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Author(s): Simon Wong, ICHEC

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[32] HPC Carpentry, https://hpc-carpentry.github.io/

List of Acronyms and Abbreviations

AI Artificial Intelligence

CERN Conseil Européen pour la Recherche Nucléaire (European Council for Nuclear

Research)

CoE Centre of Excellence CPU Central Processing Unit

CUDA Compute Unified Device Architecture (NVIDIA)

EUDAT CDI EUDAT Collaborative Data Infrastructure

F2F Face-to-Face

FAIR Findable, Accessible, Interoperable and Reusable

GPU Graphic Processing Unit

HPC High Performance Computing; Computing at a high performance level at any

given time; often used synonym with Supercomputing

MB Management Board (highest decision making body of the project)

ML Machine Learning

MOOC Massively open online Course MPI Message Passing Interface

PATC PRACE Advanced Training Centre

PRACE Partnership for Advanced Computing in Europe; Project Acronym

PTC PRACE Training Centre

RIKEN Rikagaku Kenkyusho (Institute of Physical and Chemical Research, Japan)

R-CCS RIKEN Center for Computational Science

SKA Square Kilometre Array

List of Project Partner Acronyms

BSC Barcelona Supercomputing Center - Centro Nacional de Supercomputacion,

Spain

CCSAS Computing Centre of the Slovak Academy of Sciences, Slovakia

CÉCI Consortium des Équipements de Calcul Intensif, Belgium

CENAERO Centre de Recherche en Aéronautique ASBL, Belgium (3rd Party to

UANTWERPEN)

CINECA CINECA Consorzio Interuniversitario, Italy CSC CSC Scientific Computing Ltd., Finland EPCC EPCC at The University of Edinburgh, UK

EUDAT EUDAT OY

ETH Zurich (CSCS) Eidgenössische Technische Hochschule Zürich – CSCS, Switzerland

D4.1

GCS Gauss Centre for Supercomputing e.V., Germany

GÉANT Vereniging

GRNET National Infrastructures for Research and Technology, Greece

ICHEC Irish Centre for High-End Computing

IT4I Vysoka Skola Banska - Technicka Univerzita Ostrava, Czech Republic

IUCC Machba - 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-UU)

KULEUVEN Katholieke Universiteit Leuven, Belgium (3rd Party to UANTWERPEN)
NCSA NATIONAL CENTRE FOR SUPERCOMPUTING APPLICATIONS,

Bulgaria

PRACE Partnership for Advanced Computing in Europe aisbl, Belgium

SNIC-UU Uppsala Universitet, Sweden

SURFsara Dutch national high-performance computing and e-Science support

center, part of the SURF cooperative, Netherlands

TU Wien Technische Universität Wien, Austria UANTWERPEN Universiteit Antwerpen, Belgium

UIBK Universität Innsbruck, Austria (3rd Party to TU Wien)

UL UNIVERZA V LJUBLJANI, Slovenia

ULFME University of Ljubljana Faculty of Mechanical Engineering, Slovenia

UmU Umea University, Sweden (3rd Party to SNIC-UU)

VSC Vienna Scientific Cluster, Austria

VSC Vlaams Supercomputer Centrum (Flemish Supercomputer Center),

Belgium

Executive Summary

The Training Work Package (WP4) of the PRACE-6IP project is responsible for the design and execution of a comprehensive range of HPC training activities. This includes an extensive, annual programme of short courses that are delivered by a network of now 14 PRACE Training Centres (PTCs), a series of Seasonal Schools, on-demand events, Massive Open Online Courses (MOOCs) which are underpinned by the PRACE Training Portal. This deliverable is the interim, mid-term report of all PRACE-6IP training activities up to Month 18 of the project.

The COVID-19 pandemic has had an obvious effect on training activities, in particular face-to-face courses and schools that are no longer feasible due to travel and social distancing restrictions. While this had caused disruptions and the postponement and cancellations of some 20+ events (PTC courses, a Seasonal School, the 2019 International HPC Summer School, the EuroHPC Summit Week 2020 hands-on workshops), there has been a quick pivot to providing courses online. Since the onset of the pandemic in March 2019, WP4 had still managed to deliver 29 PTC courses and the PRACE Autumn School 2020 online, not the mention converting the PRACE Summer of HPC into a virtual mentoring programme and continuing the Massive Open Online Courses (MOOCs).

The network of PTCs has expanded by four new members (from Austria, Belgium, Slovenia and Sweden) in late 2019 for a total of 14 partners who are involved in delivering an annual joint programme of courses. From May 2019 to September 2020, the PTCs have collectively delivered 119 courses, representing 326 days of training with 3,549 participants. This includes the 2019-2020 PTC programme in which almost a quarter of its courses had to be delivered online. As trainers continue to learn and improve the online learning experience, indications are that online courses have proven to be attractive to participants from all over Europe including non-PTC hosting countries. These lessons will be brought into the 2020-2021 programme with a target of 138 courses, representing 338 training days.

WP4 had targeted the delivery of eight Seasonal Schools during the course of the PRACE-6IP project. The first PRACE Autumn School in 2019 was held in Slovenia organised in a fast-tracked manner. While the schedule of Seasonal Schools, including location and organising partners, were finalised by early 2020, the COVID-19 pandemic caused the 2020 PRACE Winter School in Austria to be aborted after its first day. The subsequent 2020 Autumn School in Slovenia was successfully delivered in a hybrid face-to-face and online format. Therefore, two Seasonal Schools have been fully delivered with a total of 128 participants. A modified schedule is being finalised for delivery of remaining Seasonal Schools in 2021.

Apart from Seasonal Schools, two on-demand events have been held in 2019 that involved collaborations with the EUDAT and the BioExcel CoE projects. Meanwhile, WP4 has co-organised another successful International HPC Summer School 2019, in collaboration with partners from Canada, Japan and the U.S., which was held in Kobe, Japan in July 2019, with 80 participants including 30 from Europe. The 2020 International HPC Summer School was planned to take place in Toronto, July 2020 but has been cancelled due to the COVID-19 pandemic; the event is being rescheduled to 2021 in the same venue. Plans are ongoing to organise an advanced PRACE extreme-scale workshop, taught by a pool of instructors from PRACE partners, in 2021.

The PRACE Summer of HPC programme, where European students are mentored by HPC experts across participating PRACE partner sites, hosted 25 projects for 25 visiting students at HPC centres in 2019. While travel restrictions in summer 2020 had looked to curtail this programme in 2020, WP4 managed to transform it into a remote mentoring programme where 50 students partnered up to partake in 25 projects across HPC partners.

With the addition of another new MOOC developed by WP4, PRACE now has a repertoire of six MOOCs that are being run on the FutureLearn platform on a periodic basis. During the first half of the project, 5 MOOCs were delivered across 8 instances (i.e. some repeat runs of the same MOOC), which had attracted a total of 7,475 active learners (16,568 enrolments). Development of new MOOCs are planned for the second half of the project.

Training collaboration has always been an important aspect of PRACE. WP4 has engaged with a variety of external projects and research infrastructures to identify potential synergistic activities. Some of the engagements so far include the planning of joint training event with RedCLARA (South America), potential joint activities with CERN / GÉANT / SKA and working with FocusCoE and CASTIEL to ensure alignment in activities and providing a platform for exchange of ideas and best practices. New approaches to develop basic training materials are being investigated with the intention to contribute towards the collaborative efforts of HPC Carpentry.

Finally, the PRACE Training Portal and Events Portal have been updated and improved with new functionalities to improve the user experience. The Training Portal underwent a redesign to be consistent with the main PRACE web site, with the adoption of a new events registry system with additional metadata that makes it easier for users to identify relevant courses.

1 Introduction

Training has always been a critical PRACE activity as there is an ever-growing demand for HPC competences that can make the best use of available software and hardware to tackle big and complex problems. As we enter the EuroHPC and exascale era, the onus to develop HPC competences is even greater for Europe to remain globally competitive. With support from the Implementation Phase (IP) projects, PRACE plays a key central role in the European HPC training landscape with a comprehensive training programme. This programme encompasses many activities such as training courses or events, mentorships, online learning materials, Massive Online Open Courses (MOOCs), as well as online portals/resources related to training.

In this document, the activities of WP4 for the first 18 months of the PRACE-6IP project are presented with details. Undoubtedly, the COVID-19 pandemic has made considerable impact on planned training activities. A general overview of some of these effects, and the WP4 response to them, are outlined in Section 2. Section 3 describes the activities of the network of PRACE Training Centres (PTCs) which has been expanded during the PRACE-6IP project to a total of 14 members. Section 4 presents two complete Seasonal Schools that have been realised so far in the project and plans for upcoming schools together with the Extreme-Scale workshop that is being planned for 2021. Section 5 provides a summary of PRACE training events that have been organised on an ondemand basis, typically in collaboration with other projects. Section 6 reports on the International HPC Summer School which has been an ongoing, successful training collaboration. Section 7 describes work so far in sustaining the Summer of HPC mentoring programme that is typically aimed at undergraduate students or recent graduates. Section 8 reports on developing and running Massive Online Open Courses (MOOCs). Section 9 highlights some of the latest developments of the PRACE Training Portal, and the related events portal, which represents the online hub for PRACE training activities. Section 10 covers collaboration with other stakeholders such as CERN, SKA, GÉANT, RedCLARA, FocusCoE, CASTIEL, etc. Lastly, some concluding remarks are presented in Section 0.

2 Covid-19 Pandemic: Effect and Response

The Covid-19 pandemic and its effects on travel, gatherings, etc. have had an obvious impact on PRACE training activities; and it may continue to do so for the foreseeable future. While there have been disruptions to planned events, WP4 in general have reacted in a pragmatic manner to pivot its activities towards an online setting where possible.

At a project level, the PRACE-6IP project has announced two directives to ensure that all PRACE meetings including training events were to be organised in an online or hybrid (face-to-face plus online) format. While this has provided clarity to organisers, WP4 has made the following efforts in response to the pandemic:

Activity	Impact or response
PRACE Training Centre courses	While some PTC courses had to be postponed or cancelled, tremendous effort is being used to pivot courses online. 29 online courses have been delivered in this reporting period. Future events will be organised under an "online delivery" assumption with possibility of partial or full face-to-face participation as an unexpected bonus.
Seasonal Schools	The PRACE Winter School 2020 was interrupted mid-way by lock-down measures; this event is proposed to be organised again in 2021. The Seasonal School timetable has been re-configured with some events postponed to 2021.
Summer of HPC 2020	After consultation with student applicants, the programme has been transformed into an online offering where student projects are being supervised remotely by mentors.
International HPC Summer School	The 2020 International HPC Summer School, originally scheduled to take place in July in Toronto, had to be postponed until 2021. This will be held as an online event as the default planning assumption. If conditions allow, some face-to-face participation may be facilitated. The format of some of the sessions will have to be adjusted.
EuroHPC Summit Week – Hands-on Workshops	WP4 made preparations to deliver hands-on training workshops during the EuroHPC Summit Week, originally scheduled to take place in Porto, 23-27 March 2020. The workshops have been cancelled along with the main event.

Table 1 Summary of WP4 activities that have been affected by the Covid-19 pandemic, and some of the actions taken in response.

While the disruptions caused to WP4 are considerable, there have been some minor positives, e.g. the wider geographic reach of online courses (Section 3.2). Those who contributed to WP4 activities have also learned valuable lessons from conducting online training. Hence for the second half of the project, some coordination efforts will be invested to share some of these online training lessons and experiences both within the project, e.g. PRACE partners exchanging ideas and learning from one another, and similarly with external projects, e.g. establishing on training, open to participation from other projects such as the CoEs, FocusCoE and the EuroCC national competence centres.

3 PRACE Training Centres

The mission of the PRACE Training Centres (PTCs) is to serve as European hubs of high-quality training for researchers working in the computational sciences. The PTCs provide and coordinate training and education activities needed to achieve the best utilisation of the PRACE Research Infrastructure by the community. The PTCs promote a common PRACE brand, representing the whole PRACE community rather than only the hosting sites, and implement a jointly developed programme of courses, designed and coordinated by PRACE with advice from external experts.

The network of centres was initially established in six PRACE partner countries, where they were referred to as the PRACE Advanced Training Centres. This was expanded in 2017 to include four additional centres, which coincided with a re-branding of all centres to PRACE Training Centres. In 2019, the PRACE Management Board (MB) agreed to a new call for establishing additional PTCs. Consequently, four more partner countries, Austria, Belgium, Slovenia and Sweden were successful in their application to host PTCs, as described below in Section 3.1. Therefore, as of December 2019, the network of PTCs consists of partner sites from 14 countries.

From May 2019 to September 2020 (including the 2019-2020 PTC programme), the PTCs collectively delivered 119 courses, representing 326 days of training with 3,549 participants, which amount to 10,073 participant-training days. This period coincides with implementation of the full 2019-2020 PTC annual programme as examined in Section 3.2. The 2020-2021 PTC programme was also compiled during this time (Section 3.3). Of course, the Covid-19 pandemic has had an obvious impact on the delivery of PTC courses on both the 2019-2020 and 2020-2021 programmes as highlighted in the respective sections. However, the PTCs have made significant efforts to pivot from face-to-face to online teaching even though 25 courses had to be postponed or cancelled. Since the onset of restrictions caused by the Covid-19 pandemic in March 2020, a total of 29 online PTC courses have been delivered by end of September 2020.

3.1 Selection of new PTCs

In 2019, the PRACE-6IP Management Board (MB) had discussed and approved the launch of a new call for PRACE Training Centres in order to expand the reach of the PTC network, coinciding with renewed enthusiasm from several PRACE partners with growing experience in delivering HPC training. This led to a new call for PTCs together with processes for evaluation and selection that occurred in late 2019.

The entire process, from the initial call to the evaluation and selection procedures, closely resembled that of the one used for the previous call for PTCs in 2017 [1]. The call was announced in October 2019 with a deadline for application set in November 2019.

A key difference between the 2019 PTC call and the 2017 call was that selection of new PTCs was based on applications that exceed a certain threshold score, rather than via a ranking of application scores, i.e. any application that exceed the threshold score was recommended for selection as a PTC. There was no limit on the number of successful applications prior to call. Another key difference was that any new PTC established in this later call were not expected to receive any additional funding from the PRACE-6IP project, although existing PMs in the project can be reassigned for PTC training activities. An evaluation committee with five persons (representing PRACE-6IP PMO, MB, WP4, PRACE BoD and PTCs) was set up to review the applications.

A total of four PTC applications were received by the deadline of 15 November 2019. The applications were reviewed and scored by all five reviewers individually based on 6 key criteria:

- Ability to carry out the requested number of training events.
- Consistency and track record of training activities.
- Pool of local trainers.
- Range of expertise and experience of local trainers.

- Justification for the tentative training programme as proposed in the application.
- The suitability of the hosting site for attracting students from local and surrounding regions, in particular "filling in the gaps" of the geographical coverage of the PTC network.

The scoring scheme was based on a mix of both quantitative and qualitative assessment of each application. The evaluation committee all completed the scoring process by December 2019 and convened to resolve any potential conflicts in the evaluation and to deliberate on the final selection. The committee found no major conflicts in the scoring system and reached consensus in concluding that all four applications had exceeded the threshold score, which was derived (based on the 2017 call) and announced by the evaluation committee prior to the application. It was recommended that all four applicants should be established as new PTCs who became operational from January 2020 onwards. In December 2019, the PRACE MB approved the decision to establish the following new PTCs, expanding the network to include 14 countries:

- TU Wien representing VSC (Vienna Scientific Cluster) Research Center, Austria.
- UANTWERPEN representing VSC (Vlaams Supercomputer Centrum) & CÉCI (Consortium des Équipements de Calcul Intensif), Belgium.
- University of Ljubljana representing the HPC center Slovenia.
- SNIC, Sweden.

3.2 The 2019-2020 PTC Programme

The 2019-2020 PTC programme was originally conceived to deliver 104 courses that represent 265 days of training. Table 2 shows the key output and statistics from 14 PTCs achieved for the 2019-2020 programme compared to past ones. The number of PTCs was expanded from 6 to 10 from the 2017-18 programme onwards.

		2012-	2013-	2014-	2015-	2016-	2017-	2018-	2019-
Programme	Pilot	13	14	15	16	17	18	19	20
Date from	Mar-	Aug-							
	2012	2012	2013	2014	2015	2016	2017	2018	2019
Date to	Jul-								
	2012	2013	2014	2015	2016	2017	2018	2019	2020
Number of courses	19	71	81	77	73	78	93	99	81
Total duration (days)	56	204	233	219	203	215	244	261	220
Number of participants	511	1,547	1,682	1,786	1,567	1,658	2,259	2,499	2,502
Number of participant-	1,715	4,702	5,187	5,384	4,601	4,881	6,121	6,690	7,285
days									
Female (%)	-	12.9%	14.4%	16.3%	17.6%	19.3%	21.0%	19.3%	20.9%
Non-academic (%)	-	9.9%	12.3%	15.6%	22.2%	19.4%	18.5%	25.0%	12.5%
Non-host country (%)	-	20.6%	25.4%	29.5%	16.3%	16.2%	21.9%	15.4%	29.6%
Non-PTC country (%)	-	13.8%	17.7%	19.9%	8.9%	11.9%	8.7%	7.5%	14.7%
Feedback response rate	-	63%	64%	53%	52%	65%	53%	52%	48%
(%)									
Average overall rating (0	-	8.5	8.4	8.4	8.4	8.5	8.5	8.4	8.2
– waste of time; 10 -									
excellent)									

Table 2. Key statistics from the implementation of PTC programmes since 2012. "Non-host country" indicates the proportion of participants affiliated with institutions from anywhere outside the country hosting the PTC

course. "Non-PTC country" indicates the proportion of participants affiliated with institutions from non-PTC hosting countries.

