanese participants supported by RIKEN AICS, and 10 seats for Canadian participants supported by Compute Canada. Each partner is responsible for the selection and support of the candidates from each country/continent. The geographic distribution of the selected candidates is shown in Table 4.

Country	Number of participants
Austria	1
Canada	10
Czech Rep.	1
Denmark	1
Finland	1
France	2
Germany	5
Greece	1
Israel	1
Italy	2
Japan	10
Netherlands	1
Poland	1
Serbia	1
Spain	2
Sweden	3
Switzerland	1
UK	6
USA	30

Table 4. Geographic distribution of the participants (according to institutional country) at the International HPC Summer School 2017.

The school proved to be another success, subsequent follow-up analysis of the feedback resulted in the following key findings (see Annex 12.6 for raw feedback results):

- The school was extremely successful in promoting knowledge of high performance computing and its applications in various scientific domains,
- An overwhelming proportion of participants have rated their experience at the school a success, or have met their objectives,
- The school has also encouraged friendships and collaborations among an international mix of participants and presenters from a wide range of backgrounds,
- The international audience is a unique characteristic of the school that contributes to the learning experience and sets it apart from many other training events.

Following on from the success of 2017, the location of the 2018 iteration of the school was designated to be Ostrava, Czech Republic, with the PRACE partner IT4Innovations in charge of local organisation. This school will be held on 7-13 July 2018. Since the announcement of the school in December 2017, a total of 335 applications was received by February 2018. A total of 80

candidates has been selected to attend the school. A more detailed report on this school will follow after its completion.

6 PRACE Summer of HPC

PRACE Summer of HPC (SoHPC) [6] outreach and training programme for undergraduate students and early stage post-graduates entered its fifth edition in 2017. The SoHPC 2017 edition [7] transitioned from PRACE-4IP WP3 to PRACE-5IP WP4. Preparations for programme launch started under WP3 with a *Call for Projects* [8] to hosting sites and then under WP4 *Call for participation* [9] was issued in early January 2017 and closed mid-February 2017 with 86 applications received [10]. Selections of participants were performed with double review of applications and two consensus meetings for the final selection of 21 students [11] to be hosted by 10 PRACE partners. Site coordinators organised travel and accommodation for the students.

The training week [12] was organised at the IT4Innovations HPC centre [13] in Ostrava as a start of the students' summer project work. Each student had a mentor for their project [8] and during the summer, weekly teleconferences were organised by SoHPC coordinating team to monitor the progress and advertise achievements on SoHPC Facebook [14] and Twitter [15] accounts.

Figure 2: PRACE Summer of HPC 2017 participants at the training week in Ostrava

During the summer, students wrote 64 blog posts [16] about their project and work at hosting sites. The programme finished at the end of August 2017 with project presentations [17] upload on YouTube. Students wrote popular scientific articles describing their achievements from the project work, which was used by PRACE dissemination team for outreach communication and PRACE Digest [18] highlights. A SoHPC Awards selection panel was formed and selected the winners of the SoHPC 2017 Ambassador and Visualisation Award. The award ceremony was held on 31 October 2017 in Ostrava [19].

The SoHPC 2018 edition timeline [20] started with 11 PRACE partners expressing interest already during SoHPC 2017 run. The call for the SoHPC 2018 project proposals was issued at end of November 2017, along with the call for the training week site and award ceremony venue. Within the evaluation of the project proposals the SoHPC 2018 coordinating panel agreed among the partners that the SoHPC training week will be organised by EPCC in Edinburgh, UK and the award ceremony to be held in Juelich, Germany.

PRACE-5IP Summer of HPC programme was included as part of WP4 – Training activities, thus the main focus of the programme is to educate, inspire and motivate young students towards future studies in HPC and computational sciences. Because of this, it was decided that the "Best Visualisation Award" is no longer applicable to the programme, and instead a "Best Performance Award" was decided to replace it. The awarding SoHPC participants should excel and be motivated for the programme. They may work on theoretical or optimisation computational problems which do not create any forms of visualisations, but are still very valuable HPC contributions. With 23 project proposals the call for applications was launched in January 2018 and closed with 58 registrants at the end of February 2018. Review and selection at consensus meeting allocated successful participants to projects. Right after invitations were accepted the site coordinators started preparations for travel to and from the training week together with selected participants looking ahead for a new successful Summer of HPC edition.

7 Massive Open Online Courses

PRACE piloted "Supercomputing" and "Managing Big Data with R and Hadoop" Massive Open Online Courses (MOOC) under PRACE-4IP as a new training method hosted on FutureLearn [21] platform. Each developed MOOC will be offered twice a year with constant improvements by each MOOC team. The starting dates for these MOOCs were 28 August and 9 October 2017, respectively, and both finished after 5 weeks. Learners have two additional weeks to finish the course and are therefore available for 7 weeks.

After the pilot MOOCs period ended under PRACE-4IP, in May 2017, a Call for new MOOC Proposals was issued under PRACE-5IP. The plan in PRACE-5IP proposal was to develop two to three additional MOOCs.

Currently, the following three new courses are being developed:

1. *Python in high performance computing*, CSC
   "Python programming language has become popular in scientific computing due to many benefits it offers for fast code development. Alas, the performance of pure Python programs is often sub-optimal, but fortunately, there are ways to remedy it. In this course we teach various ways to optimise and parallelise Python programs."
2. *The new MPI-3 Shared Memory Interface*, HLRS, IUCC, SURFSara
   "MPI-3.0 added two new routines to enable shared memory windows within MPI: `MPI_COMM_SPLIT_TYPE` and `MPI_WIN_ALLOCATE_SHARED`. In this MOOC, we will present how to use the new methods. The course starts with a refresh of MPI 1-sided communication and describes ways how to use the new interface with use-case examples.

Within shared memory windows one can directly access the data by expressions or assignments in C/C++ or FORTRAN, i.e., without calling `MPI_PUT` or `MPI_GET` RMA routines."

3. *Defensive programming and debugging*, CENAERO, KU Leuven
   "This course shows a number of defensive programming techniques, and introduces the concept of assertions and unit tests. In many contexts command line debuggers are the only tool at hand, and the concepts transfer easily to GUI debuggers, so gdb will be taken as an example in a small cases and then advanced debuggers with GUI will be shown."

All new courses are being developed based on the experience gained from the pilot MOOCs. Target dates for launch of new MOOCs are expected to be in September-December 2018. As with the pilot MOOCs that received great attention we plan to advertise new MOOCS through PRACE channels and topical magazines [22][23].

7.1 Supercomputing MOOC

This MOOC was designed as a 5-week introduction to Supercomputing at a conceptual level. The weeks cover the following topics:

1. Supercomputing: motivation, parallelism, computational science and basic HPC concepts,
2. Parallel Computers: hardware components, distributed and shared-memory architectures,
3. Parallel Computing: programming using message-passing and threads,
4. Computer Simulations: basic concepts illustrated using weather forecasting,
5. Case Studies: a range of real scientific applications.

Each week comprises a mixture of articles, videos, discussion boards and quizzes. Although it does not require any programming skills, there are discussion topics which explore deep concepts such as deadlock in message-passing programing and resource contention in shared-memory systems. Course tutors monitor the discussion boards and answer questions or suggest additional topics. There are also two "Ask an Expert" sessions where the most liked questions are answered in short videos, which are then uploaded to the site. It has been run three times so far: 6 March 2017, 28 August 2017 and 15 January 2018.

The FutureLearn platform provides summary statistics on the attendees which includes the number of "joiners" (those who expressed an interest in the course at any stage), the number of learners (who visited some part of the course), the number who completed more than 90% of the steps and the "Run Retention Index" (see Table 5).

	6 Mar 2017	%	28 Aug 2017	%	15 Jan 2018	%
Joiners	3,265		3,101		1,825	
Learners	1,725	52.80 %	1916	61.80 %	1,218	66.70%
Learners with > 90% step completion	219	12.70 %	194	10.10 %	119	9.80%
Run Retention Index		36.1%		34.5%		33.3%

Table 5: FutureLearn Platform statistics for Supercomputing MOOC

We see a fairly consistent picture of around 10% of learners completing the course, which is in line with what is typical for this kind of free MOOC. Inspired by the H-Index for academic publications, the run retention index gives a measure of how long learners followed the course; for example, for the first run 36.1% of activated learners completed at least 36.1% of the course. The Retention Index can be used to compare the effectiveness of two runs of the same course against each other. The numbers are lower for the most recent run – we think this was because it was perhaps too close in time to the second run. The fourth run is planned for September 2018.

