E-Infrastructures
H2020- INFRAEDI-2018-2020

INFRAEDI-01-2018: Pan-European High Performance Computing infrastructure and services (PRACE)

PRACE-6IP

PRACE Sixth Implementation Phase Project

Grant Agreement Number: INFRAEDI-823767

D4.2

Final Training Report

Final

Version: 1.2
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Date: 21.12.2022

Project and Deliverable Information Sheet

PRACE Project	**Project Ref. №: INFRAEDI-823767**	
	Project Title: PRACE Sixth Implementation Phase Project	
	Project Web Site: https://www.prace-ri.eu/about/ip-projects/	
	Deliverable ID: D4.2	
	Deliverable Nature: Report	
	Dissemination Level: PU *	**Contractual Date of Delivery:** 31 / December / 2022
		Actual Date of Delivery: 21 December 2022
	EC Project Officer: Leonardo Flores Añover	

* - The dissemination level are indicated as follows: **PU** – Public, **CO** – Confidential, only for members of the consortium (including the Commission Services) **CL** – Classified, as referred to in Commission Decision 2005/444/EC.

Document Control Sheet

Document	**Title: Final Training Report**	
	ID: D4.2	
	Version: 1.2	**Status:** ***Final***
	Available at: https://www.prace-ri.eu/about/ip-projects/	
	Software Tool: Microsoft Word 2016	
	File(s): D4.2_v1.2.docx	
Authorship	**Written by:**	Tiina Leiponen, CSC
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	Reviewed by:	Andrew Emerson, CINECA Veronica Teodor, JUELICH
	Approved by:	MB/TB

Document Status Sheet

Version	Date	Status	Comments
0.1	23/10/2022	Draft	
0.2	11/11/2022	Draft	Comments LK,ZK,NA
0.3	18/11/2022	Draft	Update
0.4	21/11/2022	Draft	Version for 1st internal review
1.0	12/12/2022	Draft	Version for 2nd internal review
1.1	14/12/2022	Draft	Version for MB/TB approval
1.2	21/12/2022	Final	Final version for EC

Document Keywords

Keywords:	PRACE, HPC, Research Infrastructure, HPC Training, PTC, MOOC, SoHPC, PRACE Training Centres, Seasonal Schools, Training Portal, HPC in Europe Portal

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List of Acronyms and Abbreviations

3D-QSAR	three-Dimensional Quantitative Structure-Activity Relationships; web application for pharmaceutical chemistry
AI	Artificial Intelligence
aisbl	Association International Sans But Lucratif (legal form of the PRACE-RI)
AWS	Amazon Web Services; the world's most comprehensive and broadly adopted cloud platform
CASTIEL	Coordination and Support for National Competence Centres (NCC) on a European Level
CFD	Computational Fluid Dynamics
CoE	Center of Excellence
CPU	Central Processing Unit
CUDA	Compute Unified Device Architecture (NVIDIA)
EC	European Commission
ETP4HPC	European Technology Platform (ETP) for High-Performance Computing (HPC)
EUDAT CDI	EUDAT Collaborative Data Infrastructure
EHPCSW	European HPC Summit Week
GPU	Graphic Processing Unit
GROMACS	GROningen MAchine for Chemical Simulations; a free, open source molecular dynamics (MD) software package originally developed by the University of Groningen (The Netherlands)
IHPCSS	International High Performance Computing Summer School
HADDOCK	High Ambiguity Driven protein-protein DOCKing; an information-driven flexible docking approach for the modeling of biomolecular complexes
HPC	High Performance Computing; Computing at a high performance level at any given time; often used synonym with Supercomputing
HTP	High Throughput Processing
LMS	Learning Management Systems
MB	Management Board (highest decision making body of the PRACE project)
MD	Molecular Dynamics
ML	Machine Learning
MOOC	Massively Open Online Course
MPI	Message Passing Interface
OpenFOAM	Open-source Field Operation And Manipulation; a free, open source computational fluid dynamics (CFD) software package released by the Open FOAM Foundation
PTC	PRACE Training Centres (formerly PATC, PRACE Advanced Training Centres)
PMO	Project Management Office
PMX	a versatile (bio-) molecular structure manipulation package (formerly pymacs)
PRACE	Partnership for Advanced Computing in Europe; Project Acronym
RedCLARA	Latin American Cooperation of Advanced Networks (Cooperación Latino Americana de Redes Avanzadas)
RI	Research Infrastructure
RIKEN	Rikagaku Kenkyusho (Institute of Physical and Chemical Research, Japan)
R-CCS	RIKEN Center for Computational Science
SKA	Square Kilometre Array

SSO	Single Sign On; an authentication method that enables users to securely authenticate with multiple applications and websites by using just one set of credentials
TB	Technical Board (group of the PRACE Work Package leaders)
Tier-0	Denotes the apex of a conceptual pyramid of HPC systems. In this context the Supercomputing Research Infrastructure would host the Tier-0 systems; national or topical HPC centres would constitute Tier-1
UEABS	Unified European Application Benchmark Suite
WP	Work Package
XSEDE	Extreme Science and Engineering Discovery Environment

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 CDI	EUDAT Collaborative Data Infrastructure
ETH Zurich (CSCS)	Eidgenössische Technische Hochschule Zürich – CSCS, Switzerland
GCS	Gauss Centre for Supercomputing e.V., Germany
GÉANT	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
SURF	SURF is the collaborative organisation for ICT in Dutch education and research
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

This deliverable is the final report of all PRACE-6IP WP4 (training) activities. These training activities were sustained during the two extension periods of the PRACE-6IP project.

The COVID-19 pandemic has had an enormous effect on training activities, boosting the transition of face-to-face courses and schools to online format. Despite the postponement and cancellations of some courses and training events in this exceptional timeframe WP4 still managed to deliver 396 PTC courses, delivered eight Seasonal Schools in Slovenia, Belgium, Slovakia, Slovenia, Bulgaria, Austria, Finland, and Israel, converted the PRACE Summer of HPC (SoHPC) into a virtual programme and delivered eight MOOCs and two BOFs for students during ISC 2021 and 2022. An advanced online workshop was organised as a collective effort by three PTCs, which was delivered as three online events in spring 2022.

PTCs network expanded by Austria, Belgium, Slovenia and Sweden in 2019. From May 2019 to December 2022, the PTCs have collectively delivered 396 courses, representing 1,045 days of training with 13,225 participants. This includes the 2019-2020, 2020-2021, 2021-2022 and fall 2022 PTC programmes. The COVID-related changes to online courses have been attractive to participants from Europe. Most PTCs have continued mainly with online training up to the end of PRACE-6IP project – this has allowed a wider participant scope and range than in face-to-face training.

Three on-demand events were organised in the PRACE-6IP project, in 2019 with the EUDAT and BioExcel CoE projects, 2021 in Slovenia as online event. Three International HPC Summer Schools (IHPCSS) were organised: 2019 School in Kobe, Japan, 2020 school was postponed to 2021 due to pandemic, as an online event, and 2022 live edition in Athens, Greece.