As expected, the Covid-19 pandemic has greatly affected the delivery of courses in the final few months of the 2019-2020 programme. Hence a total of 81 courses (220 training days) were delivered compared to the 104 courses (265 training days) as originally envisaged. Of the 81 courses, 60 of these (161 training days) represent face-to-face courses while the remaining 21 courses delivered (59 training day) were conducted online. In many cases, courses had to be cancelled at the last minute (6 courses) or postponed to future dates (17 courses). Effort is ongoing to assess if most postponed courses can be refactored as online courses, but this may not always be possible (e.g. dependence on external instructors, access to infrastructure, nature of the course). However, 21 online courses have been organised as part of the 2019-2020 programme, which makes up for over a quarter of all PTC courses delivered.

The statistics shows that while the number of courses has been reduced, the 2019-2020 programme still managed to attract the target number of participants of around 2,500. Interestingly, there is a notable hike in the relative proportion of participants who come from another country from that of the host (e.g. in a face-to-face setting, a visiting participant from another country), as well as a rise in participants who come from non-PTC hosting countries.

Table 3 summarises a few key observations between face-to-face and online courses that were delivered during the 2019-2020 programme. The natural, intuitive expectation is that online courses would generally attract more participants from abroad because the barrier to entry due to travel is removed. Indeed, there are appreciable differences between face-to-face and online courses that reflects this trend. For online courses, it can be seen that more than half the participants were from countries outside that of the course provider. These courses also attract more (nearly a quarter of) participants from countries that currently do not host PTCs, which is significant given that there are now 14 PTC hosting countries compared to just 6 from 2012 to 2016.

	F2F courses	Online courses
Number of courses delivered (2019-2020 programme)	60	21
Number of participants	1,714	788
% of participants from outside hosting country	18.7%	52.9%
% of participants from non-PTC hosting countries	10.2%	24.3%

Table 3. Comparison of face-to-face versus online participants at PTC courses during the 2019-2020 programme.

The pivot to online courses by the PTCs has been challenging with some very valuable lessons learned. Even during the final few months of the 2019-2020 programme, PTC instructors have already highlighted through experience lessons such as the following:

- Online courses are typically much more labour-intensive with extra personnel required to manage chat sessions, hands-on sessions (e.g. using break-out rooms).
- Without the possibility of physical oversight (i.e. shoulder surfing) and interaction, more time may have to be allocated to participants to complete the same exercises. Or else the exercises should be refactored for an online audience.

• For access to infrastructure for hands-on experience, much more care and time are needed before the course to make suitable arrangements. Participants are no longer all logging in from the same physical location via the same network.

3.3 The 2020-2021 PTC Programme

In early 2020, the PTCs (including the 4 new members for a total of 14 PTCs) have jointly conceived a preliminary 2020-2021 programme that encompasses 138 courses, representing 338 training days. The programme contains a diverse range of courses that covers comprehensive aspects of HPC performance engineering and parallel programming skills. This is complemented by some domain specific courses (often in collaboration with the CoEs) and those that combine HPC with Big Data and machine learning.

During the current reporting period, or the initial three months of the 2020-2021 programme, a total of 20 PTC online courses have been delivered. A more comprehensive analysis of the programme, expected to be implemented mostly online, will be carried out in the next reporting period.

Early planning for the 2020-2021 PTC programme was carried out before the onset of the Covid-19 pandemic. While there was initial optimism that some face-to-face courses may be possible during the time frame of August 2020 to July 2021, the continuing uncertainties over whether or when face-to-face teaching can realistically take place have changed expectations for PTC courses.

Similar to PRACE events and meetings, the online or hybrid (a mix of face-to-face and online delivery, where local conditions allow) format has been set as the default for all PTC courses until the end of 2020. As for future course in 2021, the inherent preference will be for online delivery. The ability to deliver a course in hybrid face-to-face and online format, or face-to-face format only, would be treated as an exception rather than the rule.

4 Seasonal Schools

Since 2008 the PRACE Seasonal Schools are conducted as part of the PRACE educational program offering top-quality face-to-face training events organised around Europe, with the purpose to improve the necessary skills in order to use 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.

The Seasonal Schools, since 2012, have been running simultaneously with the PRACE Training Centres, offering training opportunities mainly in countries where PTCs are not in operation. To maximize PRACE training coverage around Europe, PTC hosting countries have lower priority in the selection process for hosting Seasonal Schools.

4.1 Selection Process

In order to ensure fairness and transparency, the selection process of the hosting countries for the eight (8) available Seasonal Schools slots in PRACE-6IP, was the same that was followed in PRACE-4IP and -5IP, and was a result of the big demand for hosting Seasonal Schools and the small number of available slots. The establishment of PTC hosting countries had proved to restrict the number of applications, something that was also a problem in PRACE-5IP. For this reason, the eligibility criteria were looser in PRACE-6IP call, allowing PTC hosting countries to apply with lower priority. In total, seven countries applied to host nine different Seasonal Schools. Due to lack of time, two applications were evaluated and approved in fast-track processes in order not to lose the first two available slots. One application was withdrawn by a country who requested two Seasonal Schools, in order to focus on one of them. As a result, a total of eight applications were evaluated and sorted to cover all eight available slots of Seasonal Schools for PRACE-6IP.

The PRACE-6IP MB approved the selection of a total of eight Seasonal Schools, the first Seasonal School in September 2019, the second in (early) January 2020 and the selection of the six remaining Schools in (late) January 2020. Table 4 summarises the Seasonal Schools dates, location and main subject.

School	Location	Date/Period	Main Subject
Autumn 2019	Slovenia	17-20 September	Big Data and HPC
		2019	
Winter School	Austria	9-12 March 2020	GPU programming with CUDA
2019/20			
Spring School 2020	Slovakia	May 2020	Modelling materials using HPC and
		(postponed)	AI/ML
Autumn School	Slovenia	15-18 September	HPC and FAIR Big Data
2020		2020	
Winter School	Belgium	October-November	Introduction to Machine Learning
2020/21		2020	for scientist
Spring School 2021	Finland	April - May 2021	Harnessing the EuroHPC pre-
			exascale systems
Autumn School	Bulgaria	September-	Neural Networks and Deep
2021		November 2020	Learning for Social, Behavioural,
			and Economic Sciences by
			Utilization of High-Performance
			Computing
Winter School 2021	Israel	November -	Fueling Scientific Discovery with
		December 2021	HPC

Table 4. Seasonal School schedule as approved by PRACE-6IP MB in early 2020.

4.2 Seasonal Schools Overview

During the first eighteen months of the Project, only two Seasonal Schools have fully taken place and one more was interrupted due to COVID-19 restriction measures. The Autumn 2019 School in Slovenia was the only one that was organised and took place before the pandemic breakout. The Winter 2019/20 School in Austria had to be cancelled after the first day due to rapid onset of

COVID-19 measures; a full delivery of this school has now been planned for 2021. The Spring 2020 School in Slovakia was postponed due to COVID-19 quarantine measurement and the Autumn 2020 School in Slovenia took place in a hybrid manner, half face-to-face and half remotely at the same time.

In this section, we provide a summary of the Seasonal Schools that have been realised so far in the PRACE-6IP project (Table 5).

School	Venue	Date	Participants
PRACE Autumn school	University of Ljubljana,	17-20/09/2019	46 participants
2019 – Big Data and	Slovenia		from 4 countries
HPC			
PRACE Autumn School	University of Ljubljana,	15-18/09/2020	82 participants
2020 - HPC and FAIR	Slovenia		from 18 countries
Big Data			
		Total:	128 participants

Table 5. Seasonal Schools delivered during the current reporting period of the PRACE-6IP project.

4.2.1 PRACE Autumn School 2019 – Big Data and HPC (Slovenia)

In today's competitive product development, high performance computing (HPC) delivers outstanding value and investment return. Parallel computing increases understanding, productivity and accuracy of the simulation - a faster turnaround, reduced costs, systematic design variations and more complex models.

In this training course the focus was on classical Big data topics (using Hadoop and Rhadoop for big data management and analysis) and very recent container technologies. This was a four-day course.

The PRACE Autumn School 2019 targeted at (20-30) experienced industrial users and some academics. Case studies and hands-on tutorials were carried on the ULFME cluster. The tutorials were held in sessions, depending on the applicants' interest indicated in the registration questionnaire.

4.2.2 PRACE Autumn School 2020 – HPC and FAIR Big Data (Slovenia)

The content of the PRACE Autumn School 2020 is largely similar to the PRACE Autumn School 2019, which are both organised in Slovenia by the same partner. However, the 2020 edition had one major difference: the 2020 school includes sessions on handling and processing scientific data, data life cycles and the FAIR (Findable, Accessible, Interoperable and Reusable) principles. The school was also conducted in a hybrid format, where instructions were provided to a mix of both an online audience and local participants on-site.

4.3 Upcoming Seasonal Schools

Due to travel restrictions that followed the continuing pandemic effects, Seasonal Schools were so far stopped, postponed or organised in hybrid mode. The restrictions will not be easily lifted in the coming months. For this reason a contingency plan is necessary. Discussions have already been

made among the Seasonal Schools' hosts and the WP4 leaders, co-leaders and T4.1 leader and they are prepared to organise next Seasonal Schools online if needed. In any case, they do not intend to cancel any of them, on the contrary there is the strong will to repeat the Winter 2020 Seasonal School which was stopped (even online if necessary) and make another round of the Autumn 2020 Seasonal School that took place in hybrid manner, since the available amount offered by PRACE-6IP project was not spent. A new plan is drawn (Table 6), so that all Seasonal Schools fit in the remaining shorter time frame. Seasonal Schools with different target audience will be allowed to be organised in close time periods. The modified timetable is subject to formal approval by the PRACE-6IP MB.

School	Location	Date	Main Subject
Winter School	Belgium	October-November	Introduction to Machine Learning for
2020/21		2020	scientist
Spring School	Finland	April/May 2021	Harnessing the EuroHPC pre-exascale
2021			systems
Spring School	Slovakia	May/June 2021	Modelling materials using HPC and
2021			AI/ML
Autumn School	Slovenia	September 2021	HPC and FAIR Big Data
2021			
Autumn School	Bulgaria	September-November	Neural Networks and Deep Learning
2021		2021	for Social, Behavioral, and Economic
			Sciences by Utilization of High-
			Performance Computing
Autumn School	Austria	September-November	GPU programming with CUDA
2021		2021	
Winter School	Israel	November/December	Fueling Scientific Discovery with
2021		2021	HPC

Table 6. Modified Seasonal School timetable in response to COVID-19 impact

4.4 PRACE Extreme-Scale Workshop

A pilot initiative that has been proposed in the PRACE-6IP project is the organisation of an intensive, advanced extreme-scale workshop or bootcamp that would bring pool together instructors from PRACE partners and attract some of the most talented European researchers and HPC application developers. While this type of workshop is typically best conducted in a face-to-face setting, an online version is being planned for 2021.

5 On-demand Events

The On-demand events organised in the context of PRACE-6IP 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-6IP 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-6IP partner institution. The trainings need to be given in English to accommodate the international participants.

5.1 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 I.

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: PRACE BoD representative, PRACE-6IP MB representative, PTC representative and two 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 PRACE-6IP 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.

5.2 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.

5.3 On-demand Events Overview

This subsection summarises the On-demand Events that took place during the first 18 months of the project (Table 7).

Location	Date	Main Subject	Participants
Trieste,	23-27 September	Summer School on managing	26 participants
Italy	2019	scientific data from analysis to long	from 19
		term archiving	countries
Espoo,	9-11 October 2019	Advanced Gromacs, HADDOCK +	24 on-site + 10
Finland		PMXWorkshop	on-line
		Total:	60 participants

Table 7. On-demand events in the current reporting period of the PRACE-6IP project.

5.3.1 EUDAT CDI/PRACE - Summer School on managing scientific data from analysis to long term archiving

The school aimed to provide students from diverse backgrounds knowledge and experience of using data and compute resources/services from EUDAT and PRACE respectively. It provided an ideal opportunity and setting for students to learn about both projects and how they can work in synergy to support research.

The programme was designed to take students on a 5-day journey through a typical research data lifecycle (data discovery; data processing; data analysis; data preservation and publishing) together with sessions on addressing compute-intensive challenges.

5.3.2 CSC-BioExcel – Advanced Gromacs, HADDOCK +PMI Workshop

The workshop was jointly organised between BioExcel, CoE and CSC. It taught participants new developments and best practices in BioExcel bioinformatics software on the exascale; GROMACS providing molecular dynamics simulation, HADDOCK modelling molecular interactions and PMX for automated alchemical free energy calculation setup. The developers from BioExcel presented their software packages themselves.

GROMACS is one of the most significant application codes in European HPC centres. At CSC it uses the most CPU-time as a single application code. Therefore, it is of great importance that these, often large, simulations are done as efficiently as possible. GROMACS has a wide user community that will benefit from advanced training for challenging performance optimisation and advanced simulation protocols - which in turn will have the most impact at European HPC sites. There has not been an advanced GROMCAS event in Finland for years. As a PRACE event the workshop was open for all and additionally streamed for remote participation. BioExcel is an optimal collaborator as it develops the tools (Gromacs, HADDOCK, PMX) and as developers guarantee high quality substance.

Typical research workflows, e.g., antibody-antigen interaction design, use a combination of two or three of GROMACS, HADDOCK and PMX. Users learnt how these packages may interact in typical research and are invited to bring up their own day-to-day research. Apart from enabling users to full use of all three softwares, the interaction with workshop participants with concrete research scenarios also serves to foster collaboration between developers of the respective software packages.

5.4 Future plans

On-demand events mainly fund or co-fund expenses of face-to-face trainings. For this reason, pandemic breakout eliminated some of the driving factors for these events. For the foreseeable future at least, these type of on-demand events may simply be online events where PRACE collaborates with other projects and partners by contributing to a joint programme and pool of trainers, see Section 10 for examples of potential collaborations.

6 International HPC Summer School

The annual International HPC Summer School has been an ongoing collaboration between PRACE, the U.S. National Science Foundation's eXtreme Science and Engineering Discovery Environment (XSEDE) project, Canada's SciNet HPC Consortium and the RIKEN Center for Computational Sciences (R-CCS) for close to a decade. The PRACE-6IP project aimed to sustain support for this collaborative event, typically held in July, for three years (2019 to 2021).

The objective of the annual series of international summer schools is to familiarise the best students in computational sciences with major state-of-the-art aspects of HPC for a variety of scientific disciplines, catalyse the formation of networks, provide advanced mentoring, facilitate international exchange and open up further career options. Typically, leading Canadian, European, Japanese and American computational scientists and HPC technologists are invited to offer instructions in parallel sessions on a variety of topics as:

- HPC challenges in major scientific disciplines
- HPC programming proficiencies
- Performance analysis and profiling
- Software engineering
- Numerical libraries
- Big data analysis and analytics
- Machine learning
- Scientific visualisation
- Canadian, European, Japanese and U.S. HPC-infrastructures

Since this is an ongoing, annual event, with similar objective year on year, the format of the international summer schools has remained relatively stable over the past years with minor adjustments. The programme combines elements of scientific conferences – but where HPC is a dominant theme rather than any specific scientific or engineering discipline – together with elements of HPC training courses where participants engage in learning programming tools and techniques through a mix of presentations and hands-on sessions. The programme of the school is also designed to actively promote interaction between the participants and the presenters, through the mentoring programme, the electronic poster sessions as well as group activities.

The organisation of the school has been fine-tuned over the years where there is now an established system of processes that are implemented every year to execute the event with considerable success. This includes different teams dedicated to tasks such as setting up the website, launching

the call and accepting applications, evaluation of applications, managing scientific talks, hands-on sessions, mentoring sessions, etc. These are overseen by the planning committee, whose make-up has also remained relatively stable each year with limited turnover of personnel from each collaborating organisation. The school typically attracts huge interest from students and the feedback from past participants have been extremely positive.

6.1 International HPC Summer School 2019 (Japan)

The planning for the International HPC Summer School 2019 actually began during the PRACE-5IP project, i.e. towards late 2018. The call for application was announced in December 2018 and 373 applications were received by the deadline in February 2019 for 80 seats at the school. This included 154 European applications allocated to PRACE who is responsible for the selection of ~30 students based in Europe to participate in the international summer school.