7.2 Managing Big Data with R and Hadoop MOOC

The MOOC is designed as introductory course that teaches the big data management by hands-on on a virtual machine prepared and required for following the course. Furthermore, it introduces R statistical language in conjunction with basic big data tools such as Hadoop and map-reduce concepts. Comparing to Supercomputing MOOC the Big data MOOC is quite technical for learners that in five weeks get introduction from Linux to RHadoop with the following titles:

1. Welcome to BIG DATA
2. Working with Hadoop
3. First steps in R and RHadoop
4. Statistical learning with RHadoop: clustering
5. Statistical learning with RHadoop: regression and classification

In the last week of the second MOOC run we included a possibility to access real big data cluster at UL through RStudio web interface that allows larger exercises than with virtual machine..

	2 Apr 2017	%	9 Oct 2017	%	23 Apr 2018	%
Joiners	4,133		1,723		In progress	
Learners	1,920	46.5%	1,059	61.50 %		
Learners with > 90% step completion	90	4.2%	43	4.1%		
Run Retention Index		27.8%		25.9%		

Table 6: FutureLearn Platform statistics for Big data MOOC

The statistics in Table 6 reflect two runs while third is scheduled for end April 2018. Surprisingly, larger number of joiners (4133) for the first run when comparing to the first run of Supercomputing MOOC (3265) can be explained by attractive topic. Lower number of completion and retention index is due to quite technical approach that requires hands on computer by downloading and installing virtual machine and remote RStudio. Second run received 1723 joiners, that is substantially less than first run, can be explained by appearance of similar courses and timely placement in September.

8 Training and Events portal

8.1 Events Portal

The main focus during the reporting period was preparing the major version upgrade of PRACE Events portal [24] called Indico 2.0. This version was released early 2018, but preparatory work including installation of test systems, and testing migration itself was started at the beginning of PRACE-5IP. WP4 team worked closely together with Indico developers participating to conferences and solving issues together, as PRACE is hosting more events accommodating more users than typical Indico portals around the globe.

One of the main concern of migration was the customised theme developed in PRACE-4IP, as the theming system is quite complicated and was completely rewritten in version 2.0. WP4 team is currently working to finalise material template for events on Indico 2.0 to offer near identical design after migration.

8.2 Training Portal overhaul

The aim of this task was to replace the current training portal [25] to a completely new system due to its current limitations of lacking advanced search and proper categorisation of training materials. Initial findings suggested using a Repository system instead of a CMS would be more suitable for such a task, as it provides the aforementioned features along with the capability of storing science related documents with metadata persistently (see Figure 3).

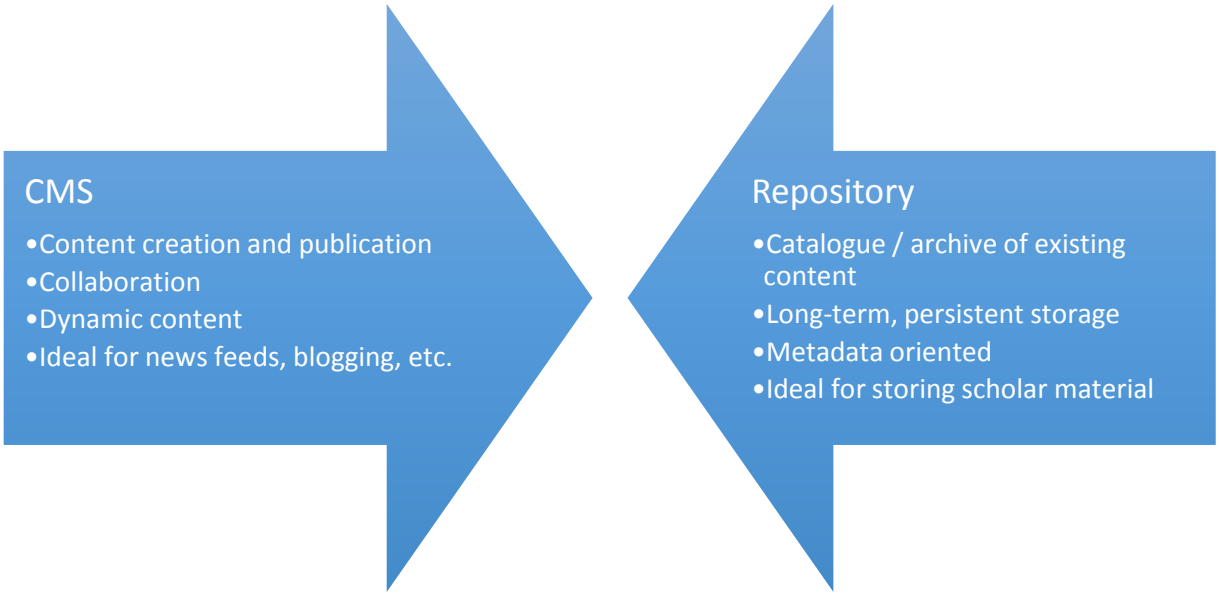

Figure 3: Comparison between CMS and Repository systems

Expectations for the document repository:

- Functional, customisable and ergonomic front page with latest design,
- Sophisticated categorisation system with advanced search functionality,
- Offers preview / embedding (e.g. video materials for streaming),
- Support integration with events portal, CodeVault and prace-ri.eu webpage, along with partner training portals.

We have investigated three reputable repository systems: DSpace [26], Invenio [27] and ePrints [28]. We decided to try all three and offer test environment, install them and make a public test version for the WP4 team to compare them extensively.

The **Invenio** Digital Library Framework is developed by CERN. Our team installed and tested all three main versions available for this software. During the testing, we contacted several developers of the Invenio team, who were trying to respond to the questions and problems. The experiences and feedback about the versions:

- 1.x old stable: lacks several features we want to be integrated, not supported anymore,
- 2.x version: they do not recommend installing Invenio v2 as it is not supported anymore; after installation we have encountered problems with some features, (e.g. multimedia streaming) otherwise it was generally functional,
- 3.x version: expect a final release of Invenio v3.0 by end-May 2018, has now problems not yet fixed, we are waiting for final release to be deployed.

DSpace is another widely used repository. The system is widely used within academia (e.g. Massachusetts Institute of Technology (MIT) Libraries, Texas Digital Library). The developer maintain this software day-by-day basis.

We installed the 6.2 version without any difficulty with 2 frontend: XMLUI and JSPUI. We can easily customise these UIs and these seemed to be stable. The greatest disadvantage of the DSpace is that it does not offer integrated multimedia (video and audio) streaming by default. However, there is a paid plugin to offer such a functionality.

Regional academia use **ePrints** open source software and their feedbacks are positive, we decided to install this system as well.

The initial impressions are positive it supports the multimedia content better than the other repositories (e.g., it generate preview images to the video and it converts to web compatible format etc). We had only difficulty with the video embedding to the page of the document. At this moment, we have managed to change the code for the online playback to work flawlessly.

We are in the process of comparing these three systems together with WP4 team, how they perform as a repository of training materials. Depending on the feedback, we will move forward with the customisation of the system to provide similar functionality as the current Portal then to add more features and new design. Last but not least, we plan to integrate this with other PRACE portals.

9 CodeVault

CodeVault is a repository/storage facility for the needs of PRACE. Apart from WP4-Training, other WPs also need repository facilities for storing content in an organised way. However, in this particular section, we will focus on the CodeVault aspect concerning WP4.

CodeVault was initially conceived and developed as a central storage facility where information could be stored and managed in an organised way. The specification was that multiple persons from each WP and Training Centre could store information in the CodeVault. Additionally, even more people (i.e. the trainers and trainees of various activities) should have fast and meaningful access to the stored information.

The first version of CodeVault was created as a repository in the gitlab.com git-repository hosting service. The complete CodeVault is till nowadays, a single git repository located at gitlab [29]. The hierarchy/organisation of the CodeVault is achieved using folders. In the highest level there are two folders named "`hpc_kernel_samples`" and "`training_materials`", respectively. The first one is for WP7 to store HPC kernels and the second one is for WP4 training purposes.

In its current form, CodeVault hosted some exercises and training material that served several trainings. However, it was soon realised that there were two drawbacks that kept CodeVault from being fully utilised by the PRACE Partners.

The first drawback was the concern that, since CodeVault is being implemented in a non-PRACE facility (i.e. gitlab.com), people were reluctant to fully commit on it, since they were unsure for the future of the particular facility.