The PRACE Summer of HPC is a summer internship programme for students mentored by HPC experts from participating PRACE partner sites. In 2019, 25 projects and 25 students were hosted at HPC centres. In 2020, SOHPC was transferred to remote mentoring programme of 50 students participated in 25 projects across HPC partners. In 2021 edition, the collaboration with CERN, PRACE HPC centres and GÉANT network was used to benchmark High Throughput Processing (HTP) on PRACE TIER-0 systems with 66 students working online in 33 projects. The 2022 edition was prepared as an in-kind contribution by the partners, with 29 students and 22 projects provided with face-to-face and online mentoring.

PRACE has delivered eight MOOCs running on the FutureLearn platform on a periodic basis (i.e. some repeat runs of the same MOOC), which have attracted a total of 7475 active learners (16568 enrolments). The PRACE Training and Events Portals were updated with new functionalities to improve the user experience. The Training Portal was redesigned to be consistent with the PRACE web site, and made easier for users to identify relevant courses. Training materials were made to match the Carpenter style of study packages in modified CodeVault.

Training collaboration has been an important asset in PRACE. The training development collaboration has continued with CERN, GÉANT and SKA. Training alignment with FocusCoE and CASTIEL has been continued in creating a joint training platform and exchange of best practices as well as workshop organisation together with ETP4HPC especially related to training for industry.

1 Introduction

Training has been one of the key activities of PRACE because of the ever-continuous demand for HPC skills and competences enabling the effective use of hardware and software needed in solving universal challenges. The PRACE training brand has had unique value that has been derived from its deep roots in the European HPC ecosystem. The long PRACE tradition and rich network of experts in HPC-related fields across Europe have been widely recognised. Together they have been providing short courses on intermediate to advanced topics for all academic and industrial HPC users free of charge, and coordinated their work via a pan-European curriculum. Since the beginning of PRACE training activities (including statistics from PRACE-6IP WP4 activities described in this report), it has delivered over 1,000 training events that attracted close to 29,500 participants as shown in Table 1.

Activity/Course	**#events**	**#training days**	**#participants**	**#participant-training-days**
PRACE Training Centres	955	2,608	26,081	73,778
Seasonal Schools and workshops	45	175	2,161	8,665
International HPC Summer School	11	54	808	3,980
On-demand events	14	43	388	1,272
TOTAL (short courses)	**1,025**	**2,880**	**29,438**	**87,695**
Summer of HPC	Organised annually for 10 years since 2013; mentored 289 students in Europe.			
MOOCs	8 MOOCs developed since 2017; a total of 37,929 people joined these courses.			

Table 1: All-time PRACE training achievements in numbers.

In the EuroHPC and exascale eras, HPC competences represent the key assets for Europe to build its competitiveness in the global race of innovation and progress. PRACE has been the dominant player in the European HPC training landscape as a provider of a comprehensive training programme and impressive material storage. The PRACE training has consisted of several activities: short training courses, longer training events, mentoring programme for students, online learning materials, Massive Online Open Courses (MOOCs), and online portals/resources for training. The intended audience for PRACE training was set as academia and industry since the beginning of PRACE training history. WP4 has carried out and coordinated the training and education activities enabling the European academic researchers and industry to utilise the computational infrastructure available through PRACE and provide the highest quality education and training opportunities for computational scientists in Europe. PRACE training has been focused mainly in interdisciplinary, advanced and intermediate level face-to-face HPC events at a global scale.

In this document, the activities of WP4 of the PRACE-6IP project are presented in detail. PRACE-6IP WP4 consists of three tasks. Each task has had an impact to the reviewed volume quality and scope of the training.

- Task 4.1 Training events: This task is responsible for organising the Seasonal Schools, on-demand events, the International HPC Summer Schools and the Summer of HPC programme;
- Task 4.2 PRACE Training Centres: The task consisted of the jointly-coordinated annual training programmes delivered by a network of 14 PRACE Training Centres around Europe, offering 100+ high-quality courses per year that are renowned in the European HPC community;
- Task 4.3 Online training: The task includes managing the PRACE Training and Events portals, developing the training section of the HPC in Europe portal [3], delivering Massive Open Online Courses (MOOC) on the Future Learn platform [4] and managing the CodeVault repository providing training material samples enabling trainers to find and use ready-made coding exercises and solutions.

The common objective for all training tasks has been the design and delivery of an extensive training programme for European research and industry. Each activity has provided the special means and impact planned for reaching the many target audiences set for PRACE training. In the last project year, the scope has been extended into covering the archiving of the PRACE training materials. This document describes and analyses the training activities and summarises the outcomes during the whole PRACE-6IP project in detail.

Section 1 describes the training activities and their impact. Section 2 describes the effects of the COVID-19 pandemic on the PRACE training and WP4's reaction to those changes, as well as the outcomes and impact in training practices. Section 3 provides a thorough summary of the Seasonal Schools activities. Section 4 reports the on-demand events. Section 5 describes the summer internship and mentoring programme of the Summer of HPC. Section 6 lists the outcomes of the International HPC Summer Schools. Section 7 explains the PRACE Training Centres and illustrates the impact and scope of these activities. Section 8 focuses on the online training activities within PRACE 6IP. Section 9 highlights the latest developments of the PRACE Training Portal, and the related Events Portal, which represents the online hub for PRACE training activities as well as the archiving process of the PRACE training legacy. Section 10 covers PRACE training collaborations with other stakeholders such as CERN, SKA, GÉANT, RedCLARA, FocusCoE, CASTIEL, ETP4HPC and EuroHPC, etc. Finally, some concluding remarks are presented in Section 11.

2 The Impact of COVID-19 Pandemic

The COVID-19 pandemic has affected the PRACE training events more than any other single phenomenon. The impact on travel and the cancellations of large gatherings, hit the PRACE training activities hard in 2020, and ever since new training methods had to be invented and implemented to be able to carry out the training activities. WP4 and PRACE Training Centres mostly reacted in a very pragmatic manner, by adapting online training procedures where and whenever possible.

Since March 2020, PRACE-6IP internal meetings and training events were dramatically reduced due to the extreme situation caused by COVID-19 all over Europe within the past two years. The PRACE-6IP project reacted to this situation by providing altogether six directives to ensure that all project internal meetings and training events were to be organised in an online or hybrid (face-to-face plus online) format. These project guidelines have been adapted to the changing situation, also building on growing experience of the PRACE partner with online and hybrid events. With the decline in new COVID-19 infections in spring 2022, the project recognised this encouraging development and adapted the guideline allowing for face-to-face PRACE events to be organised again as long as its pan-European target audience had access to these events. This meant events needed also to cater for those who could not participate in person due to local COVID-19 related regulations, i.e. by accommodating online participants to the same event in such cases. All events also had to consider for an easy transition to pure online events in case of a worsening situation, e.g. during autumn or winter 2022.