The European (PRACE) selection committee consisted of six scientists and HPC experts from Ireland, Italy, France, Germany, Spain, Sweden and the UK. The 154 applications were reviewed according to the following criteria:

- Strong scientific/technology reason for participation
- The international summer school can contribute to advancing the research goals
- Engagement in code development activities
- Experience with HPC programming

A total of 30 students, based in 12 European and PRACE partner countries, were selected to participate in the school. They joined other successful candidates from Canada (11), Japan (13), the U.S. (27) for a total of 81 participants at the school.



Figure 1. Participants of the International HPC Summer School 2019 at the Shinto Shrine, Kobe, Japan.

The school took place during 7-12 July 2019 at the venue of the RIKEN R-CCS in Kobe, Japan. The full programme of the school can be found on the school's website [2]. While the content of the school has remained roughly similar to previous year where participants were exposed to scientific talks and technical sessions related to HPC, the 2019 school incorporated new sessions on high performance data analytics that is emerging as an important HPC technology.

Overall, the school was a huge success which is reflected in the overwhelmingly positive feedback from participants. From 71 survey responses, the participants indicated the following:

Overall

A general measure of the perceived quality of this event was the response to the statement "Overall I would rate my experience as successful"; to this an overwhelming 97% of respondents were in agreement that the event was a successful experience for them.

• Learning outcome

93% of respondents indicated that their goals of attending the event were achieved; 96% stated that the skills they have learnt will significantly contribute to their research; 93% are aware of the next step to build on what they have learned.

• Organisation

97% of respondents found the school to be well organised and 95% were satisfied with technical assistance available.

• International audience

89% of respondents indicated that participation of students from other countries contributed to their learning; 94% have meaningfully engaged with other students at the school.

• Mentoring

85% respondents have stated to have meaningfully engaged with their assigned mentor during the school, with 68% planning to keep in touch with their mentors after the school.

• Compute resources

92% of respondents are interested in learning more about the resources/opportunities available through the partner organisations as a result of their experience; 85% plan on obtaining access to such resources after the school.

6.2 International HPC Summer School 2020 (Canada)

The International HPC Summer School 2020 was originally planned to take place in Toronto, Canada on 12-17 July. Similar to previous years, organisation of the event started almost 9 months prior, in 2019. The call for application for the 2020 school was opened and announced in late November 2019 along with a deadline set in January 2020. A total of 339 applications were received by the end of the deadline. 96 of these were European applications to be managed and reviewed by PRACE to fill 30 available seats at the school for Europe. Using the same evaluation committee and criteria as for 2019 (see above), 30 European candidates from 16 countries were selected to participate in the 2020 school towards the end of February.

The onset of the Covid-19 pandemic and resulting travel restrictions have initially caused a waitand-see approach from the planning committee. Selected students have been informed of their successful applications, but they would not receive formal invitations and make any travel arrangements until the pandemic and travel restrictions subsides. Feedback was then sought from both students (about their willingness to travel should the pandemic situation improved) and speakers/instructors (about the potential of teaching similar/modified material in an online setting). The feasibility of online mentoring session was also explored. As some of the unique value-add of this summer school include interaction with international students from diverse fields, as well as extensive one-to-one mentoring opportunities with leading HPC experts at the school throughout the week, transforming the International HPC Summer School to be taught online while keeping the same unique benefits was always going to be extremely challenging. However, there was enthusiasm among the instructors that an online version of the school could still be delivered, as long as the accepted candidates concur.

By May 2020, it was clear that a face-to-face event would not be feasible and selected candidates were asked of their preference to either attend an online version of the school, or to defer the event, and their seats, until 2021. There was a clear majority for the latter hence the school was cancelled for 2020 and deferred to Toronto, 2021.

Preliminary discussions have already begun for the 2021 school in Toronto. It is expected that accepted candidates from 2020 will be offered seats automatically. While discussions with all partners are ongoing, an online version of the school is likely going to be offered to students should Covid-19 induced restrictions persist until summer 2021.

7 Summer of HPC

PRACE Summer of HPC (SoHPC) [3] outreach and training programme for late stage undergraduates and/or master students entered its seventh edition in 2019. The aim of the programme is to ensure a positive experience for all students and through that experience to encourage them in their path to become the next generation of HPC users, while visiting PRACE HPC sites providing mentoring for projects. The programme runs between July and August of each year, with a kick-off training week at the start of July attended by all participants. At the end of each SoHPC edition projects are presented with short reports and video presentations. Two awards are presented to most successful participants at the award ceremony.

7.1 Summer of HPC 2019 (training week: Italy)

The SoHPC 2019 edition transitioned [4] from PRACE-5IP to PRACE-6IP in a sense that preparations for programme launch started under PRACE-5IP with a Call for Projects [5] to hosting sites and then a Call for participation [6] was issued in early January 2019 and closed mid-February 2019 with 106 applications received. Selections of participants were performed with double review of applications and two consensus meetings for the final selection of 25 students [8] to be hosted by 11 PRACE partners. Site coordinators organised travel and accommodation for the students. The training week [7] was organised at the CINECA HPC centre in Bologna as a start of the students' summer project work.



Figure 2. Summer of HPC 2019 training week participants in Bologna.

Each student had a mentor for their project and during the summer, weekly teleconferences were organised by SoHPC coordinating team to monitor the progress and advertise achievements on SoHPC Facebook [10] and Twitter [11] accounts. During the summer students wrote 91 blog posts [12] about their project and work at hosting sites. Programme finished at the end of August 2019 with project presentations [13] on YouTube. From the project work students wrote popular scientific articles describing their achievements, which will be used by PRACE press team for outreach communication and PRACE Digest [14] highlights. SoHPC Awards selection panel was formed and decided about winners of the SoHPC 2019 ambassador and best performance award. Award ceremony [15] was be held on 6 November 2019 at PRACE office in Brussels.

7.2 Summer of HPC 2020 (training week: online/Austria)

SoHPC 2020 edition prepared 25 project proposals [17] with 12 HPC hosting sites providing mentoring. The preparations and the timeline [16] were similar to the previous SoHPC editions. During the selection of 81 received applications the Covid-19 situation forced selection committee to convert the programme into online edition. The mentors were asked to double participants per project. Before selection, all participants were asked if they still want to participate in online edition. After receiving positive confirmation from all participants, 50 students were selected [18] for 25 projects, to work in pairs as a team on the same or adapted project goals. Training week [19] was prepared by VSC, Vienna along with Slack channels [20] channels for collaborative chat per project. The online training week included many social activities, including yoga time break sessions, virtual visit to VSC supercomputing facility, Mural wall collaboration and Zoom breakout rooms for common work with many instructors available to help when needed at hands-on sessions.



Figure 3. Summer of HPC 2020 online training week participants.

During the intensive summer work and weekly meetings participants wrote 99 blog posts and presented 26 project videos [21] on YouTube and the same number of popular scientific articles describing project outcomes. Award selection is underway.

Considering all implications of pandemic, we may conclude that SoHPC 2020 edition was successfully converted online and may be a guideline for future editions if visiting HPC sites will still be under risk.

8 Massive Open Online Courses (MOOCs)

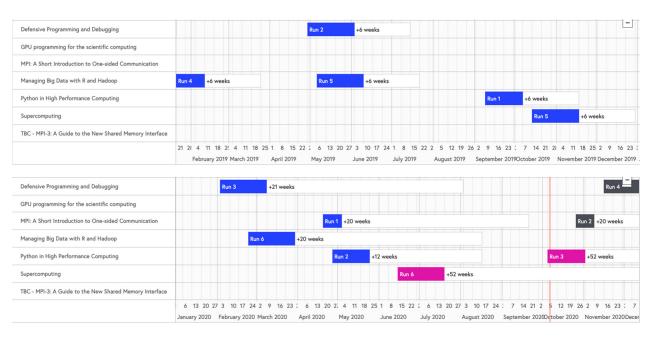


Figure 4. PRACE MOOC schedule in 2019 (top) and 2020 (bottom). Blue or pink bars indicate periods where staff from PRACE partners are actively involved in teaching the MOOC content or moderating interactions. The adjacent number of weeks indicates the period in which the MOOC remains active/open for participants to join and to follow the materials in their own time.

Massive Open Online Courses (MOOCs) started under PRACE-4IP and extended within PRACE-5IP as a different training method hosted on FutureLearn [22] platform. Each existing 5-weeks

MOOC is offered twice a year with constant improvements by each MOOC team. Figure 4 shows the schedule of each course in years 2019-20. In 2020 the courses were offered in prolonged way to address Covid-19 situation. Furthermore, Supercomputing [23] started run 6 with an extended enrolment period of 52 weeks (through to July 2021) as constant offering with lower facilitation provided by instructors. Supercomputing remains available for learners to join at any time, and they can start learning immediately. The course will remain to be run in this way, unfacilitated, and a new run will only be needed to accommodate major updates of the content. The number of joiners during this run 6 extended enrolment increased substantially during the summer of 2020 from 680 to 1617. For that also Python in High Performance Computing Course started with extended enrolment in October 2020 (both courses red in Figure 4).



Figure 5. PRACE MOOC's high level metric and their increase in 2020 when compared to the same period in the previous year 2019.

Statistics in Figure 5 show that additional course MPI: A short introduction to One-sided Communication MOOC [25] started in 2020. Overall, the numbers for all PRACE courses increased in 2020.

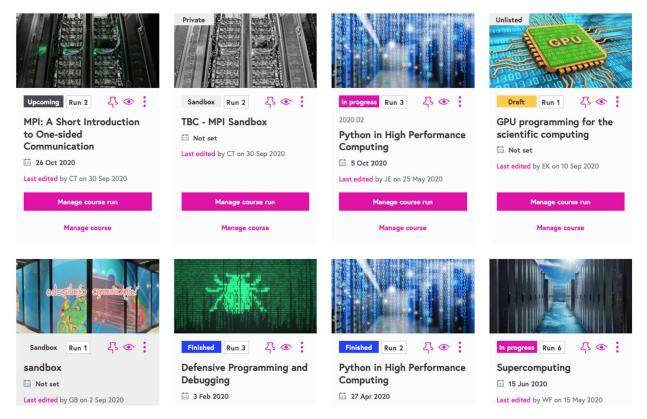


Figure 6. Dashboard of all PRACE MOOCs Course Creator with trailer introductory videos.

The plan in PRACE-6IP proposal was to develop two to five additional MOOCs. The Short MPI course [25], that stated development in PRACE-5IP and will enter second run in October 2020 is being upgraded with a new "full" MPI course developed under sandbox as shown in Figure 6. The "FORTRAN in scientific computing" course developed by CENAERO, KU Leuven started its development and recorded all video materials; it will be completed by end of 2020 and start its first run in the beginning of 2021. A third new run expected to be delivered in 2021 is "GPU programming for scientific computing" and is under development lead by University of Luxembourg.

Overall, PRACE-6IP WP4 works in close contact with FutureLearn "partnership support" team with a mission on improving the impact of the courses. This means analysing and addressing weak points in courses where substantial participants drop-off is observed. For "Defensive Programming and Debugging" [25] that is planned for third run in December 2020 and for "Managing Big Data with R and Hadoop" [27] starting in January 2021 we plan to improve virtual images and HPC cluster access.

9 Training and Events Portal

PRACE put a one stop shop portal for its training related offerings called Training Portal into production. PRACE Training portal is strongly integrated with PRACE Events Portal which

manages all PRACE related events available at https://events.prace-ri.eu [28] and complete with PRACE Material portal available at https://materials.prace-ri.eu [29] holding materials.

9.1 Events Portal

The software called Indico required constant maintenance and reaction to updates which often caused the site to change is behaviour which interfered with operation and needed to be fixed quickly. To avoid common errors during upgrade, a test infrastructure is maintained. These upgrades often introduced new and useful features requiring support of administrators.

With the Events Portal being the central location of storing events organised by PRACE, the system feeds other sites (e.g. Training Portal and PRACE website, etc) with different filters required to setup for new versions of those sites.

One of the newest addition to site functionality is the support integration with PRACE Remote Platform pilot using SSO method called 'Edugain' developed and offered by GÉANT, which allows European Research and Educational affiliates to use their Institutions ID to log into Events Portal and register to an event, and use that ID to login to Remote Platform in the future.

A new tool was developed to filter and export edugain registrants from registrant lists to make Remote Platform integration easier. A global registration export functionality was also introduced to allow administrators to work easier. All of these new functions were developed with using proper edugain based access measures.

During COVID-19 pandemic, new tags were put into the names of the events to refer whether they are held online, or postponed, according to local measures to make attendees find the safest way to participate those events.

A new branding introduced by the new website was uploaded with a completely new header.

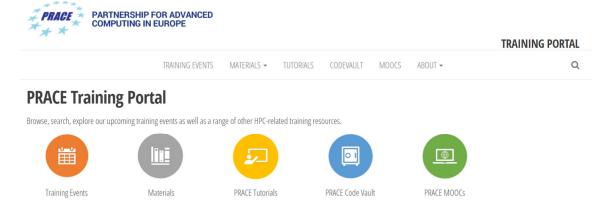
9.2 Training Portal

All existing content was migrated and new content was uploaded to offer a more visually inviting structure at the Training Portal. In collaboration with FocusCoE, a new training registry was developed to aggregate pan-European HPC training event details. This registry is dependent upon a third party service, time.ly [30], which is to be maintained by PRACE.

During the pandemic, a new structure of events was introduced to filter to online events only.

A new banner was added and responsive design was developed along with the addition of new buttons and design. Setup was made for appropriate access to portal configuration to partners.

An updated training material portal was introduced into production as well with customised landing page and improved detailed search functionality.



Upcoming PRACE Training Courses

Due to the Covid-19 pandemic, all in-person PRACE courses have been suspended until at least August 2020. Nevertheless, a considerable number of PRACE courses can now be taken online as indicated below — courses prefixed with [ONLINE] represent synchronous courses while those prefixed with [MOOC] indicate asynchronous course delivery. We are monitoring the situation closely across Europe and hope to offer in-person courses again once conditions allow.

Any in-person courses listed below from September 2020 onwards will be subject to change depending on the prevailing circumstances. They may have to be converted to an online course, be postponed or cancelled on short notice. Please allow some flexibility and understanding when registering for these courses.

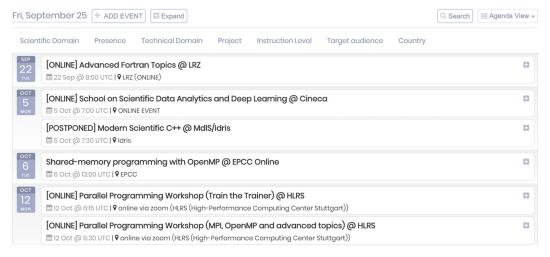


Figure 7. New PRACE Training Portal based on WordPress



Figure 8. New PRACE material portal based on ePrints

9.3 CodeVault

The PRACE CodeVault [31] was initially developed as an open repository of sample HPC codes that could be adopted, and improved upon, for training and/or demonstration purposes, e.g. examples of how sequential codes (often kernels) are parallelised using different approaches. While the repository has been populated with various parallelised HPC kernels as well as sample codes for parallel programming exercises, usage of the repository has remained low. The situation will likely persist unless trainers begin to take an active role in using the repositories for courses. There is also the challenge of supplementing hands-on exercises from courses with additional instructions, explanations and comments for these to be useful to others. Hence the question remains whether the nature of CodeVault needs to be updated – not just a repository of codes but embellished with extra content so they become self-contained lessons.

10 Training Collaboration

WP4 has always placed great emphasis on collaborating with other WPs with the project, as well as working with external projects and partners. The different modes for collaboration are typically dependent upon a joint ambition or desired outcome that leads to different activities.

10.1 EuroHPC Summit Week - Hands-on Workshops

WP4 has worked with the 2019 organising committee of the EuroHPC Summit Week (EHPCSW), in which PRACEdays19 is a major component, to organise hands-on training workshops at the event. This included providing mobility support to a limited number of students across Europe to participate at the workshop; participation from local user communities was also expected. A total of 5 workshops, taught by PRACE trainers, were organised on the following topics:

- Big data analysis with R Hadoop
- Introduction to Spark
- Introduction to machine learning/AI
- Development of modern authentication and authorization mechanisms
- Introduction to HPC computing

There was a total of 44 participants at these workshops, with 20 students provided with mobility support, i.e. travel costs to the event and back. The workshops were very well received, although time was limited to accommodate all 5 workshops, i.e. future iterations should reduce this slightly to a manageable number.

Preparation were made to deliver again a series of workshops locally at the EHPCSW20 in Porto, Portugal. However, none materialised due to COVID-19 induced curtailment of the main event. Considerations are being made to conduct similar workshops again for EHPCSW in 2021, even virtually. But it remains questionable whether these online training workshops really do benefit from being "co-located" with, presumably, a virtual EHPCSW.