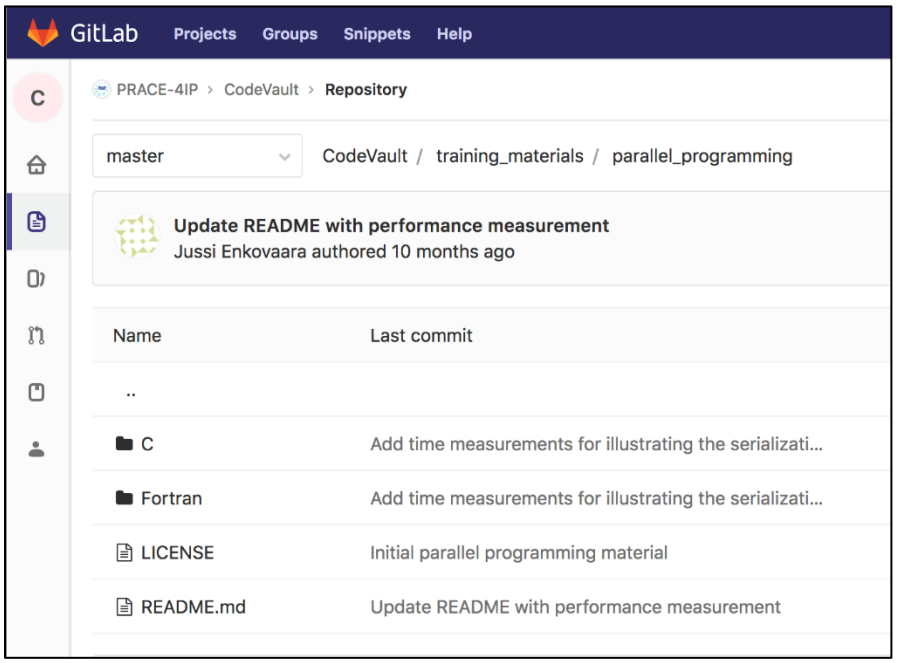

Figure 4: CodeVault in its current form at gitlab.com facility.

The second drawback, that mainly affects WP4 Training activities, is that the actualisation of CodeVault as a single repository makes it difficult to retrieve (`git clone`) a particular exercise or workshop from the whole repository. Trainers that have initially tried it during training events realised that trainees (especially those without a computer science background) had considerable troubles following the tedious instructions that would permit them to retrieve a subset of the whole repository. Imagine that in order for trainees to download a few files with instructions and code, they should pass the process of typing several obscure terminal commands. Both trainers and trainees were discouraged and preferred accessing instead a URL that offered them easily the corresponding files as a zip archive.

For the aforementioned reasons (mainly), it was decided that CodeVault will be moved to a PRACE owned facility. Furthermore, a different organisation structure would be followed that would make the usage of CodeVault easier for training purposes.

WP6 was responsible for that task of re-instantiating CodeVault as a complete gitlab facility on PRACE's own infrastructure [30], which essentially resolves the first aforementioned drawback.

Moreover, since CodeVault is now a full gitlab facility (and not one repository), PRACE can utilise multiple git repositories to store and serve the training content. That essentially means that trainers can create meaningful chunks of files under the same repository and the files be easily fetched using a simple `git clone` command by the trainees.

It was also decided that the training material would be stored in hierarchical way, which would make its search easier for the interested parties. WP4 approved the following structure during its recent January 2018 face-to-face meeting in Poznan, Poland:

```
Parallel_Programming
├── MPI
├── OpenMP
└── Python
GPU_Programming
├── CUDA
├── GPU_Python
└── OpenACC
PGAS_Languages
├── Chapel
└── Coarray_Fortran
Data_Processing
├── Python
└── R
Debugging
├── C
├── Fortran
└── Python
Profiling
├── C
├── Fortran
└── Python
Best_Practice_Guides
├── C
├── Fortran
└── Python
```

As far as WP4 is concerned, the next steps of CodeVault include its population with projects/git repositories suitable for various trainings. In collaboration with WP6, we will create the necessary accounts for all people planned to provide PRACE trainings. In this way, they will be capable of uploading all the necessary material to CodeVault, which can then be repetitively used in multiple trainings. We will also assess the possibility of permitting people outside PRACE to create `git pull` requests, in order to enlarge the pool of potential people that can correct or expand the training exercises/workshops. The final decision on whether a git pull request is accepted will belong to the owner of the corresponding repository.

10 The PRACE Training Strategy

Since the beginning of PRACE, there has been a growing emphasis on training the community of researchers and developers to maximize efficiency and productivity on large HPC systems. This has resulted in a diverse range of activities in PRACE that have grown organically (from Seasonal Schools, to PRACE Training Centres, On-demand events, MOOCs). While these activities are sometimes differentiated internally due to operational differences – Seasonal Schools are organised in different ways to On-demand events but ultimately they both provide a face-to-face training service to the community – the collective set of activities contribute to an overarching list of objectives, which are as follows:

1. Develop an advanced base of researchers and developers for exploiting exascale and EuroHPC systems (PTCs),
2. Support a community of intermediate to advanced HPC users and developers, enabling availability of a diverse range of HPC courses across Europe, the stepping stones to more advanced courses (PTCs, Seasonal Schools),

3. Bring new user groups and scientific disciplines, such as SMEs, bio- and life sciences, digital humanities, into HPC (PTCs, Seasonal Schools, On-demand events),
4. Actively pursue training collaborations with other organisations and projects and contribute to invited training events (PTCs, Seasonal Schools, On-demand events, International HPC Summer School),
5. Build a pan-European web portal that is a "one stop shop" for users to find HPC & computational science courses all around Europe, as well as access to material, self-learning resources (e.g. Training Portal, CodeVault),
6. Take advantage of new online platforms to grow the range of PRACE remote learning services to reach larger audiences (e.g. MOOCs),
7. Promote HPC training to undergraduates and universities (e.g. SoHPC, PRACE for Universities in WP3).

This section aims to set out the PRACE training strategy that will provide improved clarity to the approach taken in the planning, implementation and impact assessment of the various activities.

10.1 The European HPC User Base and Target Audience

Somewhat similar to the European HPC infrastructure landscape that can be divided into Tier-0, Tier-1 and Tier-2 systems in a pyramid representation, the HPC user base in Europe consists of a large group of users with a basic knowledge of HPC, followed by a smaller group of "intermediate level" users, and finally an even smaller group of advanced users, as shown in Figure 5.

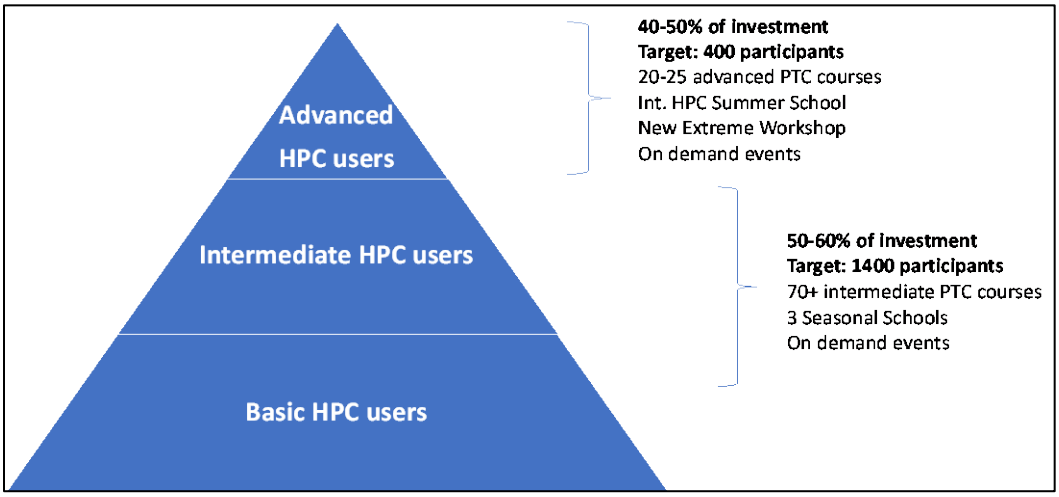

Figure 5: The HPC user pyramid, in context of HPC training

While recognising that PRACE cannot be responsible for providing the necessary training for the entire European HPC user base, the strategy of PRACE is to:

- Recognise that most basic to intermediate level HPC training remain the responsibility of national HPC training programmes.
- Focus a significant proportion of its resources on face-to-face training services that grow the community of advanced users who would gain the prerequisite experience and know-

how to exploit pre-exascale and EuroHPC infrastructure. This investment is targeted towards a relatively small audience of 400 participants per year (Figure 5). It will also organise advanced training that no individual HPC centre can provide by pooling European HPC expertise.

- Dedicate its remaining resources to enable a diverse range of intermediate level HPC courses across Europe, the stepping stones to more advanced courses. Some effort is put also into training that brings new user groups (SMEs, new scientific disciplines) into HPC. This investment is more diffused relative to that for advanced users because the target audience is 1,400 participants per year (Figure 5). But it is a necessary and cost-effective investment by PRACE (in terms of cost per participant) to ensure continued accessibility and dissemination of such courses to all European researchers.

It is important to note that without the investment of resources and coordination by PRACE for both advanced level and some intermediate level courses, HPC training provision in Europe would be disjointed and fragmented; only a handful of large countries may have the training resources to cater for its HPC user base across all levels.

10.2 Regular programme – PTCs, Seasonal Schools

Target audience: intermediate to advanced HPC users.