This meant clarity to the course organisers, and caused the following efforts in certain activities listed in Table 2 below to take place as response to the pandemic:

WP4 Activity	Impact or response
PRACE Training Centre courses	Some PTC courses were postponed or cancelled, but maximal effort was made in transforming most of courses online. 305 online courses have been delivered in PRACE-6IP. Online delivery has been the dominant course format. Hybrid or face-to-face format was regarded as an extra bonus.
Seasonal Schools	The PRACE Seasonal Schools 2020-2022 had to be postponed and rescheduled but all of them were delivered online or in a hybrid mode.
Summer of HPC 2020-2022	After consultation with students and mentors, the online format was adopted where student projects were being supervised remotely by mentors. The latest 2022 edition took place in hybrid format.
International HPC Summer School	The 2020 International HPC Summer School, originally scheduled to take place in July in Toronto, was postponed to 2021 and was delivered as an online event to three continents in different time zones.
EuroHPC Summit Week – Hands-on Workshops	Prepared hands-on training workshops during the EuroHPC Summit Week 2020 were cancelled along with the event.

Table 2: Summary of WP4 activities affected by the COVID-19 pandemic, and some of the actions taken in response

2.1 Lessons learned during the Pandemic

The most important lesson learned was the pressing need for a change in the training style, which was demonstrated in the changed mindset of trainers. The willingness of the trainers was needed to enable their shift from their normal teaching style to online training setting, which

was not ideal for them and sometimes totally out of their original training comfort zone. Mostly the traditional face-to-face HPC training is found most useful and natural in the advanced and intermediate course levels; it was crucial that the events were still adopted despite the discomfort and enormous extra work and the adoption of new tools.

The second important lesson learned was the sharing of best practices in online events. Online events and material sharing to HPC trainers around the world paid off and was an important tool in introducing new ways of teaching to a larger audience. Training of the online training tools and interactive trainer skills were also used to facilitate the change. Online training methods and tools were introduced and shared by professionals, trainer peer groups and colleagues and then adopted into HPC training when relevant and feasible.

Some examples of e-learning tools collected in the PTC network: online learning platforms (mostly Moodle), Zoom/Teams videoconferences, recordings, pre-recorded training lecture videos and online materials, quizzes, breakout rooms, online partner work exercises, discussion forums in the Learning Management Systems (LMS), slack channels, trainer online advisory channels, white marker boards to assist the code and math demonstration, coderunner programming teaching tool, collecting feedback with Mentimeter, course interaction boosting with avatars and game applications, and more. The MOOC and online course production was more work intensive but has also given the trainer a much larger audience, increased the number of participants and expressed the increased need of interactivity in every possible manner in online training.

Since COVID-19 pandemic the adaptation to various online training tools have been experimented. The aim of experiments was using and adopting the full potential of online training tools to facilitate online PRACE training.

In addressing the recommendations from the interim review, a list of tools (Annex 12.1) were tested and adopted into use based on availability, capabilities and resources of each PTC. Most university-based centres have the resources available but the need for extra support staff has been found as a bottleneck for PTCs. Moreover, the effort expended to deliver online courses had been larger than anticipated due to the need of more trainers required to manage online courses, breakout rooms and exercises. Some learning tools are also better suited for longer-term education rather than the short courses PRACE offers. Nevertheless, some training for online tools and digital pedagogy as well as interactive trainer training was offered to PTCs during the reporting period 2019 and 2021.

The availability of all training material and easy to find for self-study has also been on WP4 task list for some time. The question about the ownership of the training material is still valid. PRACE has been given the resources for the delivery but not for the development of the course material. The copyright of the courses sometimes belongs within the PTC centres or individual trainers and thus PRACE does not have the right automatically to share materials publicly, i.e. not all training content can be placed online.

Typically HPC courses have mostly been very long making the recordings very long as well. The online delivery of long PowerPoint presentations or trainer lecture videos has not proven to be a very popular and effective way of sharing courses to self-study. Participants prefer shorter pieces of training sets, which is understandable. Both ways of delivery have been tested. Also some course materials have also been edited for shorter videos with accessibility regulations considered. This takes a lot of extra time of support staff, which is not always available, as well as the accessibility law forcing the trainers to use transcripting tools explaining figures, tables etc., but again, this has proven to be very time consuming and expensive way of producing the material, because the automated transcript tools are still not efficient enough and required a lot of hand work correcting the transcripts.The list of the various tool used in the PTCs to support the online learning experience can be found in Annex 12.1.

3 PRACE Seasonal Schools

PRACE Seasonal Schools have been organised as part of the PRACE educational programme since 2008, offering top-quality face-to-face training events around Europe, and designed to improve the necessary skills needed in the use of the HPC ecosystem. The Seasonal School topics have ranged from generic intermediate to advanced programming techniques, to more specialised topical schools that e.g. focus on a specific topic, such as big data, or offer discipline specific parallel tracks.

Since 2012, the Seasonal Schools have been run simultaneously with the PRACE Training Centres offering training opportunities mainly in countries where PTCs were not in operation. To maximise PRACE training coverage around Europe, PTC hosting countries had a lower priority in the selection process for hosting Seasonal Schools.

3.1 Selection Process

In order to ensure fairness and transparency, the selection process of the hosting countries for the eight available Seasonal Schools slots in PRACE-6IP, was the same as that 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 only 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.

3.2 Seasonal Schools implemented

The PRACE-6IP MB had 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. Due to the COVID-19 pandemic, the planned schedule of the schools needed to be revised (see interim PRACE-6IP training report [2]).

Ultimately, Table 3 shows the list of Seasonal Schools that were organised during PRACE-6IP. The Seasonal Schools with different target audiences were allowed to be organised in near-concurrent timeframes.

School	Location	Date	Main Subject
Autumn School 2019	Slovenia	September 2019	Big data and HPC
Spring School 2021	Belgium	April 2021	Introduction to OpenFOAM
Spring School 2021	Slovakia	June 2021	Modelling materials using HPC and AI/ML
Autumn School 2021	Bulgaria	September 2021	Fundamentals of Bimolecular Simulations and Virtual Drug Development
Autumn School 2021	Slovenia	September 2021	Big Data with Hadoop and Keras
Autumn School 2021	Austria	October 2021	GPU programming with CUDA
Autumn School 2021	Finland	October 2021	Harnessing the EuroHPC Flagship Supercomputers
Winter School 2021	Israel	December 2021	Converging HPC Infrastructure & Methodologies

Table 3: Seasonal Schools organised during PRACE-6IP

3.2.1 Autumn School 2019, Slovenia - Big data and HPC

This school took place 17-20 September 2019 in Ljubljana, Slovenia. The training focused on classical big data topics (using Hadoop and Rhadoop for big data management and analysis) and to very recent container technologies. The four-day PRACE Autumn School 2019 collected over 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' interests.

3.2.2 Spring School 2021, Belgium - Introduction to OpenFOAM

This school was conducted as an online event from 20-21 and 27-28 April 2021, due to pandemic restrictions. It was a collaborative organisation of five universities (University of Antwerp, Gent University, Vrije Universiteit Brussel, Hasselt University and KU Leuven) that form the Flemish Supercomputing Centre (VSC).