10.2 European and International Projects

There has also been ongoing work to develop relations and identify opportunities for collaboration with other European and international entities, e.g. projects, institutions, infrastructures. These include:

- Engagement with RedCLARA:- A number of meetings have been held with representatives
 from the RedCLARA organisation, who oversees Latin America's academic computer
 networks, including some HPC competences. Talks are ongoing to determine whether joint
 online training courses can be arranged on areas such as scientific visualisation, parallel
 and GPU programming.
- Talks with Research Infrastructures:- WP4 presented its activities at the recent CERN-GÉANT-PRACE-SKA kick-off workshop (online, 29 September 2020). There has since been dialogue with some of the partners, e.g. CERN, about the potential of delivering joint

- training courses, as well as the possibility of accepting third parties to some PRACE programmes, e.g. whether external projects can host students as part of the Summer of HPC activity in PRACE.
- WP4 has been examining innovative approaches to developing training materials that are more accessible and easily maintained via collaborative efforts. The HPC Carpentry [32] approach has been identified to be a promising avenue. However, a level of internal upskilling is needed for many of the partners in order to adopt this approach to training development. Plans are ongoing to work with existing developers of the initiative and deploy PRACE efforts in the second half of the project. The expectation is that the development of such a pool of training content in this style and format would be much more amenable for re-use by other trainers, which also facilitates their potential adoption by universities.
- Training portal development with FocusCoE and CASTIEL:- As mentioned earlier, development of the training registry involved collaboration with the FocusCoE project to derive technical solutions and relevant metadata fields, which has resulted in an operational European HPC training course aggregating service/calendar. Further discussions have since been held with FocusCoE and CASTIEL with regards to a joint vision or understanding in planning for new web portals as well as creating a platform to share experiences and ideas between PRACE-6IP partners, CoEs and the EuroHPC National Competence Centres, e.g. best practices for online training, training portal functions.

11 Conclusions

In conclusion, WP4 has delivered a significant and effective training programme despite the challenges posed by COVID-19 disruptions. Collectively, Table 8 summarises some of the key output statistics of close to the first half of the PRACE-6IP project (i.e. until end of September 2020).

	Number of events/instances	Number of training days	Number of participants
PTCs	119	326	3,549
Seasonal Schools	2	8	128
On-demand Events	2	8	60
Int. HPC Summer School	1	5	80
MOOCs (active learners)	8	-	7,475
	11,292		

Table 8. Key WP4 output statistics for the first 17 months of the PRACE-6IP project.

In total, WP4 organised 124 training events, 8 MOOC instances (5 different courses), representing 347 training days, for an aggregated audience of 11,292 participants. In addition, the Summer of HPC programme hosted 50 projects and mentored 75 students over the summers of 2019-2020. Much effort has been invested in the pivot to providing online training opportunities with valuable lessons learnt by trainers. The PRACE Training Portal has continued to be updated with new functionalities that provides better information for visitors. There have been ongoing engagements with external stakeholders and projects to collaborate on training activities, e.g. hands-on workshops at the EuroHPC Summit Week, planning of joint courses.

In the remaining 18 months of the PRACE-6IP project, there will be a focus on sustaining a training programme with online delivery being the default mode of teaching; the possibility of reverting to hybrid face-to-face and online, or purely face-to-face events, will of course be welcomed but this will become less of an expectation for planning purposes. There is already recognition that the project provides an ideal platform for trainers to exchange ideas and pool resources where appropriate. WP4 will continue to engage with external projects such as the CoEs, FocusCoE and the EuroCC Competence Centres to expand this type of forum for discussion.

12 Annex I: 2019 Call for PTCs

The following shows the full text of the call for PTCs that was launched in 2019, resulting in the establishment of four new PTCs.

PRACE Training Centres – Call for Hosts

Opening of call: 16th October 2019 Closing of call: 15th November 2019

Start of operation: January 2020 (subject to MB approval)

Introduction

This call aims to establish new PRACE Training Centres (PTCs) which will collectively provide a coordinated programme of training courses on HPC and computational science for European researchers. The newly established PTCs will complement the activities of the 10 existing PTCs in Czechia, Finland, France, Germany, Greece, Ireland, Italy, the Netherlands, Spain and the United Kingdom to widen the reach of PRACE training across Europe.

The PTCs will implement a collective training programme jointly coordinated by PRACE, where each PTC will focus on subject areas that may be of particular relevance or interest to industry and/or the research communities of the local and surrounding region. Each PTC is expected to deliver 2-3 training events annually, representing up to 9 training days. Courses should be open to all researchers, free of charge (for participation) and preferably given in English.

Scope of the call

This call is aimed at PRACE-6IP project partners (apart from those located in PTC-hosting countries). Its purpose is to invite applications for hosting a PRACE Training Centre for at least the duration of the PRACE-6IP project. All interested sites/centres are encouraged to submit an application.

Roles and responsibilities of the PTCs

Each selected PTC is expected to contribute to the planning and delivery of a joint PTC training programme that is jointly coordinated by PRACE. The responsibilities of each PTC includes:

- Planning of its courses (e.g. make course proposals, and modify according to feedback if requested) ahead of each academic year (1 Aug to 31 Jul). Courses may have to be planned far ahead in advance (e.g. up to 18 months before delivery in some cases).
- Dissemination and delivery of courses (up to 9 course days per year) utilising local resources (e.g. instructors, facilities). Limited "out-sourcing" is allowed (e.g. recruiting external PTC trainers for local course delivery for training local trainers).
- Reporting of its activities (e.g. participant statistics, course evaluations) for PRACE deliverables and dissemination.

- Provide a single point of contact to represent the PTC and to facilitate communication (including participation in PRACE teleconferences to coordinate its activities).
- Work with a "mentor" PTC site (if suitable) for guidance.

PTC courses are expected to conform to the following:

- Every PTC course must be open to all researchers, free of charge (for participation).
- Course material must be in English, and made available on the PRACE Training Portal where feasible.
- Courses are to be delivered verbally in English by default to ensure accessibility; although verbal instruction may be provided in a local native language provided sufficient justification.
- Each PTC course must be set up on the PRACE events website (events.prace-ri.eu) for consistency of providing course information, and collecting registrations, evaluations, etc.
- Each PTC course is expected to be 1-3 days in duration, i.e. a PTC programme should not consist of a series of half-day courses over a term.

Process

The call is open from 15th October until 15th November 2019, 17:00 CET. All submitted applications are then evaluated and marked by 5-person evaluation panel (see below). Any PTC application that exceeds a threshold score, as determined by the evaluation panel (to be determined and announced by 1st November 2019), will become new PTCs with the final results subject to approval by PRACE management (MB). After MB approval, the PTCs are expected to commence operations immediately to prepare for the 2020-21 PTC training programme.

The evaluation panel shall consists of five individuals: Simon Wong (PRACE WP4 co-leader and MB representative), Volker Weinberg (PTC representative at LRZ, Germany), Georg Zitzlsberger (PTC representative at Czechia), Stephane Requena (BoD representative) and Florian Berberich (PMO representative).

Eligibility

All PRACE-6IP project partners are eligible for hosting a PTC (apart from those located in PTC-hosting countries). In order to be selected as a host, availability of basic resources needs to be demonstrated in the application (e.g. training facilities and prior track record in training delivery). Each application must come from a single country. Each PTC, when selected, shall commit at least 3 PMs for PTC-related activities in WP4 of the PRACE-6IP project; partners with insufficient WP4 PMs should state in their application a commitment of staff effort for PTC activities (e.g. in-kind contribution, re-allocation of resources from other WPs). Newly established PTCs in this call are also expected to make in-kind contributions to the running costs (i.e. Other Direct Costs) associated with delivery of PTC courses for the duration of the PRACE-6IP project.

How to apply

Applications (free-form text in PDF format, max 6 pages excluding an Annex for reference information) are to be sent via e-mail to the following persons via e-mail no later than 15th November 2019 17:00 CET:

• Simon Wong, simon.wong@ichec.ie

Please note that all applications should include a tentative proposal for the 2020-21 PTC training programme.

Evaluation criteria

Each applicant must have some basic resources, and a commitment to provide such resources if selected, before being considered to be a candidate PTC hosting site, i.e. the application needs to demonstrate:

- Availability of appropriate physical training facilities, e.g. room for at least 20-25 students with AV equipment. On-site workstations for students is not a compulsory requirement. Please describe such resources and how they are made available in the application.
- Prior track record in event organisation, e.g. local/national/PRACE events (minimum score of 2 pts in each evaluation criteria A and B below).
- Availability of local trainers, e.g. availability of local trainers and/or staff representing future trainers (minimum score of 2 pts in evaluation criteria C below).

Having met the basic requirements, applications are then scored by the evaluation panel on the following criteria:

- A. [Weight: 20%] Ability to carry out the requested number of training events [0-4 pts, highest number of HPC training days in a year, from the past two years: 0.4pt per training day, maximum 4pt for 10 or more days]. Please, list in the annex for each training event the location; the dates; the number of days; the title (and topics), percentage of beginners, intermediate and advanced level; percentage of training covered mainly by local trainers, by other trainers from the own country, and by trainers from abroad; number of participants; name of the lecturers.
- B. [Weight: 20%] Consistency and track record of training activities [0-4 pts, +1pt if apart from the criterion above there is another year with 10+ training days, +1pt if there are three training events in the past year with each more than 2 days and more than 25 participants, +1pt if there is at least one international training event in the past two years, +1pt if the future training plan is consistent (within 70%) with the previous year in activities]
- C. [Weight: 20%] Pool of local trainers [0-4 pts, 0.5pt per local trainer, maximum 4pts for 8+ trainers] Please list in the annex for each trainer, his/her name, were she/he is located, selected courses or course topics, and the years of his/her course experience.
- D. [Weight: 10%] Range of expertise and experience of local trainers [0-2pt, +1pt for top four applications regarding the expertise covers a wide range of HPC topics, +1pt for the top four applications regarding the level of experience of the HPC trainers]
- E. [Weight: 10%] Justification for the tentative training programme as proposed in the application, i.e. the benefits of setting up the PTC in question, regarding:
 - a. Special relevance/interest to local communities.
 - b. Interest to the wider community across Europe.
 - c. Coverage of subject areas that are not in prior PTC training programmes.
 - d. Development of local capabilities in training.
 - e. Value-add potential or commitment shown by the applicant to enhance the PTC programme if selected.
 - f. [0-2pts, +0.5pt for each subtopic, maximum of 2pts]

[Weight: 20%] The suitability of the hosting site for attracting students from local and surrounding regions, in particular "filling in the gaps" of the geographical coverage of the PTC network. [0-4 pts, ranked 1pt for

10 participants/course in the past, 2pt for 15, 3pt for 20, and 4pt for more 25 and more, (average from at least 3 HPC events per year)]

13 Annex II: PTC courses

The following lists all the PTC courses that were delivered from the beginning of the PRACE-6IP project until the end of the 2019-2020 PTC programme (end July 2020).

Programme	Course title PTC Location		Start date	Duration (days)	
2018-2019	Scalable Parallel Computations with PETSc	CSC	Espoo, FI	2019-05-02	2
2018-2019	Fortran for Scientific Computing	GCS	Stuttgart, DE	2019-05-06	5
2018-2019	DAVIDE OpenPower GPU cluster@Cineca	CINECA	Rome, IT	2019-05-06	2
2018-2019	HPC code optimisation workshop	GCS	Garching, DE	2019-05-20	3
2018-2019	Performance Analysis and Tools	BSC	Barcelona, ES	2019-05-20	2
2018-2019	Data, lights, camera, action! Scientific visualization done beautifully using Blender	SURFsara	Amsterdam, NL	2019-05-21	3
2018-2019	HPC for Industry 4.0@Cineca	CINECA	Milan, IT	2019-05-21	1
2018-2019	Node-level performance optimization	CSC	Espoo, FI	2019-05-22	3
2018-2019	OpenMP GPU Directives for Parallel Accelerated Supercomputers - an alternative to CUDA from Cray perspective	GCS	Stuttgart, DE	2019-05-22	2
2018-2019	Heterogeneous Programming on GPUs with MPI + OmpSs	BSC	Barcelona, ES	2019-05-22	2
2018-2019	Heterogeneous Programming on FPGAs with OmpSs	BSC	Barcelona, ES	2019-05-24	1
2018-2019	High-performance scientific computing in C++	GCS	Juelich, DE	2019-05-27	3
2018-2019	Uncertainty quantification	MdS	Saclay, FR	2019-05-27	3
2018-2019	Deep Learning and GPU programming workshop	GCS	Garching, DE	2019-06-03	4
2018-2019	School on Scientific Data Analytics and Deep Learning	CINECA	Rome, IT	2019-06-10	5
2018-2019	Fundamentals of Deep Learning for Computer Vision	IT4I	Ostrava, CZ	2019-06-11	1
2018-2019	Introduction to High-Performance Machine Learning	SURFsara	Amsterdam, NL	2019-06-11	2
2018-2019	Parallel Programming with MPI and OpenMP	SURFsara	Amsterdam, NL	2019-06-17	3
2018-2019	High-performance computing with Python	GCS	Juelich, DE	2019-06-17	3
2018-2019	Turbulence and Heat Transfer - Introduction to Code Saturne	EPCC	Manchester, UK	2019-06-19	2
2018-2019	33rd VI-HPS Tuning Workshop	GCS	Juelich, DE	2019-06-24	5
2018-2019	Introduction to PETSc	MdS	Orsay, FR	2019-06-24	2
2018-2019	Advanced OpenMP	EPCC	Manchester, UK	2019-06-25	3
2018-2019	Node-Level Performance Engineering	GCS	Stuttgart, DE	2019-06-27	2
2018-2019	Efficient Parallel Programming with GASPI	GCS	Stuttgart, DE	2019-07-01	2
2018-2019	Introduction to GPU programming with OpenACC and OpenMP	MdS	Orsay, FR	2019-07-02	1
2018-2019	Introduction to Parallel Programming with HPX	GCS	Stuttgart, DE	2019-07-04	2
2018-2019	Practical Software Development	EPCC	Leeds, UK	2019-07-10	2
2018-2019	Message-passing Programming with MPI	EPCC	Edinburgh, UK	2019-07-17	3
2018-2019	Advanced MPI	EPCC	Oxford, UK	2019-07-22	2

Programme	Course title	PTC	Location	Start date	Duration (days)
2018-2019	Python in HPC	ICHEC	Dublin, IE	2019-07-29	4
2018-2019	Single Node Performance Optimisation	EPCC	London, UK	2019-07-30	2
2019-2020	Parallel Design Patterns	EPCC	Durham, UK	2019-08-07	3
2019-2020	Modern C++ for Computational Scientists	EPCC	Glasgow, UK	2019-08-27	2
2019-2020	Advanced Fortran Topics	GCS	Garching, DE	2019-09-09	5
2019-2020	Fortran Programming for Scientific Computing	CSC	Espoo, FI	2019-09-25	3
2019-2020 2019-2020	Advanced Usage on Irene Joliot-curie: parallelism, optimization, IO, tools Programming the ARM64 processor	MdS EPCC	Bruyères-le- Châtel, FR	2019-09-30 2019-09-30	3 2
	•	CSC	Cambridge, UK		2
2019-2020	GPU Programming with OpenACC		Espoo, FI	2019-10-14	
2019-2020 2019-2020	Parallel Programming Workshop (MPI, OpenMP and advanced topics) Parallel Programming Workshop	GCS BSC	Stuttgart, DE Barcelona, ES	2019-10-14 2019-10-14	5
2019-2020	Productivity tools for High Performance Computing	IT4I	Ostrava, CZ	2019-10-16	2
2019-2020	Introduction to Parallel Programming	CSC	Espoo, FI	2019-10-23	3
2019-2020	Data Carpentry	EPCC	Cardiff, UK	2019-10-29	2
2019-2020	Data Management with iRODS and Compute	SURFsara	Amsterdam, NL	2019-10-30	1
2019-2020	Hands-on Introduction to HPC for Life Scientists	EPCC	Birmingham, UK	2019-10-30	3
2019-2020	Introduction to Spark for Data Scientists	EPCC	London, UK	2019-10-31	2
2019-2020	Inria autumn school "High Performance Numerical Simulation"	MdS	Bordeaux, FR	2019-11-04	5
2019-2020	Introduction to Parallel Programming	GRNET	Athens, GR	2019-11-05	3
2019-2020	Get Started with Intel and Nvidia Artificial Intelligence Technolo gies	IT4I	Ostrava, CZ	2019-11-11	2
2019-2020	Optimization	MdS	Montpellier, FR	2019-11-12	3
2019-2020	Earth Sciences Simulation Environments	BSC	Barcelona, ES	2019-11-12	3
2019-2020	Shared-memory Programming with OpenMP	EPCC	Online	2019-11-13	2
2019-2020	Introduction to Deep Learning and Tensorflow	CINECA	Rome, IT	2019-11-18	3
2019-2020	Data science with R	CINECA	Rome, IT	2019-11-25	3
2019-2020	Big Data Analysis with Apache Spark	CSC	Espoo, FI	2019-11-27	2
2019-2020	School on Numerical Methods for Parallel CFD	CINECA	Rome, IT	2019-12-02	5
2019-2020	HPC and natural hazards: modelling tsunamis and volcanic plumes us ing European flagship codes	BSC	Barcelona, ES	2019-12-02	4
2019-2020	Data, lights, camera, action! Scientific visualization done bea utifully using Blender	SURFsara	Amsterdam, NL	2019-12-03	1
2019-2020	Node-Level Performance Engineering	GCS	Garching, DE	2019-12-03	2
2019-2020	High Performance Bioinformatics	CINECA	Bologna, IT	2019-12-09	3
2019-2020	HPC Carpentry	EPCC	Edinburgh, UK	2019-12-09	2
2019-2020	Efficient Use of HPC Systems	GRNET	Athens, GR	2019-12-11	2
2019-2020	MPI	SURFsara	Leuven, BE	2019-12-11	2
2019-2020	Practical Deep Learning	CSC	Espoo, FI	2019-12-12	2
2019-2020	Introduction to machine learning in Python with Scikit-learn	MdS	Paris, FR	2019-12-18	1
2019-2020	GPU Programming with CUDA	EPCC	Edinburgh, UK	2020-01-09	2
2019-2020	[ONLINE] Using non-volatile Memory	EPCC		2020-01-15	2