- PRACE "Extreme Scalability & Performance Workshop" (to be piloted in the PRACE-6IP project): the PTCs will pool their resources (trainers) to invite some of the most talented software developers to attend a week-long event that focuses on cutting edge HPC technologies.
  - Advanced MPI
  - Advanced threading
  - Accelerators
  - I/O performance at scale
  - Programming for exascale, tools and new paradigms

  The special format and features of the school will include the following:

  - Set aside time for ad hoc sessions between participants and trainers to focus on particular codes/solvers/paradigms.
  - Most trainers will spend the whole week at the event to facilitate communication and interaction.
  - Limited to 40 participants.
  - Prerequisite: code developers with 1-2 years with MPI/OpenMP, preferably those already actively developing parallel code on Tier-1 or Tier-0 systems.
- PTCs: collectively offers 20-25 advanced courses per year on cutting edge HPC topics, exploiting maximum performance and scalability using available and new HPC hardware, software and programming paradigms.
  - The objective is to train researchers and developers to exploit pre-exascale systems.

  - Prerequisites: code developers with extensive experience in developing parallel codes (MPI, OpenMP, accelerators) with some know-how in performance analysis and optimisation.
- PTCs: in addition to advanced courses, another 70+ PTC courses per year receives support from PRACE that offers a diverse range of courses aimed at intermediate HPC users that:
  - Adheres to consistent standards of quality.
  - Are readily made available to all European researchers through PRACE dissemination channels and common registration platform.
  - Prerequisites: mainly HPC users and developers with some basic knowledge of HPC code development and/or deployment.
  - Small portion of courses (< 10) maybe targeted for new user groups with only a little previous HPC experience.
- Seasonal Schools: offer HPC and computational science courses in non-PTC hosting sites targeted at all levels of users that:
  - Caters for any regional interests
  - Allow each hosting site to organise courses that cannot be delivered by itself, via support for external trainers to these schools
  - Prerequisites: None required.
- International HPC Summer School: attracts top students from Europe, US, Canada and Japan to participate in a prestigious school that:
  - Is taught by international HPC experts.
  - Provides an overview of HPC challenges in different scientific domains.
  - Prerequisites: Experience with parallel programming, top students with strong motivation and research plans that will benefit from the school.

10.3 Impact Review of PTC Courses

A number of key statistics (e.g. number of participants, training days, overall course ratings) are currently used as indicators of impact of PRACE face-to-face training activities. But there are additional mechanisms that can be implemented in future PTC programmes to gauge other aspects of impact (e.g. whether PRACE courses are catering for some of the most advanced European users/developers). These include:

- Advanced content assessment:
  - Examine the implementation of advanced courses.
  - Ensure that these attract top researchers and developers (prerequisites, profiles of participants).
  - PRACE Scientific Steering Committee (SSC) and Board of Directors (BoD) to provide recommendations on topics.
  - Potentially, follow up surveys/analysis of impact on participants.
- Intermediate content assessment:
  - Ensure a good balance of topics.

- SSC and BoD to provide recommendations on topics.
- Prerequisites examined.

10.4 On-demand Opportunities

PRACE will continue to work with relevant organisations and projects (e.g. CoEs, EUDAT [31]), contributing to external events and/or organise joint events. This requires budget and planning flexibility in order to address more *ad hoc* On-demand opportunities.

10.5 Training Portal

PRACE Training portal acts as the main access point for PRACE training activities. All the PRACE training events are announced on the portal, and the registrations are carried out within it. The portal provides also access to the training material, and provides view to other PRACE online resources, such as MOOCs and CodeVault.

10.6 Remote Learning

While the face-to-face trainings remain the core of the PRACE training, remote learning complements the face-to-face activities by providing more scalable training which is not tied into a place or into a time. The PRACE remote learning activities target mainly the same user groups as face-to-face trainings.

- Massive Open Online Courses (MOOCs) are developed both for intermediate and advanced users. Small part of the effort is put on introducing HPC to new user groups,
- Short video tutorials are available for all interested users,
- CodeVault provides a repository of code samples that can be used in self-learning,
- The lecture and exercise material of past PRACE face-to-face events is provided in the training portal,
- Some face-to-face events provide also remote participation possibility.

10.7 Outreach to Universities

The main target audience of PRACE Training is researchers (including early stage researchers i.e. Ph.D. students). However, PRACE Training has also outreach and dissemination role in introducing HPC to undergraduates and promoting PRACE training to universities. The main activity is the PRACE Summer of HPC which provides early-stage postgraduate and late-stage undergraduate students a two month placement at top HPC centres around Europe with the opportunity to learn and share more about PRACE and HPC. Summer of HPC includes also a training week.

10.8 Summary of PRACE Training strategy

With the increasing importance of HPC in various fields of science and industry, PRACE has central role in proving state-of-the art training for European HPC ecosystem. PRACE has special focus on advanced training which targets to exploiting the pre-exascale and future exascale systems, however, developing a solid base of advanced users requires significant amount of training also in the lower parts of the user pyramid.

PRACE will place special emphasis (~40-50% of its investments in face-to-face training for ~400 participants per year) on offering courses that cater for advanced user communities in Europe. These will be offered on a regular, sustained basis by the PTCs, the International HPC Summer School, and a special "Extreme Scalability and Performance Workshop" (to be piloted in the PRACE-6IP project) that will pool together European HPC training expertise.

While recognising advanced training that caters for European Tier-0 users is well aligned with the PRACE position, and acknowledging that more basic HPC training should mostly be supported on a national level, it is important that PRACE maintains some level of support (albeit more "diluted" level of support) for intermediate courses and a small proportion of basic courses to attract new/emerging user communities. Therefore some 50-60% of investment in face-to-face training, mainly offered by PTCs and Seasonal Schools, will be on intermediate courses that will attract 1,400 participants per year. PRACE support ensures these courses are offered and advertised on a pan-European basis, free-of-charge and organised in a coordinated manner; without PRACE support, many of these courses will be much more restricted in terms of reach, organised in a fragmented manner.

Apart from face-to-face training events, PRACE will maintain and develop online resources that will provide pan-European information on face-to-face courses, training material, sample codes, online tutorials, etc. The cornerstone will be the PRACE Training Portal to facilitate users. There is also tremendous potential for PRACE partners to pool their training expertise to develop MOOCs to attract a global audience for its training offerings. Finally, PRACE will continue its outreach programme to universities to stimulate interest in HPC training among undergraduate students.

11 Conclusion

During the first half of PRACE-5IP, WP4 has continued to provide world-class training in high-performance and scientific computing. There were over 2800 participants in face-to-face courses and workshops, and over 14 000 people registered for PRACE MOOCs. PRACE has also strengthened the on-line training offering by developing the PRACE Training portal and the CodeVault repository of code samples. User satisfaction has been extremely high with an overall score of 8.5 (on a scale of 0-10) for PRACE courses.

In order to ensure continued high-impact training for the European HPC ecosystem in the future, WP4 has refined the strategy of PRACE training. The user perspective of PRACE training has also been streamlined by rebranding the previously distinct PATCs and PTCs under a common PRACE Training Centre brand.

Currently, PRACE is developing three new MOOCs. However, face-to-face events hold a very strong position in PRACE training. PRACE has continued training collaborations with CoEs and other European projects, and participation in international collaboration ensures that PRACE continues to be a key player in HPC training at a global level.