OpenFOAM is a popular open source software package for Computational Fluid Dynamics (CFD). It has a large user base across most areas of engineering and science, from both commercial and academic organisations. OpenFOAM has an extensive range of features to solve anything from complex fluid flows involving chemical reactions, turbulence and heat transfer, to acoustics, solid mechanics and electromagnetics. It is free-to-use numerical simulation software, including usage on HPC systems. During the 4-day event in total 30 attendees from six different countries participated in the 1st Spring School of PRACE-6IP.

3.2.3 Spring School 2021, Slovakia - Modelling materials using HPC and AI/ML

From 15-18 June 2021, the 2nd Spring School took place as an online event, due to the COVID-19 situation. However, it was decided to allow students to attend in person. The Slovak Academy of Sciences in Bratislava, Slovakia organised the event.

The mission of this Seasonal School was to design a programme that would cover theoretical concepts, ways of (parallel) computer implementation of pertinent algorithms, as well as efficient use of existing material science/periodic systems codes and program packages in HPC environment. The aim was to provide a crash course covering basic theory, HPC

implementation, showcasing typical applications and efficient ways of their (parallel) runs with lectures as well as hands-on sessions.

Utilization of Machine Learning workflow and various techniques was also a topic of interest, since it is being progressively applied to real chemical problems, such as discovery of new chemical compounds and materials with specific properties.

During the 4-day event, 32 participants from 10 different countries attended the course.

3.2.4 Autumn School 2021, Bulgaris - Fundamentals of Bimolecular Simulations and Virtual Drug Development

Following the COVID-19 pandemic outbreak, the 1st Autumn School of 2021, was planned as an online event, from 20-24 September. The school was organised by the BioExcel Centre of Excellence, the STFC Daresbury Laboratory, NCSA Bulgaria, and Sofia University and in partnership with AstraZeneca and NostrumBiodiscovery.

The week-long training event introduced the fundamentals of modern methods for biomolecular simulations - molecular dynamics (MD), 3D QSAR, integrative modelling, free energy and hybrid-QM/MM calculations. Widely used software applications (GROMACS, HADDOCK, PMX, ChemShell) were presented, and their usage on HPC facilities demonstrated. The school programme targeted applied scientists, who have little experience with computational methodologies and high-performance computing. It was suitable for junior researchers (post-graduates and post-docs) with a background in natural sciences and, in particular, pharmacy, biochemistry and biophysics.

Regarding participation, in total 165 attendees from 25 different countries were counted.

3.2.5 Autumn School 2021, Slovenia - Big Data with Hadoop and Keras

The 2nd Autumn School of 2021 took place from 27-30 September as an online event, because of the continuous restrictions due to COVID-19 and it was organised by the University of Ljubljana – Faculty for mechanical engineering. Due to the nature of computing course the participants were granted access to the local cluster HPCFS during the duration of the school for pre-/post- processing, job submission and calculations.

The PRACE Autumn School focuses on big data analysis with HPC using different approaches presented through Spark, Hadoop, RHadoop and TensorFlow. The success of the PRACE Autumnal School 2020 and the participants' feedback served as a basis for the programme design andhelped to achieve a better quality of the 2021 edition's programme.

In total, 22 people attended the course from 14 different countries.

3.2.6 Autumn School 2021, Austria - GPU programming with CUDA

From 4-7 October 2021, the University of Innsbruck (UIBK) and VSC (Vienna Scientific Cluster) Research Center of TU Wien, Austria (PRACE-6IP partner TU WIEN and its linked 3rd party UIBK), organised the Seasonal School in Austria as a hybrid event. There were 52 participants (34 in-person and 18 online) from 10 countries. The in-person part took place at the Campus Technik of the University of Innsbruck, Austria. For the online participants there was a separate videoconferencing instance available with the live-stream of the lectures from the main room and several breakout rooms for the exercises to facilitate collaboration within small groups of online participants.

Using GPUs can significantly improve the performance of many scientific codes. This Seasonal School addressed researchers from various domain sciences who plan to exploit the capabilities

of modern GPUs. As participants came from diverse fields, organisers focused not on just one use case but invited several speakers with different backgrounds to report on their successful projects of porting a scientific application to GPUs.

Attending this school equipped the participants with the necessary knowledge and tools such that they can make effective use of GPUs in their research. This included teaching the necessary programming paradigms. However, even more important, there was guidance to write correct and efficient code for GPUs. In addition, the trainers emphasised what needs to be done to port existing codes to use GPU acceleration. The course included many hands-on exercises such that concepts taught in the lessons could be applied immediately.

3.2.7 Autumn School 2021, Finland - Harnessing the EuroHPC Flagship Supercomputers

The 4th and last Autumn Seasonal School was conducted in Vuokatti Sport Resort, Sotkamo in Finland and organised by CSC – IT Center for Science Ltd as a face-to-face event from 11-15 October.

The PRACE Autumn School addressed the hot topics of the pre-exascale era of the HPC: programming GPUs, porting and optimising applications for GPUs and utilising machine learning methods in science. The organisers carried these out as three hands-on (learn-by-doing) learning tracks. The attendees were expected to pre-select the track that they were most interested in and to have the sufficient prerequisite information. The parallel learning sessions were supported by inspiring plenary talks on scientific success stories of utilising accelerated platforms. After the course the participants were expected to be familiar with modern GPU-accelerated supercomputers and the possibilities they offer.

Participation was active: 36 people took part in the course from 12 different countries.

3.2.8 Winter School 2021, Israel - Converging HPC Infrastructure & Methodologies

From 7-9 December 2021, the Inter-University Computation Center (IUCC) organised in Tel-Aviv, Israel the Winter School 2021 as an online event, due to the dynamic COVID-19 regulations and uncertainty.

The programme committee consisted of experts from the local HPC academic community, computational scientists close to the true need of local and regional users and computational scientists who had participated in PRACE programmes prior to this Seasonal School. The programme was designed to accommodate trainees with varying expertise levels and professional backgrounds and to give an overview in fundamental HPC topics alongside new trends in architecture, design and use cases of HPC in the cloud. Valuable input was solicited from younger students who had participated in PRACE training programmes.

A highlight of the programme was a series of HPC in the cloud sessions developed jointly with AWS Europe. AWS HPC solutions and developer architects led hands-on tutorials on a wide range of practical tools and subjects. This training model, based on collaboration between academia (IUCC/PRACE) and a commercial vendor (AWS), is perhaps one of the first of its kind. Of particular interest was AWS's presentation on how they achieved position #40 in the top 500 supercomputers in the world.

The course was attended by 76 participants coming from 20 different countries.

4 On-demand Events

The on-demand events organised by the PRACE-6IP project have been trainings specifically organised with the collaboration of research communities that have special needs for training and the expertise of PRACE trainers. Such targeted communities have been mainly the Centres of Excellence (CoEs). PRACE-6IP has continued the effort from previous PRACE Implementation Phases projects to collaborate with the CoEs in many different areas, including training. On-demand events could have been organised by any PRACE-6IP partner institution. The trainings were given in English to accommodate the international audience.

4.1 Selection Process for the On-demand Events

The selection process of the on-demand events has been lightweight, still ensuring the transparency of the process and event quality. The Call for the organisation of on-demand events was continuously open. Eligible partners sent their application forms filled in to the on-demand events evaluation committee.