Programme	Course title	PTC	Location	Start date	Duration (days)
2019-2020	Python in High-Performance Computing	CSC	CSC Espoo, FI		3
2019-2020	Parallel I/O and Portable Data Formats	GCS	Juelich, DE	2020-01-27	3
2019-2020	Advanced MPI	EPCC	London, UK	2020-01-27	2
2019-2020	Programming Distributed Computing Platforms BSC Barcelo with COMPSs		Barcelona, ES	2020-01-28	2
2019-2020	Energy Efficiency in HPC	IT4I	Ostrava, CZ	2020-01-29	2
2019-2020	Managing distributed data with Hecuba and dataClay	BSC	Barcelona, ES	2020-01-30	1
2019-2020	BIOWEEK 2020	CSC	Espoo, FI	2020-02-03	5
2019-2020	Parallel and GPU Programming in Python	SurfSARA	Amsterdam, NL	2020-02-03	2
2019-2020	Big Data Analytics	BSC	Barcelona, ES	2020-02-03	5
2019-2020	Fundamentals of Accelerated Computing with CUDA C/C++	IT4I	Ostrava, CZ	2020-02-05	1
2019-2020	Fundamentals of Accelerated Computing with OpenACC	IT4I	Ostrava, CZ	2020-02-06	1
2019-2020	Accelerator Programming	GRNET	Athens, Greece	2020-02-10	2
2019-2020	OpenMP Programming Workshop	GCS	Garching, DE	2020-02-11	3
2019-2020	Short course on HPC-based Computational Bio- Medicine	BSC	Barcelona, ES	2020-02-11	3
2019-2020	Parallel and Scalable Machine Learning	GCS	Juelich, DE	2020-02-17	3
2019-2020 2019-2020	AiiDA Hackathon: developing code plugins and robust scientific wor kflows 16th Advanced School on Parallel Computing	CINECA CINECA	Bologna, IT	2020-02-17 2020-02-24	5
	• •		Bologna, IT		
2019-2020	Introduction to Heterogeneous Memory Usage	BSC	Barcelona, ES	2020-02-25	1
2019-2020 2019-2020	Systems Workshop: Programming MareNostrum 4 Performance Analysis and Tools	BSC BSC	Barcelona, ES Barcelona, ES	2020-02-26 2020-03-02	2
	•				
2019-2020 2019-2020	Heterogeneous Programming on GPUs with MPI + OmpSs Heterogeneous Programming on FPGAs with	BSC BSC	Barcelona, ES Barcelona, ES	2020-03-04 2020-03-06	2
2019-2020	OmpSs Spring School in Computational Chemistry	CSC	Espoo, FI	2020-03-00	4
2019-2020	2020 PRACE & E-CAM Tutorial on Machine	ICHEC	Dublin, IE	2020-03-10	4
	Learning and Simulations		•		
2019-2020	Introduction for Simulation Environments for Life Sciences	BSC	Barcelona, ES	2020-03-11	2
2019-2020	[ONLINE] Programming paradigms for GPU devices	CINECA		2020-04-15	3
2019-2020	[ONLINE] Fortran for Scientific Computing	GCS		2020-04-20	5
2019-2020	[ONLINE] High Performance Molecular Dynamics	CINECA		2020-04-28	2
2019-2020	[ONLINE] Shared memory parallelization with OpenMP	VSC (AT)		2020-05-04	2
2019-2020	[ONLINE] Parallelization with MPI	VSC (AT)		2020-05-06	3
2019-2020	[ONLINE] Message-passing programming with MPI	EPCC		2020-05-14	9
2019-2020	[ONLINE] Scientific computing in R	SNIC		2020-05-27	1
2019-2020	[ONLINE] Introduction to MPI	SNIC		2020-05-27	1
2019-2020	[ONLINE] HPC code optimisation workshop	GCS		2020-06-08	3
2019-2020 2019-2020	[ONLINE] Parallel Programming with OpenMP and MPI [ONLINE] Machine Learning in HPC	VSC- CECI GRNET		2020-06-09	4
2017 - 2020	[Orderve] Machine Learning III HPC	OININE I		2020 - 00-11	4

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Programme	Course title	PTC	Location	Start date	Duration (days)
2019-2020	[ONLINE] Deep Learning and GPU programming workshop	GCS		2020-06-15	4
2019-2020	[ONLINE] Advanced topics in scientific visualization with Blender: geometry, scripts, animation, action!	SurfSARA		2020-06-15	1.5
2019-2020	[ONLINE] Introduction to Hybrid Programming in HPC	VSC (AT)		2020-06-17	3
2019-2020	[ONLINE] Efficient Parallel Programming with GASPI	GCS		2020-06-18	2
2019-2020	[ONLINE] Node-Level Performance Engineering	GCS		2020-06-29	3
2019-2020	[ONLINE] Introduction to new accelerated partition of Marconi, for users a nd developers	CINECA		2020-06-29	1
2019-2020	[ONLINE] Introduction to Molecular Modeling (materials and bio) and Molecular dynamics in HPC	GRNET		2020-06-30	2
2019-2020	[ONLINE] Reproducible computational environments using containers	EPCC		2020-07-13	2
2019-2020	[ONLINE] 34th VI-HPS Tuning Workshop	EPCC		2020-07-28	3
2020-2021	[ONLINE] Introduction to GROMACS - A SNIC/PRACE workshop in collab oration with BioExcel	SNIC		2020-09-03	2
2020-2021	[ONLINE] Deep Learning and GPU Programming Workshop	CSC		2020-09-07	4
2020-2021	[ONLINE] Introduction to High-Performance Machine Learning	SURFsara		2020-09-14	2
2020-2021	[ONLINE] 35th VI-HPS Tuning Workshop	GCS		2020-09-14	5
2020-2021	[ONLINE] Advanced Fortran Topics	GCS		2020-09-22	4
2020-2021	Parallel Visualization of Scientific Data using Blender	IT4I		2020-09-24	1

14 Annex III: Seasonal School Reports

The following subsections 14.1 to 14.2 consists of full reports from Seasonal Schools that were held during the reporting period in the PRACE-6IP project.

14.1 PRACE Autumn School 2019 - Big Data and HPC (Slovenia)

14.1.1 Basic Information about the event

14.1.1.1 Name

PRACE Autumn school 2019 - Big data and HPC

14.1.1.2 Dates

17. – 20. September 2019

14.1.1.3 Location

Ljubljana, Slovenia

14.1.1.4 Organizing sites

University of Ljubljana – Faculty for mechanical engineering

Aškerčeva 6, Ljubljana, Slovenia

14.1.2 Organizational details

14.1.2.1 Local organizing committee

Role	Name/	Institution	Contact
	Surname		
Chair of org.	Dr. Leon Kos	University of	leon.kos@lecad.fs.uni-lj.si
committee	Di. Leon Kos	Ljubljana, Slovenija	ieon.kos(w,iecad.is.um-ij.si
CoChair of org.	Dr. Pavel	University of	pavel.tomsic@lecad.fs.uni-
committee	Tomšič	Ljubljana, Slovenija	<u>lj.si</u>
Chair of progr.	Dr. Janez Povh	University of	janez.povh@lecad.fs.uni-lj.si
committee	Di. Janez Povii	Ljubljana, Slovenija	Janez.povn(<i>w</i> ,iecad.is.um-ij.si
Member of org.	Alenka Maffi	University of	alenka.maffi@lecad.fs.uni-
committee	Alelika Malli	Ljubljana, Slovenija	<u>lj.si</u>
Member of org.	Matjaž Šubelj	University of	mateja.maffi@lecad.fs.uni-
committee	Wayaz Suberj	Ljubljana, Slovenija	<u>lj.si</u>
Org. committee	Mateja Maffi	University of	matjaz.subelj@lecad.fs.uni-
secretary	iviaieja iviaiti	Ljubljana, Slovenija	<u>lj.si</u>

14.1.2.2 Venue

PRACE Autumn school 2019 took place at Faculty of Mechanical Engineering, University of Ljubljana, Aškerčeva 6, Ljubljana, Slovenia. Due to the nature of computing classrooms where max 30 seats are available and the fact that, attendees did not require their own laptops for following hands-on trainings. In cases where possible two parallel hands-on courses were organized with two lecturers and assistants in two adjacent classrooms with the required bandwidth for remote desktop connection to the supercomputer and local pre-/post- processing and job submission to the HPCFS cluster at University of Ljubljana. All the classrooms are equipped with multimedia systems, necessary for such event, as well as sufficient broadband connection.

14.1.2.3 Synergetic events

This event addresses important aspect of Big Data in HPC and possible further usage in different areas of expertise. Furthermore, Summer School on managing scientific data from analysis to long term archiving was held from 23-27 September 2019 (https://eudat.eu/eudat-prace-summer-school-2019) in nearby city of Trieste with collaboration from EUDAT CDI and PRACE. The topics addressed at the summer school have covered:

- Data processing and analysis including deep and machine learning methods,
- Data management ranging from discovery to publication and
- Data discovery.

Therefore, it was to be expected that the presented topics will be complementary for some of the participants involved in PRACE autumn seasonal school "Big Data in HPC" and they would be interested in attending both events.

14.1.3 Program & content

14.1.3.1 Program committee

Role	Name/ Surname	Institution		
Organization chair	Dr. Leon Kos	University	of	Ljubljana,
		Slovenija		
Programme chair	Dr. Janez Povh	University	of	Ljubljana,
		Slovenija		
Committee member	Dr. Pavel Tomšič	University	of	Ljubljana,
		Slovenija		

14.1.3.2 Final program

TUESDAY, 17 SEPTEMBER 2019

Beginning	End	Description
8:00	9:00	Registration

9:00	12:00	Introduction to Linux and HPC		
		Motivation to use HPC system		
		• Introduction to PRACE HPC ecosystem - HPC facilities available to		
		researchers in Europe (Slovenia)		
		HPC platforms architecture		
		 Overview of Linux operating system and introduction to HPC; 		
		• Outline of the benefits of parallelization of the numerical simulations		
		in engineering analysis using HPC.		
		 How to connect and use HPC at UL FME 		
		Convener: Dr Leon Kos (University of Ljubljana, Slovenia)		
		10:30 Coffee break		
12:00	13:00	Lunch Break		
13:00	17:00	HADOOP		
		Introduction to Hadoop		
		Hands-on tutorials on HADOOP		
		Conveners: Dr Amy Krause (EPCC, Edinburgh, UK), Andreas Vroutsis		
		(EPCC, Edinburgh, UK)		
		14:30 Coffee break		

WEDNESDAY, 18 SEPTEMBER 2019

Beginning	End	Description		
9:00	12:00	Introduction to Spark		
		• basic concepts of Apache Spark Data Analytic Framework.		
		• testing access to HPC available at UL where all necessary software		
		will be preinstalled.		
		• creating and starting own Spark working place, which will be used		
		later for running different jupyter notebooks.		
		Conveners: Dr Amy Krause (EPCC, Edinburgh, UK), Mr Andreas		
		Vroutsis (EPCC, Edinburgh, UK)		
		10:30 Coffee break		
12:00	13:00	Lunch Break		
13:00	14:00	Spark: testing different basic Apache Spark concepts by using the		
		Python language		
		Conveners: Dr Amy Krause (EPCC, Edinburgh, UK), Andreas Vroutsis		
		(EPCC, Edinburgh, UK)		
14:00	14:30	Coffee break		
14:30	17:00	Big data analysis with RHadoop		
		• basic concepts of big data management and analysis using RHadoop.		
		 How to create, store, load big data files; 		
		 How to perform basic statistics above big data files. 		
		Convener: Dr Janez Povh (University of Ljubljana, Slovenia)		

THURSDAY, 19 SEPTEMBER 2019

Beginning	End	Description
9:00	17:00	Pre- and post-processing of scientific data with SALOME framework

SALOME: a general overview
Shaper CAD modelling
• Meshing
• Visualization
Connection to solvers (MED coupling)
Hands-on with ELMER multiphysics)
Conveners: Nathalie Gore (OpenCASCADE, France), Dr Paul Rascle
(EDF R&D, France)
10:30 Coffee break
12:00 Lunch break
14:30 Coffee break

FRIDAY, 20 SEPTEMBER 2019

Beginning	End	Description					
9:00	12:00	Introduction to TensorFlow					
		Introduction through Keras					
		 Parallelization in TensorFlow through Horovod 					
		Convener: Dr Marco Rorro (CINECA, Bologna, Italy)					
		10:30 Coffee break					
12:00	13:00	Lunch Break					
13:00	17:00	Applications of TensorFlow					
		• automatic differentiation and gradient descent					
		• introduction to low-level TensorFlow API					
		• built-in parallelism and GPU acceleration with TensorFlow					
		• use cases: clustering					
		Conveners: Primož Godec (University of Ljubljana, Slovenia), Rok Hribar					
		(IJS, Ljubljana, Slovenia)					
		14:30 Coffee break					

14.1.3.3 List of trainers

Name/ Surname	Institution	Lecture	
Dr. Leon Kos	University of Ljubljana,	Introduction to Linux and HPC¶	
DI. Leoli Kos	Slovenija		
		HADOOP	
		Introduction to Spark	
Dr. Amy Krause	EPCC, Edinburgh, UK	Spark: testing different basic Apache	
		Spark concepts by using the Python	
		language	
		HADOOP	
		Introduction to Spark	
Mr. Andreas Vroutsis	EPCC, Edinburgh, UK	Spark: testing different basic Apache	
		Spark concepts by using the Python	
		language	

Dr. Janez Povh	University of Ljubljana,	Big data analysis with RHadoop	
DI. Janez Fovii	Slovenija		
Nathalie Gore	OpenCASCADE, France	Pre- and post-processing of scientific	
Nathane Gore	OpenCASCADE, France	data with SALOME framework	
Dr. Paul Rascle	EDF R&D, France	Pre- and post-processing of scientific	
DI. Faul Rascie	EDF R&D, Flance	data with SALOME framework	
Dr. Marco Rorro	CINECA, Bologna, Italy	Introduction to TensorFlow	
Primož Godec	University of Ljubljana,	Applications of TensorFlow	
Primoz Godec	Slovenia		
Rok Hribar	IJS, Ljubljana, Slovenia	Applications of TensorFlow	

14.1.3.4 Designing the program

In today's competitive product development, high performance computing (HPC) delivers outstanding value and investment return. Parallel computing increases understanding, productivity and accuracy of the simulation - a faster turnaround, reduced costs, systematic design variations and more complex models.

In this training course classical Big data topics (using Hadoop and Rhadoop for big data management and analysis) were focused at and recent container technologies were verified.

At the beginning the PRACE Autumn School 2019 targeted at (20-30) experienced industrial users and some academics. Case studies and hands-on tutorials were carried on the ULFME cluster. The tutorials were held in sessions, depending on the applicants' interest indicated in the registration questionnaire.

14.1.3.5 Description of contents

The training event was target to master and PhD students, early career researchers and engineers from industry looking for competencies in big data analysis using Hadoop, Spark, R (with RHadoop) and TensorFlow. We expected that engineers from SMEs would find this course of particular interest.

Content	Description
Introduction to Linux and HPC¶	Motivation to use HPC system in professional workflow was shown to attendees. PRACE HPC ecosystem were introduced- HPC facilities available to researchers in Europe. Different HPC platforms architecture as well as a short overview of Linux operating system was explained. Benefits of parallelization of the numerical simulations in engineering analysis using HPC were outlined. At the end an example of how to connect and use HPC at UL FME was showcased.