12 Annex

12.1 PATC and PTC Courses offered by PRACE February 2017 – April 2018

Course Title	PATC	Location	Start Date	Duration (days)
Programming Distributed Computing Platforms with COMPSs	BSC	Barcelona, ES	2017-02-02	1
Parallel Linear Algebra	MdS	Ostrava, CZ	2017-02-02	2
Big Data Analytics	BSC	Barcelona, ES	2017-02-07	4
Intel MIC Programming Workshop	LRZ	Ostrava, CZ	2017-02-07	2
24th VI-HPS Tuning Workshop	EPCC	Southampton, UK	2017-02-08	3
Advanced Parallel Programming	CSC	Espoo, FI	2017-02-13	3
13th Advanced School on Parallel Computing	CINECA	Bologna, IT	2017-02-13	5
HPC-based simulations, Engineering and Environment	BSC	Barcelona, ES	2017-02-14	3
Python in High Performance Computing	CSC	Espoo, FI	2017-03-01	3
Parallel filesystems and parallel IO libraries	MdS	Saclay, FR	2017-03-06	2
OpenMP GPU Directives for Parallel Accelerated Supercomputers - an alternative to CUDA from Cray perspective	HLRS	Stuttgart, DE	2017-03-07	2
Parallel I/O and Portable Data Formats	JSC	Juelich, DE	2017-03-13	3
Simulation Environments for Life Sciences	BSC	Barcelona, ES	2017-03-14	2
Spring School in Computational Chemistry 2017	CSC	Espoo, FI	2017-03-14	4
Fortran for Scientific Computing	HLRS	Stuttgart, DE	2017-03-20	5
Advanced Fortran Programming	CSC	Espoo, FI	2017-03-20	3
25th VI-HPS Tuning Workshop	JSC	Aachen, DE	2017-03-27	
Single-sided PGAS Communications Libraries	EPCC	Warwick, UK	2017-03-27	2
Efficient Parallel IO on ARCHER	EPCC	Durham, UK	2017-03-29	2
Metagenomics Data Analysis Workshop	CSC	Espoo, FI	2017-04-03	4
Advanced Topics in High Performance Computing	LRZ	Garching, DE	2017-04-03	4
Programming the Manycore Knights Landing Processor	EPCC	Leeds, UK	2017-04-03	2
Hands-on Porting and Optimisation Workshop: Making the most of ARCHER	EPCC	Birmingham, UK	2017-04-04	1
C-C++ multicore application programming	MdS	Saclay, FR	2017-04-18	3
Introduction to CUDA Programming	BSC	Barcelona, ES	2017-04-18	4
GPU Programming with CUDA	JSC	Juelich, DE	2017-04-24	3
Advanced usage on Curie supercomputer: Best practice for current and future HPC architectures	MdS	Bruyères-le-Châtel, FR	2017-04-25	3
Advanced Optimization and Threading	CSC	Espoo, FI	2017-04-26	3
Node-Level Performance Engineering	HLRS	Stuttgart, DE	2017-04-27	2
Introduction to OpenACC	BSC	Barcelona, ES	2017-04-27	2
Uncertainty quantification	MDLS	Saclay, FR	2017-05-02	3
Introduction to Scientific and Technical Computing in C	CINECA	Bologna, IT	2017-05-03	3
HPC code optimisation workshop	LRZ	Garching, DE	2017-05-04	1
Performance Analysis and Tools	BSC	Barcelona, ES	2017-05-08	2
Software Carpentry	EPCC	Edinburgh, UK	2017-05-09	2
Heterogeneous Programming on GPUs with MPI + OmpSs	BSC	Barcelona, ES	2017-05-10	2
Systems Workshop: Programming ARM based prototypes	BSC	Barcelona, ES	2017-05-12	1

Course Title	PATC	Location	Start Date	Duration (days)
High-performance computing with Python	JSC	Juelich, DE	2017-06-12	2
3rd School on Scientific Data Analytics and Visualization	CINECA	Rome, IT	2017-06-12	5
Workshop HPC Methods for Engineering	CINECA	Milan, IT	2017-06-19	3
Intel MIC Programming Workshop	LRZ	Garching, DE	2017-06-26	3
8th Programming and Tuning Massively Parallel Systems summer school (PUMPS)	BSC	Barcelona, ES	2017-06-26	5
Introduction to Unified Parallel C (UPC) and Co-array Fortran (CAF)	HLRS	Stuttgart, DE	2017-06-29	2
Data Analytics with HPC	EPCC	Portsmouth, UK	2017-06-29	2
Efficient Parallel Programming with GASPI	HLRS	Stuttgart, DE	2017-07-03	2
Hands-on Introduction to HPC	EPCC	Edinburgh, UK	2017-07-10	2
Message-passing Programming with MPI	EPCC	Edinburgh, UK	2017-07-12	3
Modern Fortran	EPCC	Cambridge, UK	2017-07-27	2
Hands-on Introduction to High Performance Computing for womENcourage	EPCC	Barcelona, ES	2017-09-07	1
Advanced Fortran Topics	LRZ	Garching, DE	2017-09-11	5
Advanced MPI	EPCC	Cambridge, UK	2017-09-12	2
Fortran Programming for Scientific Computing	CSC	Espoo, FI	2017-09-21	2
Systems Workshop: Programming MareNostrum 4	BSC	Barcelona, ES	2017-09-26	2
Introduction to Parallel Programming	CSC	Espoo, FI	2017-10-09	3
Parallel Programming Workshop (MPI, OpenMP and advanced topics)	HLRS	Stuttgart, DE	2017-10-16	5
Parallel Programming Workshop (Train the Trainer)	HLRS	Stuttgart, DE	2017-10-16	5
Parallel Programming Workshop	BSC	Barcelona, ES	2017-10-23	5
Introduction to Marconi KNL Cluster, for users and developers	CINECA	Rome, IT	2017-10-23	1
Mastering GPU-Acceleration on OpenPOWER Platform for Optimal Appli cation Performance	MDLS	Orsay, FR	2017-10-24	3
Programming the Manycore Knights Landing Processor	EPCC	Cambridge, UK	2017-10-31	2
Single Node Performance Optimisation	EPCC	Edinburgh, UK	2017-11-06	2
HPC methods for Computational Fluid Dynamics and Astrophysics	CINECA	Bologna, IT	2017-11-13	3
Analysing large datasets with Apache Spark	CSC	Espoo, FI	2017-11-16	2
GPU Programming with CUDA	EPCC	Daresbury, UK	2017-11-21	2
Debugging and Optimization of Scientific Applications	CINECA	Bologna, IT	2017-11-27	3
Hands-on Introduction to HPC for Life Scientists	EPCC	Edinburgh, UK	2017-11-29	3
Earth Sciences Simulation Environments	BSC	Barcelona, ES	2017-11-29	3
Node-Level Performance Engineering	LRZ	Garching, DE	2017-11-30	2
Debugging & Optimization	MDLS	Montpellier, FR	2017-12-04	5
GPU Programming with OpenACC	CSC	Espoo, FI	2017-12-04	2
EoCoE-POP Performance Evaluation Workshop	MDLS	Saclay, FR	2017-12-11	4
Advanced OpenMP	EPCC	London, UK	2017-12-12	3
High Performance Bioinformatics	CINECA	Rome, IT	2017-12-13	3
Parallel and Scalable Machine Learning	JSC	Juelich, DE	2018-01-15	3
Introduction to hybrid programming in HPC	LRZ	Garching, DE	2018-01-18	1
Python in High-Performance Computing	CSC	Espoo, FI	2018-01-29	3
Programming Distributed Computing Platforms with COMPSs	BSC	Barcelona, ES	2018-01-30	1

Course Title	PATC	Location	Start Date	Duration (days)
Big Data Analytics	BSC	Barcelona, ES	2018-02-06	4
Advanced Parallel Programming	CSC	Espoo, FI	2018-02-12	3
14th Advanced School on Parallel Computing	CINECA	Bologna, IT	2018-02-12	5
HPC-based simulations\, Engineering and Environment with Applicati ons in Bioengineering	BSC	Barcelona, ES	2018-02-14	3
Object-Oriented Programming with Fortran	EPCC	Daresbury, UK	2018-02-27	2
Hands-on Porting and Optimisation Workshop: Making the most of ARC HER	EPCC	Oxford, UK	2018-03-08	1
OpenMP GPU Directives for Parallel Accelerated Supercomputers - an alternative to CUDA from Cray perspective	HLRS	Stuttgart, DE	2018-03-12	2
Parallel I/O and Portable Data Formats	JSC	Juelich, DE	2018-03-12	3
Spring School in Computational Chemistry 2018	CSC	Espoo, FI	2018-03-13	4
Simulation Environments for Life Sciences	BSC	Barcelona, ES	2018-03-14	2
Introduction to Parallel Programming with HPX	HLRS	Stuttgart, DE	15/03/2018 (cancelled)	
Efficient Parallel IO on ARCHER	EPCC	Cambridge, UK	2018-03-20	2
Petaflop System Administration\; Marenostrum 4	BSC	Barcelona, ES	2018-03-22	2
Parallel I/O & Libraries	VSB	Ostrava, CZ	2018-03-22	2
Advanced Topics in High Performance Computing	LRZ	Garching, DE	2018-03-26	4
Advanced Fortran Programming	CSC	Espoo, FI	2018-03-26	3
High Performance Molecular Dynamics	CINECA	Rome, IT	2018-03-26	3
Advanced Threading and Optimization	CSC	Espoo, FI	2018-04-04	3
Systems Workshop: Programming MareNostrum 4	BSC	Barcelona, ES	2018-04-09	2
Fortran for Scientific Computing	HLRS	Stuttgart, DE	2018-04-09	5
Introduction to OpenACC	BSC	Barcelona, ES	2018-04-12	2
Introduction to CUDA Programming	BSC	Barcelona, ES	2018-04-16	5
Introduction to the DAVIDE OpenPower GPU cluster	CINECA	Bologna, IT	2018-04-16	2
Programming paradigms for GPU devices	CINECA	Bologna, IT	2018-04-18	3
25th VI-HPS Tuning Workshop	LRZ	Garching, DE	2018-04-23	5
Parallel filesystems and parallel IO libraries	MDLS	Saclay, FR	2018-04-23	2
GPU Programming with CUDA	JSC	Juelich, DE	2018-04-23	3

Table 7: List of PATC courses from Feb 2017 to Apr 2018.