The committee was obliged 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 was comprised of five members: one PRACE BoD representative, one PRACE-6IP MB representative, one PTC representative and two WP4 representatives. Task 4.1 leader coordinated and facilitated the process, without any power to influence the final decision.

Since the process for the selection of the on-demand events was lightweight, there was no need for PRACE-6IP MB approval after each decision of the committee. The PMO was 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 was from a PRACE partner involved in the proposal, the member was not allowed to participate in making the recommendation. The final decision was expected within 30 calendar days after the day of submission of the application.

4.2 Selection Criteria for the On-demand Events

The following selection criteria applied to the selection of the on–demand events:

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

4.3 On-demand Events Overview

Only two on-demand events were organised before the COVID-19 pandemic. The on-demand events typical funding model has been the funding or co-funding of expenses of face-to-face trainings. For this reason, pandemic breakout eliminated some of the driving factors for these events. Some of these type of on-demand event initiatives were simply cancelled and some

turned into online or hybrid events where PRACE collaborated with other projects and partners by contributing to a joint programme and pool of trainers.

This subsection summarises the on-demand events that took place during the PRACE-6IP project (Table 4).

Location	Date	Main Subject	Participants
Trieste, Italy	23-27 September 2019	EUDAT-PRACE Summer School on managing scientific data from analysis to long term archiving	26 participants from 19 countries
Espoo, Finland	9-11 October 2019	Advanced Gromacs, HADDOCK + PMXWorkshop	24 on-site + 10 on-line
Ljubljana, Slovenia	5-9 July 2021	HPC Workshop on Containers and Unikernels	Online event: 46 participants from 17 countries
		Total:	**106 participants**

Table 4: On-demand events during the reporting period of the PRACE-6IP project

4.3.1 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. The event was well received by the participants.

4.3.2 CSC-BioExcel – Advanced GROMACS, HADDOCK + PMX 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 were invited to bring up their own day-to-day research. Apart from enabling users the full use of all three software, the interaction with workshop participants with concrete research scenarios also served to foster collaboration between developers of the respective software packages. The event was well received by the participants.

4.3.3 University of Ljubljana - HPC Workshop on Containers and Unikernels

The workshop was jointly organised between University of Ljubljana, University of Oslo and CSCS and took place online due to COVID-19 restrictions.

Containers with the build-once-run-everywhere principle have become very popular for scientific use cases. The majority of HPC platforms for research now support container runtimes. Unikernels are very lightweight virtual machines that provide hypervisor level isolation and near to native performance. This workshop aimed to introduce several container platforms (Docker, Singularity, Sarus, Charlie cloud) and provide hands-on MPI and GPU examples. In addition, there was a demo on Unikernels. The event was well received by the participants.

5 Summer of HPC Programme

The PRACE Summer of HPC (SoHPC) [5] outreach and training programme for late stage undergraduates and/or master students had its seventh edition in 2019. The programme has aimed to ensure a positive experience for all students and 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 presented with short reports and video presentations. Two awards are presented to the most successful participants at the award ceremony.

5.1 Summer of HPC 2019

The SoHPC 2019 edition transitioned from PRACE-5IP to PRACE-6IP in a sense that preparations for programme launch started under PRACE-5IP with a Call for Projects to hosting sites and then a Call for Participation 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 to be hosted by 11 PRACE partners. Site coordinators organised travel and accommodation for the students. The training week was organised at the CINECA HPC centre in Bologna as a start of the students' summer project work.

Figure 1: 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 the SoHPC coordinating team to monitor the progress and advertise achievements on SoHPC Facebook and Twitter accounts. During the summer, students wrote 91 blog posts about their project and work at hosting sites. The programme finished at the end of August 2019 with project presentations on YouTube [6]. From the project's work students wrote popular scientific articles describing their achievements, which will be used by PRACE

press team for outreach communication and PRACE Digest highlights. The SoHPC Awards selection panel was formed and decided the winners of the SoHPC 2019 ambassador and best performance awards. The award ceremony was held on 6 November 2019 at the PRACE office in Brussels. The final reports of the SoHPC 2019 projects were published online [7].

5.2 Summer of HPC 2020

The 8th edition of the SoHPC 2020 programme was prepared and 25 project proposals with 12 HPC hosting sites provided mentoring. The preparations and the timeline were similar to the previous SoHPC editions. During the selection of 81 received applications, the COVID-19 situation forced the selection committee to convert the programme into online edition. The mentors were asked to double the number of participants per project. Before selection, all participants were asked if they still wanted to participate in the online edition. After receiving positive confirmation from all participants, 50 students were selected for 25 projects to work in pairs as a team on the same or adapted project goals. The training week was prepared by VSC, Vienna along with Slack channels for collaborative chats for each project. The online training week included many social activities, including yoga time break sessions, virtual visits to the VSC supercomputing facility, Mural wall collaborations and Zoom breakout rooms for common work with many instructors available to help when needed at hands-on sessions (see Figure 2 for a screenshot of and on-line session). The final reports of the SoHPC 2020 projects was published online [8].

Figure 2: Summer of HPC 2020 online training week participants

5.3 Summer of HPC 2021

The 2021 edition of SoHPC project was again organised as an online event due to the continuing pandemic. The Summer of HPC 2021 was also the largest event. It started with 65 participants and their mentors at 14 PRACE HPC sites who worked on 33 projects. Participants spent two summer months working on their projects related to PRACE technical or industrial work and produced a final report and video of their work results. An online kick-off training week was organised by the Irish Centre for High End Computing (ICHEC) (see Figure 3). The 2021 SoHPC final reports were published online [9].