	A short introduction to Hadoop for the attendees.		
HADOOP	Later on hands-on tutorials on HADOOP were		
IIADOOI	shown.		
	222 22		
	Basic concepts of Apache Spark Data Analytic		
	Framework were shown. Access to HPC available		
	at UL where all necessary software was		
Introduction to Spark	preinstalled has been presented. Additionally		
	creating and starting own Spark working place was		
	shown, which was to be used later for running		
	different jupyter notebooks.		
Spark: testing different basic Apache	Hands-on approach using Apache Spark with		
Spark concepts by using the Python	implementation through Python programming		
language	language.		
	Basic concepts of big data management and		
	analysis using RHadoop was shown with		
Big data analysis with RHadoop	explanation of how to create, store, load big data		
	files and how to perform basic statistics above big		
	data files.		
	Firstly, a general overview of SALOME has been		
	presented. The usage of SALOME was shown		
Pre- and post-processing of scientific data	through Shaper CAD modelling, meshing,		
with SALOME framework	visualization. Connection to solvers (MED		
	coupling) and hands-on with ELMER multiphysics		
	was showcased.		
	Introduction of TensorFlow to attendees through		
Introduction to TensorFlow	Keras and parallelization in TensorFlow through		
	Horovod was showcased.		
	Automatic differentiation and gradient descent was		
	explained. Introduction to low-level TensorFlow		
Applications of TensorFlow	API and built-in parallelism and GPU acceleration		
- Production of Temporation	with TensorFlow was presented. Some use cases		
	(clustering) were showcased.		
	(clustering) were showeascu.		

14.1.3.6 Computer resources

Supercomputer HPCFS-U at ULFME with accounts for the event was prepared that gave attendees KDE GUI environment with all required tools and icons required for tutorials. Nearby computing classrooms were prepared for NX client remote terminal access.

Time limited WiFi hot spot access with the same credentials as for HPC were given to all attendees so that they could access internet from their laptops and smart phones.

14.1.4 Participants & feedback

14.1.4.1 Number of participants by country

Country	No. of participants
Slovenia	39
Germany	3
UK	1
Estonia	1

14.1.4.2 Process for selecting the participants

Applicants were expected to have some experience with the topic of interest. School attendees were selected based on applications submitted through the registration form, taking into account the order of registrations. Applicants were informed about their acceptance not later than two weeks after the registration. The number of attendees was at the end higher than expected 30.

14.1.4.3 Statistics of the feedback survey

Info	ormation about th	e sch	ool was	Answered: 15
A	excellent	7	46,67%	CB
В	good	7	46,67%	CB
C	not good nor bad	1	6,67%	A
D	bad	0	0,00%	В
E	very bad	0	0,00%	
F	don't know	0	0,00%	

Reg	Registration was Answered			
A	excellent	12	80,00%	
В	good	1	6,67%	B
C	not good nor bad	2	13,33%	
D	bad	0	0,00%	
E	very bad	0	0,00%	A
F	don't know	0	0,00%	

The	The venue was Answered: 15				
A	excellent	5	33,33%		
В	good	8	53,33%	CDF	
C	not good nor bad	0	0,00%	A	
D	bad	2	13,33%		
E	very bad	0	0,00%	В	
F	don't know	0	0,00%		

Cat	Catering was Answered: 15				
A	excellent	6	40,00%		
В	good	6	40,00%	D	
C	not good nor bad	0	0,00%	C	
D	bad	3	20,00%		
E	very bad	0	0,00%	В	
F	don't know	0	0,00%		

The overall organization was				Answered: 15
A	excellent	7	46,67%	DE
В	good	5	33,33%	C
C	not good nor bad	2	13,33%	A
D	bad	1	6,67%	
E	very bad	0	0,00%	В
F	don't know	0	0,00%	

The	The topics were relevant for my work/research interests Answered: 1					
A	agree completely	2	13,33%			
В	agree	9	60,00%		C PA	
C	no strong feelings	4	26,67%			
D	disagree	0	0,00%			
E	disagree completely	0	0,00%		В	
F	don't know	0	0,00%			

I w	as inspired to new	way	vs of thinking	Answered: 15
A	agree completely	4	26,67%	EF
В	agree	6	40,00%	DETA
C	no strong feelings	3	20,00%	C
D	disagree	1	6,67%	
E	disagree completely	1	6,67%	
F	don't know	0	0,00%	В

The	The lectures were clearly presented and comprehensible Answered: 15					
A	agree completely	3	20,00%	EF		
В	agree	5	33,33%	DETA		
C	no strong feelings	4	26,67%			
D	disagree	2	13,33%			
E	disagree completely	1	6,67%	В		
F	don't know	0	0,00%			

The	pace of teaching	was r	ight	Answered: 15
A	agree completely	4	26,67%	
В	agree	6	40,00%	DEFA
C	no strong feelings	3	20,00%	
D	disagree	1	6,67%	
E	disagree completely	1	6,67%	В
F	don't know	0	0,00%	

Tea	Teaching aids used (e.g. slides) were well prepared Answered					
A	agree completely	8	53,33%	DE		
В	agree	4	26,67%	C		
C	no strong feelings	2	13,33%			
D	disagree	1	6,67%	A		
E	disagree completely	0	0,00%	В		
F	don't know	0	0,00%			

	nds-on exercises atribution to the sc		d demonstrations	were	a valuable	Answered: 15
A	agree completely	6	40,00%			
В	agree	2	13,33%		D	
C	no strong feelings	4	26,67%			A
D	disagree	3	20,00%			
E	disagree completely	0	0,00%			
F	don't know	0	0,00%		В	

Soc		an c	enjoyable and	important aspect of the	Answered: 15
A	agree completely	2	13,33%		
В	agree	4	26,67%	G A	
C	no strong feelings	4	26,67%		
D	disagree	1	6,67%		В
E	disagree completely	0	0,00%	D	
F	don't know	1	6,67%	С	
G	not applicable	3	20,00%		

What did you like most about the course?

Answered: 11

The idea of presentations, combined with hands-on exercises was great. Some of the speakers were great.

Hands-on exercises

Some practical exercises, very well organized.

The practical exercises

The encouragement that even no computer guys can work on HPC.

Combination of theoretical lectures and practical assignments.

Spark/pySpark workshop

A wide range of topics, excellent hand-on exercises.

Everything

Great overview of relevant technologies for my future work

The topic

What did you like least about the course?

Answered: 9

In practice, the hands-on part had a lot of technical issues.

I felt there were too many topics and technologies covered in the course, which meant we only got a small taste of each one.

Some of the speakers were terrible, troubled by either poor English and a verbally unclear voice, or by poor rhetorical and pedagogical ability."

Theory at some moments.

The presentation on the first morning (mr. Leon Kos) was terrible in terms of speaking capabilities and non-generality of content.

The SALOME workshop, I did not fully understand it

Speakers didn't work properly.

Some problems with setting-up the software but they were eventually overcome with the help of the staff.

Additional comments on the content, specific lectures, etc.

Answered: 6

I would suggest that future courses try to unify all hands-on exercises to be done on a single system.

Setting up accounts, clearing technical problems and learning how to operate several different clusters wasted too much valuable time."

Hands-on exercises lacked a bit of instruction of tasks. Sometimes I got lost not knowing what to do next.

CFD modelling with HPC (Fluent)

Maybe they could provide us with more instructions about how to get access to the HPC.

everything was excellent

Over	all, ho	w wou	ld you rate this	school? Answered: 15
10 = ex	cellent		0 = waste of time	
A	10	4	26,67%	
В	9	3	20,00%	
C	8	1	6,67%	
D	7	2	13,33%	G A
E	6	2	13,33%	
F	5	1	6,67%	E
G	4	0	0,00%	
Н	3	2	13,33%	D B
I	2	0	0,00%	C
J	1	0	0,00%	
K	0	0	0,00%	

	In the future, I will need training in general HPC programming (MPI, OpenMP) Answered: 13					
A	urgent need	0	0,00%	DA		
В	important need	7	46,67%			
C	some need	6	40,00%		В	
D	no need	2	13,33%	C		
E	don't know	0	0,00%			

(Hy	In the future, I will need training in advanced HPC programming (Hybrid MPI-OpenMP; next-gen HPC languages e.g. PGAS; Answered: 15 GPU computing e.g. CUDA)					
A	urgent need	0	0,00%	D A		
В	important need	5	33,33%	В		
C	some need	8	53,33%			
D	no need	2	13,33%			
E	don't know	0	0,00%			

	In the future, I will need training in code optimisation and performance analysis Answered: 15					
A	urgent need	4	26,67%			
В	important need	2	13,33%	A		
C	some need	9	60,00%			
D	no need	0	0,00%	В		
E	don't know	0	0,00%			

	In the future, I will need training in porting of existing codes to HPC architectures Answered: 15					
A	urgent need	1	6,67%	EA		
В	important need	5	33,33%	D		
C	some need	6	40,00%		В	
D	no need	2	13,33%			
E	don't know	1	6,67%			

In t	In the future, I will need training in specific HPC application(s) Answered: 15					
A	urgent need	1	6,67%			
В	important need	4	26,67%	В		
C	some need	5	33,33%	D		
D	no need	2	13,33%			
E	don't know	3	20,00%	C		

	In the future, I will need training in HPC programming and applications specific to my research community Answered: 15				
A	urgent need	2	13,33%	F Δ	
В	important need	6	40,00%		
C	some need	3	20,00%		
D	no need	2	13,33%	В	
E	don't know	2	13,33%		

Int	In the future, I will need training in visualisation techniques Answered: 15				
A	urgent need	3	20,00%		
В	important need	1	6,67%	EA	
C	some need	5	33,33%	B	
D	no need	4	26,67%	D	
E	don't know	2	13,33%	C	

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

Answered: 3

CFD modelling (Fluent).

Data science

In nature sciences, we need more and more computational power.

The	e accessibility of v	enue	(e.g. stairs	, lifts, signage, facilites) was: Answered: 15
A	excellent	10	66,67%	CB
В	good	4	26,67%	Car
C	not good nor bad	1	6,67%	В
D	bad	0	0,00%	
E	very bad	0	0,00%	A
F	don't know	0	0,00%	

	Teaching aids (e.g. slides, handouts, exercises) were clear and accessible Answered: 15				
A	agree completely	6	40,00%	o DE	
В	agree	7	46,67%	C	
C	no strong feelings	1	6,67%		A
D	disagree	1	6,67%		
E	disagree completely	0	0,00%	В	
F	don't know	0	0,00%		

Gei	Gender			Answered: 15
A	male	14	93,33%	BD
В	female	1	6,67%	
C	prefer not to say	0	0,00%	
D	other	0	0,00%	Α

Job Title or Career Stage	Answered: 13
PhD student	Master's student
Researcher	Independent Expert at HPC
Data Scientist	MSc student
Research Fellow, Ph.D.	IT
Master's student	Student
Young researcher (PhD Candidate in Bioinformatics)	Researcher
Researcher	

Ho	w easy or har	d did you	find this course?	Answered: 15
A	Very easy	3	20,00%	
В	Quite easy	6	40,00%	C
C	Moderate	6	40,00%	
D	Quite hard	0	0,00%	В
E	Very hard	0	0,00%	

D4.1

14.1.4.4 Analysis of the feedback

The feedback survey was offered to all participants of the PRACE Autumn School, but only 15 decided to provide answers. Altogether 30 questions were asked (see https://events.prace-ri.eu/event/896/manage/surveys/601/results), with purpose of gaining feedback on satisfaction and further development of similar events.

The survey has shown that the participants were satisfied with the organization and venues of PRACE Autumn School.

The selected topics were relevant to their area of expertise and accordingly prepared. Most of them were happy with the hands-on approach. There were some technical difficulties, which were successfully taken care during the length of the program. The participants successfully accepted the idea of presentations, combined with hands-on exercises. Most of the attendees feel the need of usage of HPC related tools in their further workflow.

Some of the participants proposed further expansion of the courses to cover CFD modelling and analysis.

Unfortunately, the vast majority of the participants were male, therefore some effort for promotion through female population has to be considered. Participants were mostly students/researchers and business professionals, which indicates success of attracting the proposed target group.

14.1.5 Conclusions & lessons learned

The PRACE autumn school was successful and we would like to repeat it. In our application for organizing the PRACE Autumn School we expected up to 30 attendees. At the end, altogether there were 46 participants, which is a big success in form of School importance. Most of them were locals from academia. Therefore, we need to strive for further internationalization of the attendees and to attract people from SMEs.

The presented topics were well accepted and we would like to further develop similar programs for professional community. We would like to implement additional topics and at the same time remove some of the difficulties of the organizational aspects. We strive at delivering an improved version of the PRACE Autumn Seasonal School in 2020.

14.2 PRACE Autumn School 2020 – HPC and FAIR Big Data (Slovenia)

14.2.1 Basic Information about the event

14.2.1.1 Name

PRACE Autumn School 2020 - HPC and FAIR Big Data

14.2.1.2 Dates

15-18 September 2020

14.2.1.3 Location

Ljubljana, Slovenia

14.2.1.4 Organizing sites

University of Ljubljana - Faculty for mechanical engineering, Aškerčeva 6, Ljubljana, Slovenia

14.2.1.5 Event URL

https://events.prace-ri.eu/e/CUDA-2020

14.2.2 Organisational Details

14.2.2.1 Local organizing committee

Role	Name/	Institution	Contact
	Surname		
Chair of org.	Dr. Leon Kos	University of	leon.kos@lecad.fs.uni-lj.si
committee	Di. Leon Kos	Ljubljana, Slovenia	ieon.kos(w)iecad.is.um-ij.si
Co-Chair of org.	Dr. Pavel	University of	pavel.tomsic@lecad.fs.uni-lj.si
committee	Tomšič	Ljubljana, Slovenia	paver.tomsic(w)recad.is.um-ij.si
Chair of progr.	Dr. Janez Povh	University of	janez.povh@lecad.fs.uni-lj.si
committee	Di. Janez Povii	Ljubljana, Slovenia	Janez.povn(w)recad.is.um-ij.si
Member of org.	Alenka Maffi	University of	alenka.maffi@lecad.fs.uni-lj.si
committee	Alenka Ivianii	Ljubljana, Slovenia	alenka.mam(a/jecad.is.um-ij.si
Member of org.	Matjaž Šubelj	University of	mateja.maffi@lecad.fs.uni-lj.si
committee	Maijaz Subeij	Ljubljana, Slovenia	mateja.mam(w,recau.is.um-ij.si
Org. committee	Mateja Maffi	University of	matjaz.subelj@lecad.fs.uni-lj.si
secretary	Iviaicja iviaili	Ljubljana, Slovenia	mayaz.suberj@iecad.is.um-ij.si

14.2.2.2 Venue

PRACE Autumn School 2020 took place at Faculty of Mechanical Engineering, University of Ljubljana, Aškerčeva 6, Ljubljana, Slovenia.

Due to the nature of computing classrooms where max 30 seats are available and the fact that, attendees will not require their own laptops for following hands-on trainings. In cases where possible two parallel hands-on courses will be organized with two lecturers and assistants in two adjacent classrooms with the required bandwidth for remote desktop connection to the supercomputer and local pre-/post- processing and job submission to the HPCFS cluster at University of Ljubljana.

All the classrooms are equipped with multimedia systems, necessary for such event, as well as sufficient broadband connection.

Due to restrictions regarding Coronavirus the Autumn School was organized as a hybrid event – by having some participant in-person and the majority on-line. The venue was excellent for the event!

14.2.2.3 Synergetic events

This event addresses important aspect of Big Data in HPC and possible further usage in different areas of expertise. Due to restrictions regarding Coronavirus and the fact that most of the planned events in near surroundings have been posponed, canceled ore moved on-line there was no synergetic event held in parallel. PRACE Autumn School was organized as a hybrid event - the majority of participants were on-line. Such a situation further reduces the impact of a synergetic event.