Course Title	PTC	Location	Start Date	Duration (days)
Data Management with iRODS	SURFsara	Amsterdam, NL	25/09/2017	1
Productivity Tools for High Performance Computing	IT4I	Ostrava, CZ	27/11/2017	2
Introduction in Parallel Programming	GRNET	Athens, GR	29/11/2017	3
Parallel and GPU Programming in Python	SURFsara	Amsterdam, NL	06/12/2017	2
CFD Simulations using OpenFOAM	IT4I	Ostrava, CZ	14/12/2017	2
Parallel Programming with MPI and OpenMP	SURFsara	Amsterdam, NL	05/07/2018	3
Machine Learning with Apache Spark	SURFsara	Amsterdam, NL	13/02/2018	1
Efficient Use of HPC Systems	GRNET	Athens, GR	13/02/2018	2
Introduction to High-Performance Machine Learning	SURFsara	Amsterdam, NL	14/02/2018	1
Intel Xeon Phi Programming	IT4I	Ostrava, CZ	01/03/2018	2
Introduction to Biomolecular modelling and Molecular dynamics in HPC	GRNET	Athens, GR	23/04/2018	1
Data, lights, camera, action! Scientific visualization done beautifully	SURFsara	Amsterdam, NL	24/04/2018	1
PETSc Basic & Advanced Tutorial	IT4I	Ostrava, CZ	10/05/2018	2
Accelerator Programming	GRNET	Athens, GR	22/05/2018	2
HPC in Molecular & Atomistic Simulations	ICHEC	Dublin, IE	13/06/2018	4
Parallel Programming: Basics and Beyond	ICHEC	Dublin, IE	02/07/2018	5

Table 8: List of PTC courses from Feb 2017 to Jul 2018.

12.2 Autumn 2017 Seasonal School Report, Poland

GUT – Gdańsk University of Technology, Poland
CI TASK – Academic Computer Center in Gdańsk, Gdańsk University of Technology
SCAI – Fraunhofer-Institute for Algorithms and Scientific Computing, Germany
IMP PAN – Institute of Fluid Flow Machinery Polish Academy of Science
UGLA – University of Glasgow

PRACE Autumn School 2017 – Event Report

1 Basic information about the event

1.1 Name

PRACE Seasonal School on Computational Fluid-Structure Interaction

1.2 Dates

20.11.2017 – 24.11.2017

1.3 Location

Gdańsk, Poland

1.4 Organising sites

- Gdańsk University of Technology – Academic Computer Centre in Gdańsk (CI TASK),
- Institute of Fluid Flow Machinery Polish Academy of Sciences (IMP PAN),
- University of Glasgow (UGLA)
- Fraunhofer-Institute for Algorithms and Scientific Computing (SCAI)

1.5 Mission

We know that HPC is intensely used across a wide range of academic disciplines and within industry for obtaining results for computational problems very quickly or for discovering new and novel solutions. Thus we perceive HPC as a laboratory for research and development where new or novel novel solutions to computational problems are discovered. Access to carrying out experiments in this HPC laboratory is easy for new as well as experienced HPC users. Our mission is to make HPC easily accessible and hereby enable a wide range of academic users to be able to easily apply HPC optimally in their workflows. To achieve this we would like to provide high-quality education and training service for the European HPC community. We belive that the most import thing is to get smooth combination of theory and practice.

1.6 Event URL

https://events.prace-ri.eu/event/667

2 Organisational details

2.1 Local organising committee

- Rafał Tylman, CI TASK
- Ewa Politowska, CI TASK
- Michał Białoskórski, CI TASK

- Ondrej Jakl, VSB

2.2 Venue

Seasonal school was placed at our headquarter in Gdańsk University of Technology. It is located in city centre and close to the old city centre of Gdańsk (approx 10 minutes by public transport). It is very easily to get there from airport (approx 20 min by train) and main train station (approx 5 minutes). All laboratories and lecturers were held in well equipped conference room suitable for 30 persons.

3 Program & contents

3.1 Program committee

- Geroge Barakos, UGLA
- Klaus Wolf, SCAI
- Maciej Kahsin, GUT
- Marcin Łuczak, IMP
- Michał Białoskórski, CI TASK

3.2 Designing the program

Large number of the mechanical, aerospace, civil and hydro engineering machines are operating in the complex environment. Floating offshore wind turbine or the helicopter in flight are only a reference examples of the problem. Operational loads and resulting structural response of the investigated object are coming from aerodynamic, hydrodynamic and thermal forces. Traditionally those mechanical systems are being studied w.r.t the different scientific disciplines: solid mechanics, flow mechanics, material sciences and computer methods only to name major domains. It leads to the approximate and often imprecise results of numerical simulations. Muti-physics approach is required to adequately address the complexity of the real-life operation of the mechanical systems.

Proposed Seasonal School on Computational Fluid-Structure Interaction tries to close the isolated domain analysis gap. The FSI School offers an integrated multidisciplinary training covering the comprehensive spectrum of the mathematical theorems, fluid and solid dynamics, numerical modelling techniques and all this within the framework of the HPC resources and tools able to tackle the challenging problems of the coupled multi-physics problems. Lectures will be followed with the laboratory exercises run on the CI TASK cluster. The course is addressed to wide audience ranging from PhD students to more senior researchers active in the science and industrial R&D departments.

3.3 Description of the contents

HPC – Introduction to High Performance Computing. On this seminar attendees were introduced to HPC and parallel calculation problems. On laboratories attendees were able to access to supercomputer and learn how to submit jobs to queue.

CFD – This seminar provides an introduction to the CFD methods. From basic elements to more andvaced problems. On laboratories attendees conducted by trainer write their own CFD calculation programs in Fortran

FEM – Introduction to FE modelling concept. Derivation of governing equations for 1D problems (simple approach). Formulation's generalization for 2D, ad 3D problems (weighting methods). Simplification for special cases. During laboratories attendees where working with Matlab software.

FSI – This seminar provides an introduction to the Fluid-Structure Interaction (FSI) capability using CFD and FEA codes based on MpCCI technology from Fraunhofer SCAI. FSI covers a broad scope of problems in which fluid flow and structural deformation interact and affect each other. The interaction may be thermal, mechanical, or both and can be steady or transient. Many problems involve some form of FSI. During the seminar's lectures and workshops users will learn about: Developing coupling strategies, Simulating FSI problems by co-simulation, Evaluating FSI algorithms, Using MpCCI, commercial CAE tools like Abaqus, ANSYS Fluent and open source packages like OpenFOAM, CalculiX

3.4 List of trainers

George Barakos – professor at School of Engineering of the University of Glasgow. George has so far delivered undergraduate and graduate-level courses on Fluid Mechanics, Aerodynamics, Aeroelasticity, Computational Fluid Dynamics and Thermodynamics, Simulation in Aerospace Engineering. He is the author of some 150 research papers and a regular contributor to national and international conferences on aerodynamics, fluid mechanics and CFD.

Pascal Bayrasy – Development Manager at Fraunhofer SCAI, specialised on Fluid Structure Interaction Method. Involved in R&D of MpCCI Coupling Environment software.

Nadja Wirth – engineer at Fraunhofer SCAI, specialised on Turbomachineru applications, and MpCCI software development.

Maicej Kashin, PhD – scientist and lecturer at GUT. Specialised on Finite Element Methods (FEM).

Michał Białoskórski, PhD – senior HPC specialist in CI TASK administrator involved in building first HPC clusters. During his work in CI TASK has a lot of didactic activities with students and On-demand workshops for HPC users

3.5 Computer resources

All attendees have guarantee access to CI TASK supercomputer – Tryton (https://www.top500.org/system/178552) within course accounts. There where resource reservation set for course purpose.

Laboratories were held on virtual machines with installed all software needed for course. Attendees has been connecting to the laboratory via remote desktop application.

4 Participants & feedback

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

There were 32 participants, from Poland only.

4.2 Analysis of the feedback

All participants were satisfied from the course level and contents, except one who was expecting more HPC information and less theorems.

The most attractive for attendees where CFD lab classes – 50% asks for course continuation in future.

4.3 Awareness activities, outreach

Information was published on PRACE event portal and disseminated in HPC centres in Poland as well as researchers working with fluid dynamics.

The maximal number of registrants was reached.

5 Conclusions & lessons learned

Organisation of Seasonal School was very valuable experience and it was not as difficult as we thought it would be.

The concept of laboratories run on prepared in advanced virtual machines was a just idea. The time spent on preparation of systems resulted in efficient conduct of laboratories. There were no problems with wireless network bandwidth, all remote desktops ran smoothly.