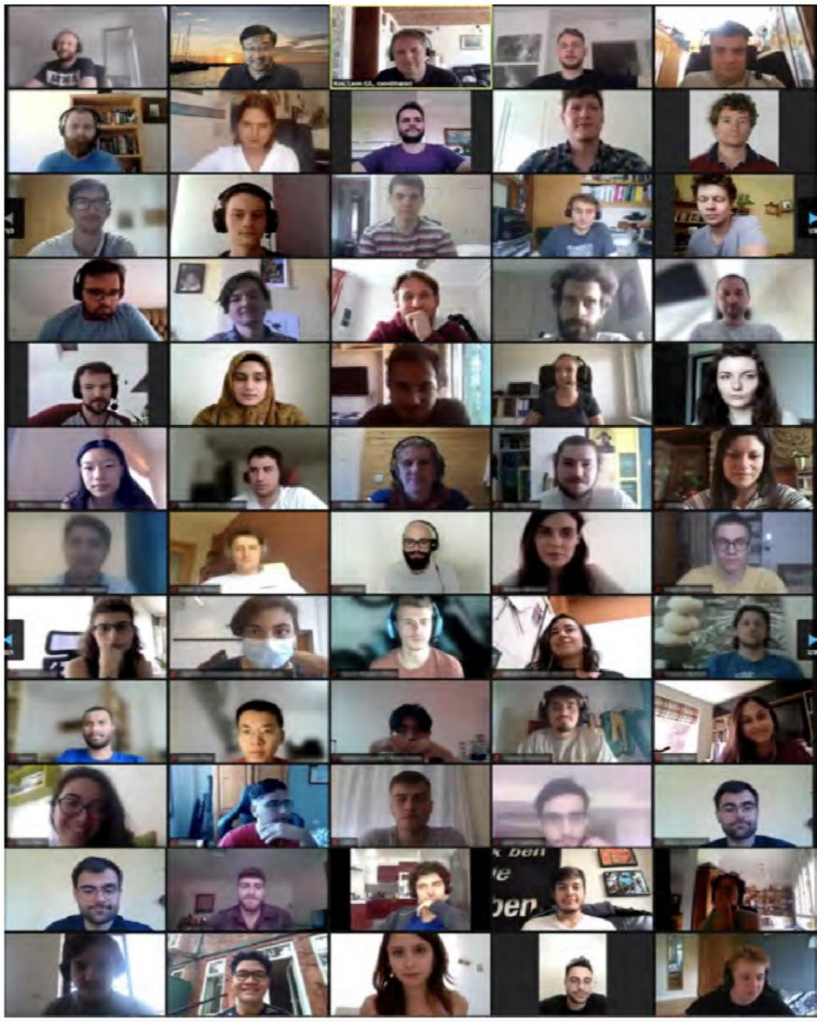


Figure 3: Summer of HPC 2021 online participants and some of their mentors

5.4 Summer of HPC 2022

The SoHPC 2022 was prepared partly as an in-kind contribution by the volunteered WP4 partners. The SoHPC call was initiated again in January 2022, during the extension of PRACE 6IP. Altogether 30 students started and worked on 21 projects. The mentors from PRACE hosting sites provided both on-site placement and face-to-face mentoring. The SoHPC2022 started with a hybrid study (online and onsite) week hosted by the University of Ljubljana starting on 4 July 2022. Half of the students participated in person while thehalf of students participated online. The final reports of the SoHPC 2022 projects were published online [10].

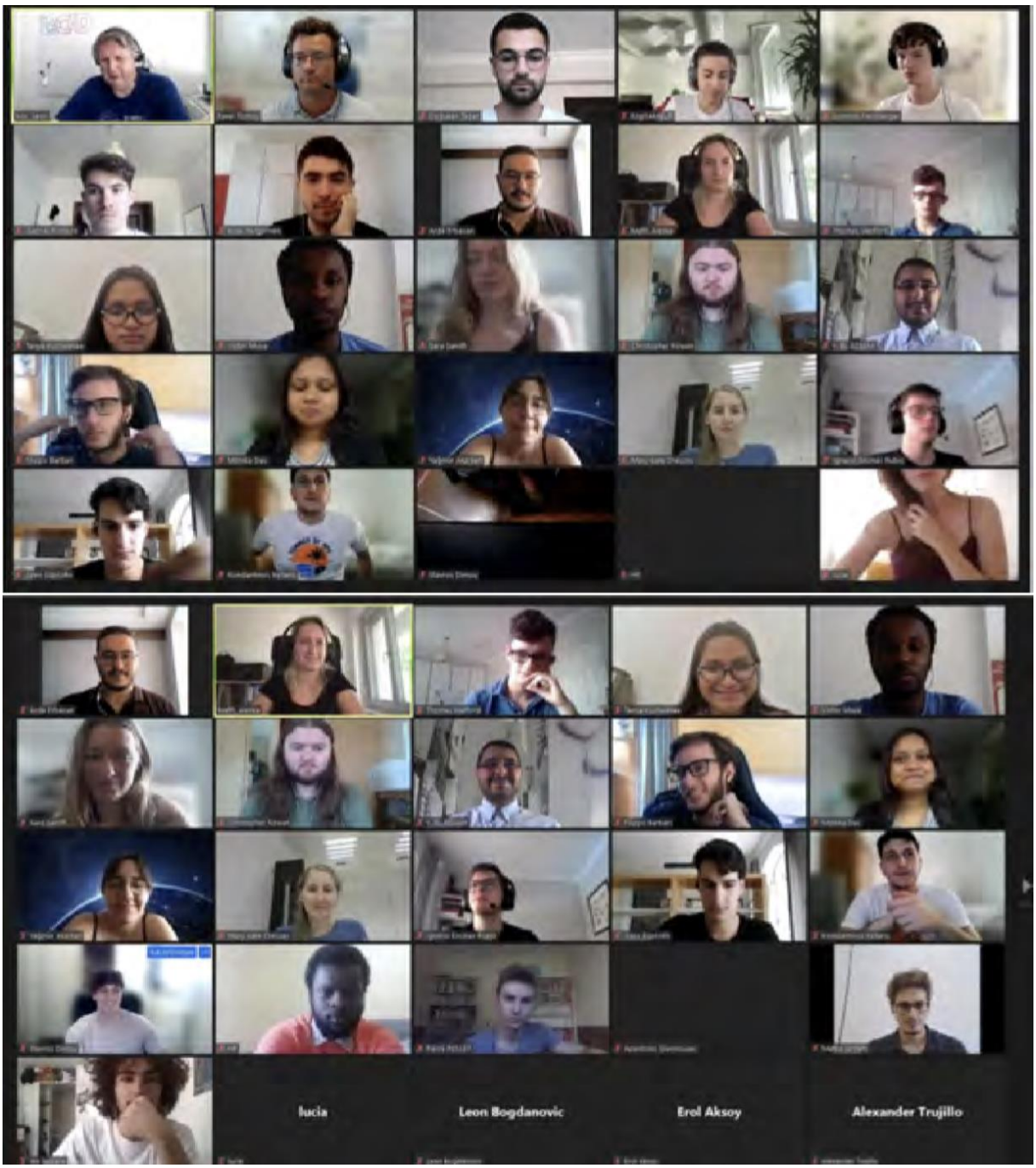


Figure 4: SoHPC 2022 participants and some of their mentors at the online training week

From the PRACE-6IP experience we can conclude that the popularity of Summer of HPC as a summer learning experience has not been decreased by the online format, but the interaction between the students and trainers needed to be emphasised in every possible way to keep the programme alive and the student support system had to be sustainable. The community building aspect has been almost as important attraction to the programme as the skills learned and needs to be taken into account in international events and social media platforms.

6 International HPC Summer School

The 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 over a decade [11]. The PRACE-6IP project has sustainably supported this collaborative event, typically held in the summer months of June/July, for four years (2019 to 2022).

The objective of the annual series of international summer schools was 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 were 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 visualization;
- Canadian, European, Japanese and U.S. HPC-infrastructures.

Since this has been an ongoing annually, with similar objectives every 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 has been 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 with an established system of processes that were implemented every year to execute the event with considerable success. This included 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 were 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 has typically attracted 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 Applications 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 was 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 5: 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. While the content of the school has remained roughly similar to previous years 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 has been a huge success which has been 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 were 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 (cancelled)

The International HPC Summer School 2020 was originally planned to take place in Toronto, Canada on 12-17 July. Similar to previous years, the organisation of the event started almost nine months earlier, in 2019. The Call for Applications 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 the 30 available seats at the school for Europe. The same evaluation committee and criteria were used 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 caused the planning committee to adopt a cautious approach. By May 2020, it was clear that a face-to-face event would not be feasible and selected candidates were asked for their preference to either attend an online version of the school, or to defer the event, and their seats, until 2021A clear majority preferred for the latter hence the school was cancelled for 2020 and deferred to Toronto, 2021.