14.2.3 Program & Content

14.2.3.1 Program committee

Role	Name/ Surname	Institution
Organization chair	Dr. Leon Kos	University of Ljubljana, Slovenija
Programme chair	Dr. Janez Povh	University of Ljubljana, Slovenija
Committee member	Dr. Pavel Tomšič	University of Ljubljana, Slovenija

14.2.3.2 Final program

TUESDAY, 15 SEPTEMBER 2020

Beginning	End	Description		
8:00	9:00	Registration		
9:00	12:00	Introduction to Linux and HPC		
		Overview of Linux operating system and introduction to HPC		
		• Outline of the benefits of parallelization of the numerical simulations in eng. analysis using HPC.		
		Motivation to use HPC system		
		HPC ecosystem - HPC facilities available to researchers in Europe (Slovenia)		
		HPC platforms architecture		
		How to connect and use HPC at UL FME		
		Convener: Dr Leon Kos (University of Ljubljana, Slovenia)		
		10:30 Coffee break		
12:00	13:00	Lunch Break		
13:00	17:00	Introduction to HADOOP (Introduction to HADOOP I)		
		Introduction to the Apache Hadoop framework		
		The Hadoop Distributed File System (HDFS)		
		- Architecture and basic usage		
		Hadoop MapReduce		

- Data partitioning
- Sorting and shuffling
- Hadoop streaming
a simple hands-on demo
Conveners: Dr Giovana Roda (TU Wien, Austria)
14:30 Coffee break

WEDNESDAY, 16 SEPTEMBER 2020

Beginning	End	Description
9:00	11:00	Introduction to HADOOP (Introduction to HADOOP II)
		Some more in-depth topics:
		fault tolerance and HDFS Erasure Coding
		The YARN resource manager
		The Mrjob library
		HDFS i/o benchmarking
		Conveners: Dr Giovana Roda (TU Wien, Austria)
		10:30 Coffee break
11:00	12:00	Introduction to R
		 creating and running own script files;
		 creating, retrieving, saving data files;
		• standard operations on data frames;
		standard matrix calculus;
		basic statistics and data visualization
		Convener: Dr Janez Povh (University of Ljubljana, Slovenia)
12:00	13:00	Lunch Break
14:00	14:30	Coffee break
14:30	17:00	Big data analysis with RHadoop
		• Basic concepts of big data management and analysis using RHadoop.
		 How to create, store, load big data files;
		How to perform basic statistics above big data files.
		Convener: Dr Janez Povh (University of Ljubljana, Slovenia)

THURSDAY, 17 SEPTEMBER 2020

Beginning	End	Description			
9:00	12:00	Introduction to Spark			
		Basic concepts of Apache Spark Data Analytic Framework.			
		• Testing access to HPC available at UL where all necessary software			
		will be preinstalled.			
		• Creating and starting own Spark working place, which will be used			
		later for running different jupyter notebooks.			

		Testing different basic Apache Spark concepts by using the Python language		
		Conveners: Dr. Slavko Žitnik (University of Ljubljana, Slovenia)		
		10:30 Coffee break		
12:00	13:00	Lunch Break		
13:00	17:00	 Data handling and processing of scientific data with FAIR principles Data Lifecycle Big data and FAIR EOSC relevance Hadoop and metadata Connection to Jupyter hub Conveners: Dr. Milan Ojsteršek (University of Maribor, Slovenia)		
		14:30 Coffee break		

FRIDAY, 18 SEPTEMBER 2020

Beginning	End	Description			
9:00	12:00	TensorFlow (Deep learning with Keras 1)			
		 Introduction to machine learning and deep learning 			
		Neural networks with Keras			
		Conveners: Primož Godec (University of Ljubljana, Slovenia), Rok Hribar			
		(IJS, Ljubljana, Slovenia)			
		10:30 Coffee break			
12:00	13:00	Lunch Break			
13:00	17:00	TensorFlow (Deep learning with Keras 2)			
		Introduction to machine learning and deep learning			
		Neural networks with Keras			
		Convolutional neural networks			
		Recurrent neural networks			
		Conveners: Primož Godec (University of Ljubljana, Slovenia), Rok Hribar			
		(IJS, Ljubljana, Slovenia)			
		14:30 Coffee break			

14.2.3.3 List of trainers

Name/	Institution	Lecture
Surname		
Dr. Leon Kos	University of Ljubljana, Slovenia	Introduction to Linux and HPC
Dr. Giovanna Roda	TU Wien, Austria	Introduction to HADOOP: Introduction to HADOOP I

	Introduction to HADOOP: Introduction to HADOOP II			
D., I., D4.	University of Ljubljana,	Introduction to R		
Dr. Janez Povh	Slovenia	Big data analysis with RHadoop		
Dr. Slavko Žitnik	University of Ljubljana, Slovenia	Introduction to Spark		
Dr. Milan Ojsteršek	University of Maribor, Slovenia	Data handling and processing of scientific data with FAIR principles		
Primož Godec	University of Ljubljana,	TensorFlow: Deep learning with Keras 1		
Fillioz Godec	Slovenia	TensorFlow: Deep learning with Keras 2		
Rok Hribar	IJS, Ljubljana, Slovenia	TensorFlow: Deep learning with Keras 1		
	, 3 3 ,	TensorFlow: Deep learning with Keras 2		

14.2.3.4 Designing the program

The PRACE Autumn School focuses on Big data analysis with HPC using different approaches presented through Spark, Hadoop, RHadoop and TensorFlow. The success of PRACE Autumnal School 2019 serves as a basis for the program design. Remarks from 2019 participants will serve as an efficient way to achieve better quality of the programme.

PRACE is presented as the main organization for HPC in Europe. Autumn school targets industry users to get acquainted with advanced technology and the possibilities of HPC.

Case studies and hands-on tutorials will be carried on the ULFME cluster. The tutorials will be held in sessions, depending on the applicants' interest indicated in the registration questionnaire.

14.2.3.5 Description of the contents

The training event was target to master and PhD students, early career researchers and engineers from industry looking for competencies in big data analysis using Hadoop, Spark, R (with RHadoop) and TensorFlow. We expected that engineers from SMEs would find this course of particular interest.

Content	Description	
Introduction to Linux and HPC	Motivation to use HPC system in professional workflow was shown to attendees. PRACE HPC ecosystem were introduced-HPC facilities available to researchers in Europe. Different HPC platforms architecture as well as a short overview of Linux operating system was explained. Benefits of parallelization of the numerical simulations in engineering analysis using HPC were outlined. At the end an example of how to connect and use HPC at UL FME was showcased.	
Introduction to HADOOP (Introduction to HADOOP I)	Short introduction to the Apache Hadoop framework, explaining the Hadoop Distributed File System (HDFS), its architecture and basic usage. Explaining the Hadoop MapReduce.	

Introduction to HADOOP (Introduction to HADOOP II)	Some more in-depth topics about fault tolerance and HDFS Erasure Coding, the YARN resource manager, the Mrjob library and HDFS i/o benchmarking.
Introduction to R	Short introduction to R by creating and running own script files, standard operations on data frames, matrix calculus and basic statistics and data visualization.
Big data analysis with RHadoop (Big data analysis with RHadoop)	Basic concepts of big data management and analysis using RHadoop.
Introduction to Spark (Introduction to Spark)	Presenting basic concepts of Apache Spark Data Analytic Framework, testing access to HPC available at UL where all necessary software will be preinstalled. Creating and starting own Spark working place, which will be used later for running different jupyter notebooks. Testing different basic Apache Spark concepts by using the Python language.
Data handling and processing of scientific data with FAIR principles (Data handling and processing of scientific data with FAIR principles)	Explaining Data Lifecycle, Big data and FAIR principles, EOSC relevance, Hadoop and metadata
TensorFlow (Deep learning with Keras 1)	Introduction to machine learning and deep learning and Neural networks with Keras.
TensorFlow (Deep learning with Keras 2)	Presenting convolutional neural networks and recurrent neural networks.

14.2.3.6 Computer resources

Supercomputer HPCFS-U at ULFME with accounts for the event was prepared that gave attendees KDE GUI environment with all required tools and icons required for tutorials. Nearby computing classrooms were prepared for NX client remote terminal access.

Time limited WiFi hot spot access with the same credentials as for HPC were given to all attendees so that they could access internet from their laptops and smart phones.

14.2.4 Participants & Feedback

14.2.4.1 Number of participants by country

Altogether 82 participant from 19 countries participated at the PRACE Autumn School 2020.

Country	No. of participants	Remote (online)	Hands-on (in person)
Belgium	23	23	0
Bulgaria	2	2	0
Egypt	1	1	0
Estonia	1	1	0
France	1	1	0
Germany	2	2	0

India	1	1	0
Iraq	1	1	0
Ireland	1	1	0
Israel	1	1	0
Portugal	17	17	0
Saudi Arabia	1	1	0
Slovenia	12	4	8
Spain	2	2	0
Sweden	1	1	0
Switzerland	1	1	0
Turkey	4	4	0
United Kingdom	2	2	0
Not specified	8	8	0
Total:	82	74	8

14.2.4.2 Process for selecting the participants

Applicants were expected to have some experience with the topic of interest. School attendees were selected based on applications submitted through the registration form, taking into account the order of registrations. Applicants were informed about their acceptance not later than two weeks after the registration. The number of attendees was at the end higher than expected 30.

14.2.4.3 Statistics of the feedback survey

Over	Overall, how would you rate this training event? Answered: 21				
A	10 - excellent	5	23,81%		
В	9	7	33,33%		
C	8	3	14,29%		
D	7	4	19,05%	E Fill	Α
E	6	1	4,76%	D	
F	5	1	4,76%		
G	4	0	0,00%		
Н	3	0	0,00%	C	В
I	2	0	0,00%		
J	1	0	0,00%		
K	0 - bad	0	0,00%		

How did you like the online format? – We switched to the online format because of COVID-19...

Answered: 20

Worked really great

Yes, it was good.

There were no complications. It could be beneficial if the speaker had a microphone - using the built in laptop mic only works when the speaker is close enough and speaking directly into it. actually this format save me time and money to my employee. I like it.

Everything worked well as if the course was given in person.

By me its perfect, because its easy the interaction directly with the instructor and the questions also.

It was efficient

great

very good and well organized

Due to the epidemic situation, the hybrid idea for the event was well thought out.

All those present were very well. It was felt a little, the fact that we were not present, but the teachers did their best to minimize this lack.

The online format seemed good and appropriate to the circumstances due to the covid-19

The process of education was effective enough and all necessary resources were provided

Excellent

It was so nice to be able to join the event from home without any worries.

I like it, online format is good in these circumstances.

It is a good alternative due to current conditions, and it allows to achieve generically the same goals. However, on-site versions allows for direct interaction among trainer-trainee and trainee-trainee, which contributes to better learning experience.

It was Ok, but the schedule was packed. I think for an on-line format it would have been better to have for instance only morning sessions.

better than traditional

The online format is much more convenient and just as effective as the presented format. Please do keep it as an option even after the pandemic.

Training event content and feedback to lecturers (e.g. topic, materials, exercises, structure): – What did you like best?

Answered: 20

Topic & materials where good.

Topics

The machine learning lectures on the last day were the most interesting.

I liked the fact that we had a lot of different lecturers, that broke the monotony. it was good.

Practical exercises were the most effective for me.

the structure online format always was convenient to according even training the best was material nd access to infrastructure HPC

The lectures on Friday were the best.

event content

Topics and materials

I like the idea of uploading the materials before the lecture so that we can get acquainted with the upcoming lecture. The other thing that was good was the screen sharing as the speakers explained the commands so that each step was followed and the material was more accessible.

The program was well prepared. I especially liked the topics, materials made available.

Regarding the practical component, it seemed appropriate and responded to expectations

I liked the topics and structure

Practical sessions

I liked the topics they were very interesting and the structure of the program

I had trouble following up with some exercises due to technical issues like server capacity.

Materials were good.

Content was at good level, including introductory level, which was important for not experts. Some topics where covered to fast.

I did like the way the instructors teached the last day, it was easy to follow and make by ourserves by using colab.research.google.com

Some topics very quite slow, some were very fast paced, maybe balance it out?

The rigor and the down-to-earth applicability of all the lectures.

Where should we improve?

Answered: 16

Some specific topics

I expected more time and energy dedicated to explaining why and how things work, and not showing how they work. As an example, one could find the syntax rules of the functions used to train a machine learning algorithm on stackoverflow/youtube/documentation, while e.g. the choice of an activation function or the number of nodes should be explained by an expert. During the lectures, it was (multiple times) explained away with "we do not worry about this" or "it just works like this". The same goes for the Hadoop lectures, I would assume everybody knows how to move files in the command line; there is no need to show this multiple times on multiple examples.

it was just a pity that some of the codes weren't tested before so it felt a bit improvised

1 - The last lecture from Friday was to profound. It would be preferable to use that time explaining how the algorithms of neuronal networks actually work and discuss which parameters to use in some classification problems. 2 - The last lecture from Thursday didn't have enough practical exercises. The presentation was too long, the slides had too much text and the lecturer has too slow to speak the information needed.

by me everything was good quality

1- To give little more time for the exercises, sometimes i got some errors and while i'm working on it, i miss the next exercise. 2- keep in mind the number of participants as in Spark exercises I stuck becouse of the number of ports and tried to set manually the port number, i prefered to just watch through zoom as I have already have some knowledge in Spark. but you can just include the instraction of setting the port manually for next time:).

There were technical problems, but this is understandable given the situation.

Unfortunately, at the moment I am unable to state any points. And, I'm referring only to distance learning. Eventually, delivering the material in advance could be a solution.

In some sessions they did the exercises very fast and it was difficult to follow them at the same time

the instructional design of the presented materials can be improved

In some of the presentations terminal commands were problematic and it led to some delay for attenders while following up with the process.

Some technical issues like sound.

It would be interesting if trainees could prepare and bring their own problems for testing during the workshop

In a mixed format (precential and on-line), when the audience ask something it should be repeated by the instructor because the on-line participants had no idea what was the question and what the instructor is talking about.

Although sound quality and picture quality were perfectly adequate, both could still be improved by using studio-like cameras and microphones.

Which future training topics would you like to be provided by PRACE or the training host?

Answered: 17

These topics covered everything.

C++, OpenFOAM

Lectures on algorithms and data structures with practical exercises and complexity analysis.

Bioinformatic Tools using HPC infrastructure

More deep learning and AI

parallel programming

more for HadoopR or Spark in R TensorFlow as unfortunately I didn't manage to attend the exercise

Probably, those ones for MPI, OpenMP and CUDA.

One of the themes that we will face is with big data modeling and parallelization, distribution is one of the very important topics. But, we must not focus only on achievement (i.e., technology).

I would like to go deeper into machine learning

Advanced image processing

I would like to delve into deep learning, machine learning and big data

HPC, Machine Learning, Deep Learning, Reinforcement Learning, Data, Digital Signal Processing, Computer Vision etc.

maybe natural language processing

Deeper course on TensorFlow and Recursive Neural Networks.

Parallel computing

I am alredy registered for the parallel programming / MPI event. My area of research involves the development of simulation codes so further events around this subject would be greatly appreciated.

Training event organisation (e.g. announcement, registration, changes due to COVID-19): – What did you like best? – Where should we improve?

Answered: 19

The quality of camera was not good sometimes.

Everything was well organised. The announcement email (with instructions to install certain software etc.) was sent too late for my liking (5pm the day before the lectures).

it was really nice to get all my emails answered by the team, thanks to them. it felt i deserved a lot of attention

Everything was good.

By me was perfect.

It was well prepared

none applicable

The remote attendance and wish that can continue after the COVID in the same way as it was very useful

I think it was well-organized.

I have nothing to comment.

I think it was very well organized. Perhaps a little more announcement was lacking.

Communication with organizers was fast, effective and without irrelevant information

very good organization and advertising can be improved

I think the organization was perfect. Thank you for your efforts.

All of them are okay but in application, sometimes it was busy, I couldn't focuse continuously

The workshop was well organized, although it would be nice to receive information in some more time advance, in order to better prepare participation.

It would have been good for the organization to ask requirements for log-in accreditation in advance and not few days before starting. It helps to plan from our sides.

very straight forward, better than traditional

Smooth and clear organization and communication.

Woul	Would you recommend this training event to others? Answere				
A	Yes	19	90,48%	BC	
В	No	1	4,76%		
С	No selection	1	4,76%	A	

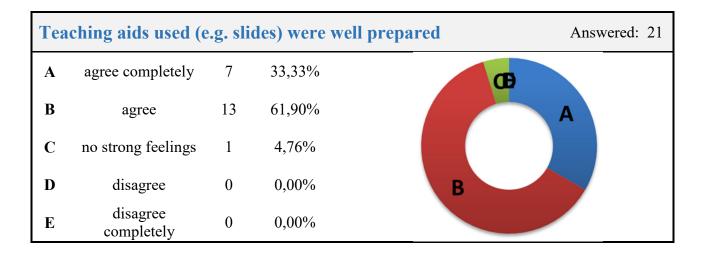
Subj	Subject of course for me was			Answered: 21
A	important	19	90,48%	BO
В	minor	1	4,76%	
C	not relevant	0	0,00%	
D	no selection	1	4,76%	A

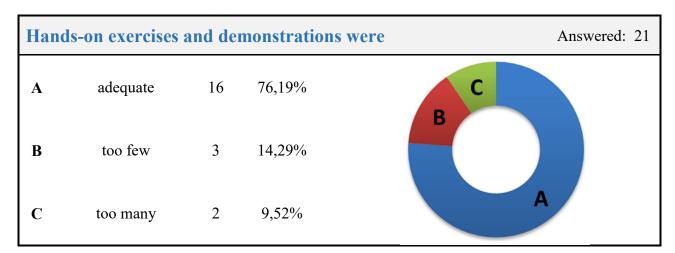
I was	I was inspired to new ways of thinking			Answered: 21
A	yes	13	61,90%	C
В	partially	8	38,10%	B
С	no	0	0,00%	

Leng	th of course wa	as		Answered: 21
A	adequate	19	90,48%	BC
В	too short	1	4,76%	
C	too long	1	4,76%	A

Depth of content was Answered:			Answered: 21	
A	adequate	15	71,43%	C
В	too superficial	5	23,81%	
C	too profound	1	4,76%	A

The p	The pace of teaching was			Answered: 21
A	adequate	18	85,71%	C
В	too slow	1	4,76%	
C	too fast	2	9,52%	A





14.2.5 Analysis of the feedback

The feedback survey was offered to all participants of the PRACE Autumn School, but only 21 decided to provide answers. Altogether 14 questions were asked, with purpose of gaining feedback on satisfaction and further development of similar events.