12.3 Winter 2018 Seasonal School Report, Slovakia

1. Basic information about the event
   1.1. Name
   PRACE Seasonal School on Bioinformatics
   1.2. Dates
   23.-26. 4. 2018
   1.3. Location
   Bratislava, Slovak Republic
   1.4. Organizing sites
   Computing Center of the Slovak Academy of Sciences (CC SAS)
2. Organizational details
   2.1. Local organizing committee (table)

Name	Organization
Dr. Lukas Demovic	CC SAS
Dr. Michal Pitonak	CC SAS
prof. Jozef Noga	CC SAS
Dr. Lubos Klucar	Institute of Molecular Biology of SAS

   2.2. Venue
   Event was organised in a conference room provided by the Plant Science and Biodiversity Centre of SAS. Conference room provided enough space to comfortably accommodate all (about) 40 participants. Venue was easy to find and reached, internet connection (wifi) was satisfactory for remote connection to our supercomputer, without delays and interruptions. The costs for renting the conference room were fractional compared to the "commercial" ones.
   2.3. Realized workload (table: person and total working hours spent for the event)

Name	PMs
Dr. Lukas Demovic	1.25
Dr. Michal Pitonak	1.25
prof. Jozef Noga	0.5

   2.4. Synergetic events
   None
3. Program & content
   3.1. Program committee (table)

Name	Organization
Dr. Lukas Demovic	CC SAS
Dr. Michal Pitonak	CC SAS
prof. Jozef Noga	CC SAS
Dr. Lubos Klucar	Institute of Molecular Biology of SAS

   3.2. Final program (table (appendix))
   See appendix
   3.3. List of trainers (full list of trainers as an appendix with contact information and description of expertises)

- Prof. Erik Bongcam Rudloff: biologist and computer scientist. He is Professor of Bioinformatics and the head of SLU-Global Bioinformatics Centre at the Swedish University of Agricultural Sciences. His main research deals with development of bioinformatics solutions for the Life Sciences community; erikbong@mac.com
- Dr. Seija Sirkiä: Data scientist at CSC - Scientific computing Ltd., Finland.; seija.sirkia@csc.fi
- Mr. Apurva Nandan: Software specialist at CSC - Scientific computing Ltd., Finland. Works in the Data Analytics group building big data and cloud based applications; apurva.nandan@csc.fi
- Dr. Kimmo Mattila: Bioinformatics specialist at CSC - Scientific computing Ltd., Finland; kimmo.mattila@csc.fi

3.4. Designing the program

The program was designed to attract more researchers from the field of biology to bioinformatics and especially HPC technologies. It is indisputable that HPC and Big Data technologies have a lot to offer to bioinformatics, however a (possible) lack of education background of “biologists” in this field often poses a barrier for successful applications. The program comprises overview of necessary mathematical theory required to understand machine learning algorithms, overview of HPC parallel computer architectures, working in (typically Unix/Linux-based) HPC environment, (parallel) programming in popular data science languages such as R and hands-on experience with the most common bioinformatics program packages for their efficient use and application limits.

3.5. Description of the contents

- Introduction to bioinformatics: General overview of the field with a special attention to use of (super)computers.
- Parallel programming with R: This lecture is aimed at R users with very limited or no experience in parallel computing. You will learn how and when taking advantage of parallel computing can help you run your R scripts in less time, when not, and how to tell the difference. More importantly, you will get an idea of how to approach parallelizing your task in practice. We will consider Intel Math kernel library (MKL) together with Microsoft R Open, and R packages snow and “foreach”, both used as backend by various Bioconductor and CRAN packages. Lecture will include live coding demos. Prerequisites: experience in using R for data analysis in research
- Analyzing large datasets with Spark: With the rapid growth in data volume that is being used in data analysis tasks, it gets more and more challenging for the user to process it using standard methods. Enter Spark, a high-performance distributed computing framework, which allows us to tackle big-data problems by distributing the workload across a cluster of machines. This two day course discusses the advantage of cloud computing for big data based computing, why should you use Spark for big data analysis and why should you care about running Spark on cloud. Next, the technical architecture and use cases of Spark, some ways to set it up, best practices and programming aspects. The first day

includes the overview, architectural concepts, programming with Spark's fundamental data structure (RDD) and basics of Machine Learning with Spark. The second day focuses on the SQL module of Spark, which allows the user to analyze data using Spark's distributed collection (Dataframes) by using the traditional SQL queries, best practices when using spark, demo of a working Spark cluster, using Spark Streaming over a live twitter data. Spark can be an ideal platform for bioinformatics when it comes to building analysis pipelines and workflows. Spark supports languages such as R, Python, and SQL which eases the learning for practicing bioinformaticians. Spark is constantly growing with new libraries for bioinformatics analysis, although widespread usage will take some time because the traditional methods need some rewriting in Spark. But, with the community constantly evolving, it is good chance to learn Spark and implement your own methods in it, for doing large scale data analysis.

- BLAST: Running BLAST in Clusters NCBI BLAST is one of the most of the most frequently used bioinformatics tools. BLAST answers to the question: "What known sequences are significantly similar to my sample sequence". Answer to this question is needed in numerous bioinformatics analyses and work-flows. As the sequence databases keep growing as well as the sizes of the data sets to be analyzed, a HPC cluster environment is often needed for BLAST analyses. In this half a day session we briefly go through the basic features of BLAST and issues related to maintaining and using BLAST in HPC cluster environments.

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)

56 node x64 infiniband cluster with Lustre filesystem under CC SAS administration. Participants used their own laptops during the hands-on sessions for accessing the cluster.

4. Participants & feedback

4.1. Number of participants by country

Country	Count
Slovakia	32
Czech Republic	1
Germany	1

4.2. Process for selecting the participants (if applicable)

No selection applied

4.3. Statistics of the feedback survey (tables (appendix))

To be added if available

4.4. Analysis of the feedback

We have 18 replies to the evaluations. Significant fraction of participant had very little experience with programming and working in HPC environment in general. We tried to bridge this gap by providing one-day tutorial, a day before the Seasonal School start. About one third of the participants took this opportunity either in person of via video conference.

Positive:

- Venue, catering, organization and registration were good or excellent
- Most of participants agree that the topic was relevant for their research and / or inspiring
- About 70% of participants rated the school with grade 8 to 10 (10 is the best).

Negative:

- 44% of attendees claim that the information about the school was worse the "good"
- 39% claim didn't agree that lectures were "clear and comprehensive"
- 40% don't completely agree with the "pace of teaching" was right.

5. Conclusions & lessons learned

   We are aware that this school may have been too advanced for non-negligible fraction of participants due to a lack of programming skills. However, if we would explicitly state, that the event is suitable for skilled programmers, we would hardly attract this many participants (especially among biologists). We nevertheless strongly believe that the school was inspiring for many of them and by enlarging the community of researched using bioinformatics tools in HPC environment, even more researchers will be attracted to this area. Despite rather small participation of foreign researchers we were positively surprise that we could attract local researcher from various institutions across the country. Most of the attendees are not HPC users (yet) that we could effectively disseminate the information not only about our local computing resources and opportunities but also about PRACE to a brand new community.

12.4 On-demand Events Application Form Template

1. **Basic information about the event**
   - **1.1. Name**
   - **1.2. Dates**
   - **1.3. Location**
   - **1.4. Organizing sites**
   - **1.5. Mission and relevance to other communities (i.e. CoE, etc)** (max ½ page)
2. **Organizational details**
   - 2.1. **Local organizing committee** (draft table)
   - 2.2. **Venue** (name, its description and why it was selected; fluid text: analysis of the facilities provided their use for the particular training) (max ½ page)
   - **2.3. Budgeting** (fluid text: reasoning behind the budget; table: the budget) (max 1 page)
   - 2.4. **Workload** (table: person or type of employee and estimation of working hours to be spent for the event
   - **2.5. Synergetic events (listing: will there be any other PRACE activity during the event which would** have utilized the venue or other effort) (max ¼ page)
3. **Tentative Program & content**
   - 3.1. **Draft program** (table listing the selected topics of the potential seasonal school, indication about parallel sessions, hands on etc.)
   - 3.2. **Expected Participants**
   - 3.3. **Number of expected participants**
4. **Planned Awareness activities, outreach** (fluid text)
5. **Any other relevant information to support your application** (fluid text)

12.5 PRACE-5IP Y1 On-demand Events Reports

12.5.1 E-CAM Workshop on Particle-Based Models and HPC

1. Basic information about the event
   1.1. PRACE E-CAM Workshop on Particle-Based Models and HPC
   1.2. 7-9.6.2017
   1.3. CSC - IT-center for science
   1.4. CSC, Aalto university
2. Organizational details
   2.1. Local organizing committee
   Jan Åström, CSC
   Mikko Alava, Aalto
   Antti Puisto, Aalto
   2.2. A workshop on particle based models and HPC, was arranged because such methods have emerged more and more as important tools for science research. In comparison to more standard methods based on numerical solution for differential equations, particle methods more directly deal with the underlying physics of a problem. In contrast, these methods are much more demanding in terms of compute power requirements.
   2.3. Workload, person ~hours
   Jan Åström ~ 150h
   2.4. Synergetic events: The workshop fit as a natural part of CSC and Aalto courses on HPC methods in science.
3. Program & content
   3.1. Program committee
   Jan Åström
   Mikko Alava
   Antti Puisto
   3.2. Final program: attached appendix
   3.3. List of trainers (appendix)
   3.4. Designing the program: The idea behind the program was to find a suitable mix of experts on particle models and HPC experts. The HPC part was focused on implementing particle models on GPUs, and the particle model part focused on models for fracture and fragmentation as well as the Lattice Boltzmann method for fluid dynamics.
   3.5. Description of the contents (brief commentary of each lecture and lab/exercise)
   3.6. Computer resources: table top work stations with GPUs in the CSC lecture room.
4. Participants & feedback
   4.1. Number of participants by country:
   Finland: 17
   Estonia: 1

Holland: 1
Hungary: 1
Germany: 1

4.2. Process for selecting the participants (all who expressed interested could attend)
4.3. Statistics of the feedback survey (only one person feedback received. Maximum positive feedback 5/5 on all points.)
4.4. Analysis of the feedback (only one person feedback – not statistically representative. On-site personal feedback at the closing overwhelmingly positive - "very useful" was the general comment.)