6.3 International HPC Summer School 2021 (online)

The planning for the 2021 school in Toronto started similarly as described in the previous paragraphs and it was expected that accepted candidates from 2020 were offered and they would accept the seats automatically. As the pandemic still persisted, finally after discussions with all parties involved, an online version of the school was offered to students in summer 2021 and the final decision was made to host the 2021 International HPC Summer School as an online event over 18-30 July. After the selection of participants from across three continents, most agreed to take part in the 2021 online event, thus there was no need to organise another Call for Applications. The event itself underwent significant changes in terms of format, pedagogical approaches, etc. but covered similar topics as before, e.g. a mix of scientific and technical talks/exercises combined with networking and mentoring, and was delivered to 64 participants online. The virtual summer school was conducted in separate sessions to accommodate participants from different time zones across continents. To achieve this, every scientific talk was replicated in two time slots – one streamed live, the other re-played, where different "shifts" of instructors were organised for practical sessions. While the feedback from participants has generally been positive, there were some aspects of the school which have suffered in terms of impact due to the online, more fragmented nature of the 2021 event.

6.4 International HPC Summer School 2022 (Greece)

The planning of the 2022 edition started optimistically but with similar uncertainty of pandemic situation and its effects on the school. The 12th International HPC Summer School took place in Athens during the extension of PRACE-6IP project and was hosted by the Partnership for

Advanced Computing in Europe (PRACE) and the local host was GRNET responsible for the local organisation. Altogether 76 participants including graduate students and postdoctoral scholars from institutions from Canada, Europe, Japan and the United States took part in the school held on 19-24 June 2022 at Novotel Athenes in Athens, Greece. The summer school was sponsored by PRACE, the Extreme Science and Engineering Discovery Environment (XSEDE), the RIKEN Center for Computational Science (R-CCS) and the SciNet HPC Consortium. The feedback of the event was very positive. Students have found the international representation and the mentoring programme adding unique value to the event. The 76 participants came from Canada (13), 17 countries in Europe (32), Japan (5) and the U.S. (26).

Figure 6: Participants of the International HPC Summer School 2022, Athens, 19-24 June 2022

7 PRACE Training Centres

The mission of the PRACE Training Centres (PTCs) was to serve as European hubs of high-quality training for researchers working in the computational sciences. The PTCs provided and coordinated training and education activities needed to achieve the best utilisation of the PRACE Research Infrastructure by the community. The PTCs promoted a common PRACE brand, representing the whole PRACE community rather than only the hosting sites, and implemented 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, and referred to as the PRACE Advanced Training Centres. This was expanded in 2017 to include four additional centres, and all centres re-branded as PRACE Training Centres. In 2019, the PRACE Management Board (MB) agreed to a new call for establishing additional PTCs. Four partner countries, Austria, Belgium, Slovenia and Sweden were successful in their application to host PTCs. Therefore, as of December 2019, the network of PTCs consists of partner sites from 14 countries.

Since their conception, PTC courses have built a preeminent reputation for delivering some of the best quality courses that are open to the European HPC community. The PTCs have been a landmark achievement of PRACE that have reacted quickly to adverse conditions (e.g. COVID-19 pandemic) and were sustained through different PRACE project extension periods, such is their importance to the community.

7.1 Selection of new PTCs

In 2019, the PRACE-6IP 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; later on due to release of funding from other project activities that could not be undertaken as planned, partial financing of the new PTCs was approved by the PTRACE-6IP MB and implemented. 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 six 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.

7.2 Implementation of the PTC Programmes in 2019-2022

From May 2019 to December 2022, the PTCs collectively delivered 396 courses, representing 1,045 days of training with 13,225 participants, which amount to 35,910 participant-training days. This period coincides with implementation of the PTC's 2019-2020, 2020-2021 and 2021-2022 annual programmes. Key statistics from these programmes are shown in Table 5 which also includes statistics from the very first establishment of the PTCs (formerly the PRACE Advanced Training Centres).

While the COVID-19 pandemic has had an obvious impact in course deliveries, as highlighted below, the PTCs have reacted constructively and effectively by pivoting rapidly to online courses; only 25 courses (out of 100+ courses PTCs deliver per year) had to be postponed or cancelled due to COVID-19.

Despite additional efforts in adapting to and delivering online courses, the PTCs has committed to delivering a large proportion of its courses online. Online delivery have also resulted in some of the highest levels of participation at PTC courses and in particular attracting some of the highest proportion of attendees from all around Europe, i.e. those who would otherwise have to travel across country borders to attend the courses if they were in-person. Since COVID-19 restrictions have been deemed sufficiently relaxed in August 2022 – participants could hence travel to PTC courses with minimal hinderance – over 70% of PTC courses have been maintained as online courses, i.e. there is no expectation whatsoever that the PTCs will return to the pre-COVID *status quo* where online courses were rare occurrences; there is a firm commitment to delivering a large part of the PTC programme online. Over the course of the PRACE-6IP project, 305 PTC courses (77% of total) have been delivered online.

Programme	Pilot	2012-13	2013-14	2014-15	2015-16	2016-17	2017-18	2018-19	2019-20	2020-21	2021-22	2022 Aug-Dec
Number of PTCs	6	6	6	6	6	6	10	10/14	14	14	14	14
Date from…	Mar-2012	Aug-2012	Aug-2013	Aug-2014	Aug-2015	Aug-2016	Aug-2017	Aug-2018	Aug-2019	Aug-2020	Aug-2021	Aug-2022
Date to…	Jul-2012	Jul-2013	Jul-2014	Jul-2015	Jul-2016	Jul-2017	Jul-2018	Jul-2019	Jul-2020	Jul-2021	Jul-2022	Dec-2022
Number of courses	19	71	81	77	73	78	93	99	81	121	124	38
Number of online courses	0	0	0	0	0	0	0	0	22	121	124	25
Total duration (days)	56	204	233	219	203	215	244	261	226	323	310	114
Number of participants	511	1,547	1,682	1,786	1,567	1,658	2,259	2,499	2,502	4,954	4,028	1,088
Number of participant-days	1,715	4,702	5,187	5,384	4,601	4,881	6,121	6,690	7,351	13,626	10,212	3,308
Female (%)	-	12.9%	14.4%	16.3%	17.6%	19.3%	21.0%	19.3%	20.9%	20.3%	21.7%	21.9%
Non-academic (%)	-	9.9%	12.3%	15.6%	22.2%	19.4%	18.5%	25.0%	12.5%	19.7%	22.6%	25.4%
Non-host country (%)	-	20.6%	25.4%	29.5%	16.3%	16.2%	21.9%	15.4%	29.6%	53.5%	59.9%	54.9%
Non-PATC country (%)	-	13.8%	17.7%	19.9%	8.9%	11.9%	8.7%	7.5%	14.7%	25.2%	32.3%	44.1%
Feedback response rate (%)	-	63%	64%	53%	52%	65%	53%	52%	48%	39%	41%	41%
Average overall rating (0 – waste of time; 10 - excellent)	-	8.5	8.4	8.4	8.4	8.5	8.5	8.4	8.2	8.0	8.3	8.4

Table 5. Key statistics from the implementation of PTC programmes from 2012 until 2022.