The survey has shown that the participants were satisfied with the PRACE Autumn School 2020. They were satisfied with the switch to the on-line format we have taken due to COVID-19. We received only positive feedback, even proposing to keep it as an option after the pandemic. Overall, the event was well organized, and everyone was satisfied with communication. Most of the participants would recommend this training event to others.

The presented training content and structure was well received. The participants were especially keen to the screen sharing option. Improvement can be in dedicating more time to explaining the basics, as some of the participants had a lack of knowledge. Dealing with larger numbers of participants, most of them presented remotely is a challenging task due to code-errors problems

when presenting a practical example. In this aspect it is easier for the presenter to have all the participants present in the classroom.

The participants showed a desire to further expand their knowledge. There are many different suggestions what topics PRACE could provide, from coding, machine learning to bioinformatics. Subject of course was important to the participants, it even inspired them to new ways of thinking.

14.2.6 Conclusions & Lessons Learned

The PRACE autumn school was successful and we would like to repeat it. In our application for organizing the PRACE Autumn School we expected up to 30 attendees. Due to problems regarding coronavirus, organizing such an event proved to be quite challenging. In the process we have changed the event type into hybrid event. We had to follow the rules at limiting the number of people in classrooms. For participants, that were interested, on-line presence was enabled. Overall this approach resulted in greater number of international participants than in 2019. This proves that the presented topics are interesting to a wider population.

Altogether 82 participant applied, coming from 19 countries, which is a big success in form of School importance. Only local participants (8) were present at in person lectures, which was to be expected. Others (74) participated through on-line presence.

After the course completion, we conducted a survey in order to obtain feedback. It has shown satisfaction with the PRACE Autumn School 2020. We received only positive feedback from going on-line, even proposing to keep it as an option after the pandemic. According to the survey, the event was well organized, and everyone was satisfied with communication.

The presented topics were well accepted and we would like to further develop similar programs for professional community. We would like to implement additional topics and at the same time remove some of the difficulties of the organizational aspects. We strive at delivering an improved version of the PRACE Autumn Seasonal School in 2021.

15 Annex IV: On-demand Events

The following subsections (15.1 and 15.2) contain the full reports from on-demand events that were organised and delivered during the reporting period in the PRACE-6IP project.

15.1 EUDAT-PRACE Summer School 2019 (Italy)

15.1.1 Basic Information about the event

15.1.1.1 Name

EUDAT-PRACE Summer School on managing scientific data from analysis to long term archiving

15.1.1.2 Dates

23-27 September 2019

15.1.1.3 Location

Trieste, Italy

15.1.1.4 Organizing sites

EUDAT, International Centre for Theoretical Physics (ICTP), PRACE (CSC, ICHEC, CINECA)

15.1.2 Organisational Details

15.1.2.1 Local organizing committee & trainers

Claudio Cacciari, SURFsara; Donatello Elia, CMCC; Giuseppe Fiameni, CINECA; Sandro Fiore, CMCC; Shaun de Witt, UKAEA; Sara Garavelli, Trust-IT Services; Ivan Girotto, ICTP; Leon Kos, University of Ljubljana; Sara Ramezani, SURFsara; Marco Rorro, CINECA; Mark van de Sanden, SURFsara; Hans van Piggelen, SURFsara; Heinrich Widmann, DKRZ; Simon Wong, ICHEC.

15.1.2.2 Venue

The Abdus Salam International Centre for Theoretical Physics (ICTP) was chosen as the venue of the Summer School. It has a long tradition of hosting visitors for both research collaborations and training/educational events. There are excellent teaching facilities on-site, as well as accommodation that is dedicated for institutional visitors.

15.1.2.3 Synergetic events

The event itself was a synergistic effort between the EUDAT and PRACE project.

15.1.3 Program & Content

15.1.3.1 Program committee

Claudio Cacciari, SURFsara; Donatello Elia, CMCC; Giuseppe Fiameni, CINECA; Sandro Fiore, CMCC; Shaun de Witt, UKAEA; Sara Garavelli, Trust-IT Services; Ivan Girotto, ICTP; Leon Kos, University of Ljubljana; Sara Ramezani, SURFsara; Marco Rorro, CINECA; Mark van de Sanden, SURFsara; Hans van Piggelen, SURFsara; Heinrich Widmann, DKRZ; Simon Wong, ICHEC.

15.1.3.2 Designing the program

The programme was designed to take students on a 5-day journey through a typical research data lifecycle (data discovery; data processing; data analysis; data preservation and publishing) together with sessions on addressing compute-intensive challenges.

15.1.3.3 Final program

SUNDAY 22 SEPTEM	MBER 2019						
18:30 - 20:30	Ice Breaker Social Event						
	Hotel Riviera & Maximilian's, Strad	la Costiera 22, 34010 Trieste, Italy	y. The hotel is 10 minute walk fron	n the ICTP Adriatico Guesthouse. I	Meeting point: Reception		
	of the ICTP Adriatico Guesthouse @	918:15 pm CEST.					
SUMMER SCHOOL I	DDOCDAMME						
30MMER 3CHOOL I	MONDAY 23 SEPTEMBER 2019	TUESDAY 24 SEPTEMBER 2019	WEDNESDAY 25 SEPTEMBER 2019	THURSDAY 26 SEPTEMBER 2019	FRIDAY 27 SEP- TEMBER 2019		
08:00 - 09:00	Registration						
09:00 - 11:00	Kicking-off the Summer School	Data Analysis (Part I)	Data Preservation (Part I)	Data Sharing & Publishing (Part I)	Real use case (Part I)		
11:00 - 11:30	Coffee & Networking						
11:30 - 13:00	Introducing the basics, from Linux fundamental commands to Python notation	Data Analysis (Part II)	Data Preservation (Part II)	Data Sharing & Publishing (Part II)	Real use case (Part II)		
13:00 - 14:00	Lunch Break						
14:00 - 16:00	Data Processing: HPC fundamentals	Data Analysis (Part III)	Meet the experts	Data Discovery	Final remarks on the Summer School & feedback collection		
16:00 - 16:30	Coffee & Networking						
16:30 - 18:00	Data Processing: Computing Architectures	Data Analysis (Part IV)	Social Event	Data Movement			
18:00 - 22:00			Social Event				

15.1.3.4 List of trainers

Claudio Cacciari, SURFsara; Donatello Elia, CMCC; Giuseppe Fiameni, CINECA; Sandro Fiore, CMCC; Shaun de Witt, UKAEA; Sara Garavelli, Trust-IT Services; Ivan Girotto, ICTP; Leon Kos, University of Ljubljana; Sara Ramezani, SURFsara; Marco Rorro, CINECA; Mark van de Sanden, SURFsara; Hans van Piggelen, SURFsara; Heinrich Widmann, DKRZ; Simon Wong, ICHEC.

15.1.3.5 Computer resources

Students brought own laptops for hands-on exercises. Access to various EUDAT data services was supported throughout the workshop. Access to the CINECA Galileo cluster was also provisioned. These resources were sufficient for the event.

15.1.4 Participants & Feedback

15.1.4.1 Number of participants by country

Total of 26 participants - Armenia (1), Belgium (1), Canada (1), Denmark (1), Germany (3, Ghana (1), India (2), Iran (2), Iraq (1), Italy (4), Nigeria (1), Qatar (1), Saudi Arabia (1), Senegal (1), Serbia (1), Sudan (1), United Kingdom (1), Turkey (1), Croatia (1)

15.1.4.2 Process for selecting the participants

Participants were asked to justify their reasons for attending the summer school. Each application was reviewed by at least 2 reviewers from EUDAT and PRACE in order to accept students whose research will benefit from the learning outcomes of the summer school.

15.1.4.3 Statistics of the feedback survey

An overall rating of 4.5 out of 5 was achieved for the school.

15.1.5 Conclusions & Lessons Learned

It was a fruitful collaboration between EUDAT and PRACE, and students were introduced to services that will help them tackle both data and compute challenges. There is good potential to make more/better use of Jupyter notebooks for teaching, even on compute clusters.

15.2 CSC-BioExcel – Advanced Gromacs (Finland)

15.2.1 Basic Information about the event

15.2.1.1 Name

Advanced Gromacs Workshop

15.2.1.2 Dates

9-11 October 2019

15.2.1.3 Location

Espoo, Finland

15.2.1.4 Organizing sites

CSC - IT Center for Science

KTH – Computational and Theoretical Biophysics Group / Prof. Erik Lindahl

University of Utrecht – Computational Structural Biology Group / Prof. Alexandre Bonvin

Supporting role: Max-Planck Institute for biophysical Chemistry – Computational Biomolecular Dynamics / Prof. Bert de Groot

15.2.2 Organisational Details

15.2.2.1 Local organizing committee & trainers

Name	Role	Home organization
Dr. Atte Sillanpää	Local organization, technical setup, hands-on	CSC
Dr. Christian Blau	Lectures, hands-on, organization from BioExcel side	KTH / BioExcel
Dr. Rodrigo Vargas	Lectures, hands-on	Utrecht University/BioExcel
Dr. Martti Louhivaara	Hands-on	CSC
Dr. Nino Runeberg	Hands-on	CSC
Dr. Vesa Savolainen	Web streaming and recording	CSC
Marina Bouianov	Practical arrangements	CSC

15.2.2.2 Venue

The event will take place at the CSC training room Dogmi.[2] It has two projectors and 24+1 workstations making it ideal for the hands-on exercises. The room has been used for tens of training events, including PRACE training, over the years with very good feedback. The training room is well suited for streaming the lectures for remote participation. The training room is connected to a lounge area for coffee breaks and networking. CSC is easy to reach by metro.



Figure 9 Dr. Christian Blau lecturing about the new Gromacs API.



Figure 10 CSC training lounge for coffee breaks and the flash talk introductory session.

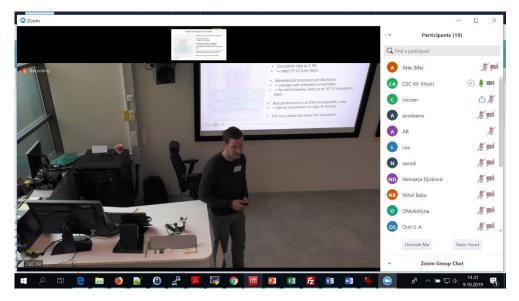


Figure 11 Dr. Christian Blau as shown in the web stream camera. The remote participants could choose the relative size of the web camera or shared screen (above the small rectangle at the top) with slides/hands-on.

15.2.3 Program & Content

15.2.3.1 Program committee

Name	Role	Home organization
Dr. Atte Sillanpää	Overall, querying interests on potential	CSC
	participants	
Dr. Christian Blau	Lectures, hands-on, organization	KTH
Dr. Rodrigo Vargas	Lectures, hands-on	Univ. of Utrecht
Prof. Alexandre	Content planning and creation	Univ. of Utrecht
Bonvin		

15.2.3.2 Designing the program

CSC has just deployed the first of the new supercomputers. Gromacs users are among those, who consume the largest amounts of CPU and GPU time on the HPC systems. Since there hadn't been an advanced Gromacs usage event in Finland for a long time, it was considered to be important to maximize efficient usage of the latest algorithms and hardware. It turned out that Gromacs developers could contribute via the BioExcel CoE and a collaboration was set up. The BioExcel CoE members suggested also other content, i.e. PMX and HADDOCK, which nicely complement the functionality of Gromacs. A query was sent out to research groups using CSC resources for their interest in the three topics, and a large majority wanted them all included. This created the backbone for the workshop. Additional tuning was made to allow interactivity (bring your own systems) and hands-on exercises on the topics covered.

15.2.3.3 Final program

Wednes	Vednesday 9th October			
11:30	Registration - training room lounge			
12:00	Lunch			
13:00	Gromacs - where are we now, what's new, what's coming in the future			
14:00	Maximizing Gromacs performance for HTC and HPC			
14:30	Hands on - Performance			
15:00	Advanced simulation protocols in GROMACS			
15:30	Hands on - Advanced simulation protocols			
18:00	Light dinner and Flash talks			
21:00	End of Day 1			
Thursd	ay 10th October			
9:00	PMX - alchemical free energy calculation setup tools introduction			
10:00	Hands on - PMX github.com/deGrootLab/pmx			
12:00	Lunch			
13:00	HADDOCK – Modelling intermolecular interactions			
14:00	Hands on - HADDOCK www.bonvinlab.org/education/HADDOCK24/			

15:00	HADDOCK – advanced topics
17:00	End of day 2
Friday 11	th October
9:00	Getting deeper into issues and questions that emerged during the workshop,
10:00	Participant contributions, Q&A, Discuss your own model systems
12:00	Lunch
13:00	Closing

15.2.3.4 List of trainers

Name	Role
Dr. Atte Sillanpää	Overall and technical support, HPC-Europa3 talk
Dr. Christian Blau	Lectures on Gromacs and PMX, hands-on support
Dr. Rodrigo Vargas	Lectures and hands-on supervision for HADDOCK
Dr. Nino Runeberg	Overall and technical support
Dr. Martti Louhivuori	Technical and Gromacs support

15.2.3.5 Description of the contents

The Training materials (Slides, links to exercises) are available on the Workshop homepage [1] The event started with Christian's review of the development of Gromacs, where it is now, and where it's heading. This was both an important introduction as well as information to plan efficient simulation setups.

15.2.3.6 Computer resources

The lectures and most of the hands-on exercises were done on the training room workstations. For the duration of the workshop, training accounts were created for all participants on the Puhti supercluster (In total 682 CPU nodes, each equipped with two latest Cascade Lake CPUs, with 20 cores each running at 2.1 GHz (Xeon Gold 6230) linked with HDR InfiniBand 200 Gbps. Additionally, the cluster has 80 nodes including also four Nvidia Volta V100 GPUs with 32 GB of memory each linked with Dual rail HDR100 interconnect [3]). An advance reservation was set up for Friday to minimize queuing for the scaling tests, while running on normal partitions was possible throughout the workshop.

15.2.4 Participants & Feedback

15.2.4.1 Number of participants by country

Participants on-site (20 in total)

Country	Number of participants
Belgium	1

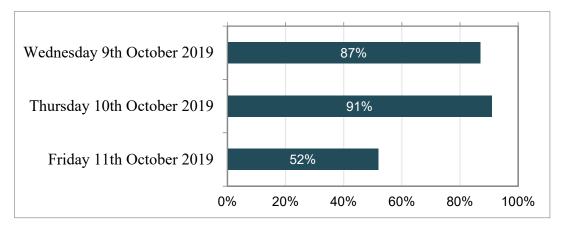
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Finland	17
Germany	1
The Netherlands	1

Participants registered for remote stream (22)

Country	Number of participants
Finland	5
Germany	2
Hungary	1
India	3
Serbia	1
Sweden	2
Switzerland	1
The Czech Republic	2
Turkey	3
USA	1
unknown	1

On-site participation was for the whole event, while the remote participation registration was as follows:



The actual daily remote participation was sampled at a few points, and highest simultaneous numbers on-line were: 17, 13, 6, for Wednesday, Thursday and Friday, respectively.

15.2.4.2 Process for selecting the participants

The first 24 registrations wishing to come on-site were selected. In addition, there was a free-of-cost possibility to participate remotely.

15.2.4.3 Statistics of the feedback survey

Q1: Information on the event seems to localize in Finland. Perhaps better PRACE visibility next time?

Q4: Heterogeneous audience from novices to experts surprisingly evenly distributed

Q8: One person disagreed that lectures were clear. Average scores were very good (content match to advertise, clarity, prerequisites, learned new skills, slides, hands-ons).

Q15: Teaching pace could have been a little slower

Q16-18: Participants gave some individual feedback which will be useful in future workshops, but which don't really require overhauling everything

Q19: Overall, the school achieved an verage score 8.65/10

15.2.5 Conclusions & Lessons Learned

Still more emphasis could be made for participants to prepare in advance for the event. Perhaps a test, that the participant can do to evaluate skill level. Some participants struggled with basic Linux command line usage. Although we clearly and strongly encouraged the participants to make sure they know the basics, and provided suitable training material to brush up before the event, some time was lost from the actual scientific content to cover the basics. On the other hand, we believe this is a sign of us attracting those researchers with a very large potential gain from these events i.e. become able to use HPC in their research. Nevertheless, even more emphasis on should be given on preparations next time. We consider the workshop a great success and plan to include a similar on as a PTC event in fall 2020 or spring 2021.