5. Conclusions & lessons learned (A very positive experience in general.)

12.5.2 Energy-aware application development for heterogeneous computing

1. Basic information about the event
   1.1. Name
   Energy-aware application development for heterogeneous computing
   1.2. Dates
   November 21st, 2017
   1.3. Location
   Barcelona
   1.4. Organizing sites
   Barcelona Supercomputing Center (BSC)
2. Organizational details
   2.1. Local organizing committee

Rosa M. Badia, Jorge Ejarque, TANGO Project, Computer Science Dept, BSC
Education and Training Team of BSC under the management of Maria-Ribera Sancho.

   2.2. Venue
   The course was hosted by BSC on the Nord Campus Premises of UPC. We used the standard set-up applied for the PATC courses we run.
   2.3. Realized workload (table: person and total working hours spent for the event)
   2.4. Synergetic events (listing: was there any other PRACE activity during the event which would have utilized the venue or other effort)
   No
3. Program & content
   3.1. Program committee
   The role of convener was assigned to Jorge Ejarque, a researcher working at the Computer Science department of BSC
   3.2. Final program (see table in Appendix))
   3.3. List of trainers (see Appendix)
   3.4. Designing the program
   With this course, we aimed to present the TANGO toolbox which provides a set of tools to simplify and optimize the usage of distributed heterogeneous computing

environments. We mainly targeted to attract students, HPC application developers and System administrators which can benefit from the tools we developed at the TANGO project.

3.5. Description of the contents

In the first lesson the student learned why heterogeneous computing is important nowadays. In the second lesson, students got an overview of TANGO toolbox components and the provided functionality.

In the third lesson, the attendees got a first lesson about the programming model and an overview of the runtime internals. The attendees programmed with COMPSs and that enabled them to start programming with this framework.

A hands-on with simple introductory exercises was also performed. The students who finished this course will be able to develop simple applications and to run them in a distributed heterogeneous platform.

3.6. Computer resources

For this course, we created accounts for Minatauro. We used the UPC network to connect to the Internet. Students were asked to bring their own laptops.

4. Participants & feedback

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

Spain 13
Brazil 1
Iran 1

4.2. Process for selecting the participants

All students registered were accepted.

4.3. Statistics of the feedback survey (tables (appendix))

There was no quality survey for this course because the number of registration were low.

5. Conclusions & lessons learned

Since we did not get the student target number, we think dissemination of our training activities should be improved at BSC

APPENDIX

PROGRAM

Session 1 / 9:00 – 10:00: Introduction

- Overview of Heterogeneous distributing computing
- Why TANGO?

Coffee Break 10:30

Session 2 / 10:00am – 12:00pm: TANGO Toolbox

- Introduction to the TANGO Toolbox Components
- Demos

Session 3 / 12:00 -13:00 Introduction to TANGO Programming Model

- Programming Model Syntax

Lunch Break 13:00 to 14:00

Session 4 / 14:00 pm- 17:30 pm: Programming Model Hands-on

- Environment Setup
- Sample application overview
- Exercise with an incomplete sample code
- Compilation and execution
- Monitoring and Debugging
- Final notes

Coffee Break 16:00

END of COURSE

LIST OF TRAINERS

Name	Institution	Contact Details
Jorge Ejarque, Workflows and Distributed computing group, Computer Sciences Dept	BSC	jorge.ejarque@bsc.es
Karim Djemame	University of Leeds	
David Garcia	Atos Research and Innovation	

12.5.3 Programming and optimizing the Knights Landing

1. Basic information about the event
   1.1. PRACE Workshop on “Programming and Optimizing the Intel Knights Landing Manycore Processor”
   1.2. Dates: 24-25.04.2018
   1.3. Location: HPC2N, Umeå University, Sweden
   1.4. Organizing sites: HPC2N, Umeå University
2. Organizational details
   2.1. Local organizing committee
   Jerry Eriksson, HPC2N
   Pedro Ojeda-May, HPC2N
   Birgitte Brydsö, HPC2N
   2.2. A two day workshop with instructors from Intel. The course focused on programming and optimizing the Intel ® Xeon Phi™ Manycore Processor, codenamed "Knights Landing (KNL)" and how to best use it efficiently. Code examples were profiled on KNL processors. Participants were encouraged to bring their own code, which Intel instructors helped them optimize.
   2.3. Workload, person ~hours
   Jerry Eriksson ~ 100h
   Pedro Ojeda-May ~ 100h
   2.4. Synergetic events: The workshop was a natural fit for HPC2N and the NLAFET group with a focus on HPC programming and optimization.
3. Program & content
   3.1. Program committee
   Jerry Eriksson
   Mikko Byckling
   Asma Farjallah

3.2. Final program: https://www.hpc2n.umu.se/events/courses/knl-spring-2018
3.3. List of trainers: Mikko Byckling and Asma Farjallah, Intel Corporation
3.4. Designing the program: The idea was to offer training on KNL programming, on vectorization, and on optimization from experts in the field.
3.5. Description of the contents: (brief commentary of each lecture and lab/exercise)
3.6. Computer resources: Kebnekaise KNL partition at HPC2N.

4. Participants & feedback
   4.1. Number of participants by country:
   Finland: 1
   Germany: 1
   Mexico: 1
   Sweden: 10
   Denmark: 2
   Jordan: 1
   Canada: 1
   Vietnam: 1
   4.2. Process for selecting the participants (all who expressed interested could attend)
   4.3. Statistics of the feedback survey (evaluation results to be added.)
   4.4. Analysis of the feedback (evaluation results to be added.)
5. Conclusions & lessons learned (A very positive experience in general. More comments to follow.)

12.6 Feedback from the International HPC Summer School 2017

Question	Strongly disagree		Disagree		Neutral		Agree		Strongly agree		Total
My goals for attending the international HPC Summer School were achieved	0%	0	2%	1	12%	8	55%	36	32%	21	66
The summer school was well organized	0%	0	0%	0	5%	3	36%	24	59%	39	66
I am satisfied with the delivery format of the summer school	0%	0	5%	3	6%	4	53%	35	36%	24	66
I am satisfied with my interaction with my mentor during the mentoring/work sessions	0%	0	3%	2	14%	9	24%	16	59%	39	66
I meaningfully engaged with a mentor during the summer school	2%	1	3%	2	14%	9	29%	19	53%	35	66
I plan on keeping in contact with my mentor after the summer school	2%	1	6%	4	18%	12	35%	23	39%	26	66
	2%	1	6%	4	23%	15	41%	27	29%	19	66

I plan on keeping in contact with a staff member after the summer school											
I am satisfied with the student/mentor matching process	2%	1	3%	2	23%	15	33%	22	39%	26	66
I meaningfully engaged with other students at the summer school	0%	0	3%	2	2%	1	32%	21	64%	42	66
The fact that students from other countries participated in the summer school contributed to my learning	0%	0	2%	1	6%	4	30%	20	62%	41	66
The knowledge/skills I gained during this summer school will significantly contribute to my work/research	2%	1	0%	0	11%	7	41%	27	47%	31	66
I know the next step for me to build on what I learned at this summer school	0%	0	2%	1	20%	13	36%	24	42%	28	66
I am interested in learning more about the resources/opportunitie s available through Compute/Calcul Canada, PRACE, RIKEN, or XSEDE as a result of this experience	0%	0	2%	1	6%	4	36%	24	56%	37	66
I plan on obtaining (or currently have) access to Compute/Calcul Canada, PRACE, RIKEN, or XSEDE resources	0%	0	2%	1	9%	6	32%	21	57%	37	65
The lodging was adequate	2%	1	5%	3	6%	4	49%	32	38%	25	65
Overall I would rate my experience as successful	0%	0	0%	0	8%	5	24%	16	68%	45	66

Table 9. Feedback from 66 responses from the International HPC Summer School 2017 in Boulder, Colorado.