In the table above, the "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.

7.2.1 The 2019-2020 PTC Programme

The 2019-2020 PTC programme was originally conceived to deliver 104 courses that represent 265 days of training. Table 5 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 2017-2018 programme and from 10 to 14 from the 2019-2020 programme onwards.

The statistics shows that while the number of courses has been reduced due to the onset of the COVID-19 pandemic, 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 (discussed in Section 7.3).

7.2.2 The 2020-2021 PTC Programme

Early planning for the 2020-2021 PTC programme was carried out before the onset of the COVID-19 pandemic. The programme contained a diverse range of courses that covered comprehensive aspects of HPC performance engineering and parallel programming skills. This was complemented by some domain specific courses (often in collaboration with the CoEs) and those that combine HPC with Big Data and machine learning.

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 allowed) format was set as the default for all PTC courses until the end of 2020. For 2021 courses, the inherent preference was for online delivery. The ability to deliver a course in hybrid face-to-face and online format, or face-to-face format only, was treated as an exception rather than the rule.

The 2020-21 programme delivered 121 courses representing 323 days of training which attracted a total of 4,954 participants (i.e. 13,626 participant-days of training). All courses were delivered online with the exception of a handful of events where hybrid (face-to-face and online) delivery was used. This was the first full PTC programme that was delivered online and had the highest level of participation per course than any other PTC programmes in the past. Similar to the 2019-2020 programme, the online courses also attracted large numbers of "visiting" participants who are based outside the hosting country (of the PTC institution), which is examined in Section 7.3.

7.2.3 The 2021-2022 PTC Programme

The 2021-22 PTC programme faced many of the same issues and challenges compared to its predecessor, in that there was a great deal of uncertainty whether face-to-face training can return but there was nevertheless a readiness from all the PTCs to deliver all courses online. Again the collective programme was devised to cover a wide range of HPC and related topics, providing a

broad spectrum of HPC programming and performance engineering courses as well as those covering topics to increase productivity (e.g. using Python in a HPC setting) or to scale up AI workloads. In addition, there were coureses aimed specifically at optimising for architectures of EuroHPC systems, or based on the particular system itself (e.g. optimising for the AMD architecture and workshop on LUMI).

This programme delivered 124 courses representing 310 days of training which attracted a total of 4,028 participants (i.e. 10,212 participant-days of training). The level of participation, while at a somewhat reduced level compared to the 2020-21 programme (with an unusual number of large events where 27 courses had 50+ participants), remains to be high compared to face-to-face courses (see also Section 7.3).

7.3 The Shift to Online Course Delivery

The interim training report of the PRACE-6IP project had made a preliminary analysis of some of the different characteristics of face-to-face versus online courses based on only the 2019-20 programme [2]. However, that was based on a sample of 21 online courses. With additional data now available, Table 6 summarises the same key attributes from face-to-face courses (two years prior to travel restrictions induced by the pandemic in March 2020) versus online courses (two years after March 2020).

The natural, intuitive expectation is that online courses would generally attract more participants in general and from abroad because the barrier to entry due to travel is removed. Indeed, the level of participation at online courses is 50-60% higher compared to face-to-face courses (adjusting for slight differences in number of courses being compared). For online courses, it can be seen that more than half the participants were from countries outside that of the course provider. Online courses also attracted many more participants from countries that were not hosting PTCs compared to face-to-face courses, which is significant given that there were 14 PTC hosting countries compared to just 6 from 2012 to 2016. All of these trends point to the successful adaptation and implementation of the PTC training programme to serve a more diverse popuplation of HPC users and potential users around Europe.

	F2F courses	Online courses
Period	Apr 2018 to Mar 2019	Apr 2019 to Mar 2022
Number of courses delivered	201	216
Number of participants	4,977	8,250
% of participants from outside hosting country	17%	55%
% of participants from non-PTC hosting countries	8%	26%

Table 6: Comparison of face-to-face versus online PTC courses (before/after onset of COVID-19 pandemic) by key statistics on level and geographic distribution of participation.

The pivot to online courses by the PTCs has been challenging with some very valuable lessons learned. 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.

7.4 PRACE Advanced HPC Workshop

While the initial pilot of this advanced workshop was intended to be a face-to-face event, it was not possible to organise this during the PRACE-6IP project. Hence an online version of a special advanced level HPC track of courses were organised as a substitute to the face-to-face event. The workshop consisted of three online training events on advanced HPC topics over May-June 2022. The advanced track began with the Message Passing Interface (MPI), the dominating programming model, continued with node-level performance optimisation and finished with hybrid programming.

A total of 30 participants took part in the advanced workshop which was comprised of the following events:

- Parallelization with MPI at VSC (TU Wien), 17-20 May 2022 (in cooperation with HLRS);
- Node Level Performance Optimization at CSC, 7-9 June 2022 (in collaboration with Intel and AMD);
- Hybrid programming in HPC - MPI+X at LRZ, 22-24 June 2022 (in cooperation with HLRS, NHR@FAU and VSC (TU Wien)).

The prescribed workshop enabled participants to be immersed in low-level, advanced topics that are key to optimising codes and scaling applications on some of the largest supercomputers in the world. All the advanced courses included effective and personalised, practical hands-on sessions with relevant exercises. The courses included also small group breakout rooms.

8 Online Training

The activities of online training consisted of ongoing activities such as:

- Maintaining and developing the PRACE portal as well as PRACE Training and Events Portals [12],[13];
- Participation in the development of European HPC in Europe Portal [3];
- Preparing the students experience and usability of material for everyday training use as well as for archiving PRACE training material for long time on data storages such as Zenodo [14].

8.1 Massive Open Online Courses (MOOCs)

PRACE-6IP WP4 aimed to develop two to five additional MOOCs hosted on the FutureLearn platform [4]. The Short MPI course, that started development in PRACE-5IP and entered second run in October 2020 was upgraded with a new "full" (4 weeks) course: "One-Sided Communication and the MPI Shared Memory Interface". The "FORTRAN in scientific computing" course was developed by CENAERO, KU Leuven. A third MOOC "GPU programming for scientific computing" was developed by University of Luxembourg. The fourth MOOC "Introduction to parallel programming" was developed by University of Ljubljana.

Each existing 5-weeks MOOC was offered twice a year with constant improvements by each MOOC in years 2019-20. In 2020 the courses were offered over a more prolonged period to address COVID-19 situation as constant offering with facilitation provided by instructors. Courses remained available for learners to join at any time, and they could start learning immediately. The courses will remain to be running in this way, unfacilitated, and will only need a start of a new course run if update of the content is needed. Overall, over 22,500 participants enrolled in eight PRACE MOOCs listed in Figure 7, with key statistics about participation in these MOOCs shown in Table 7.

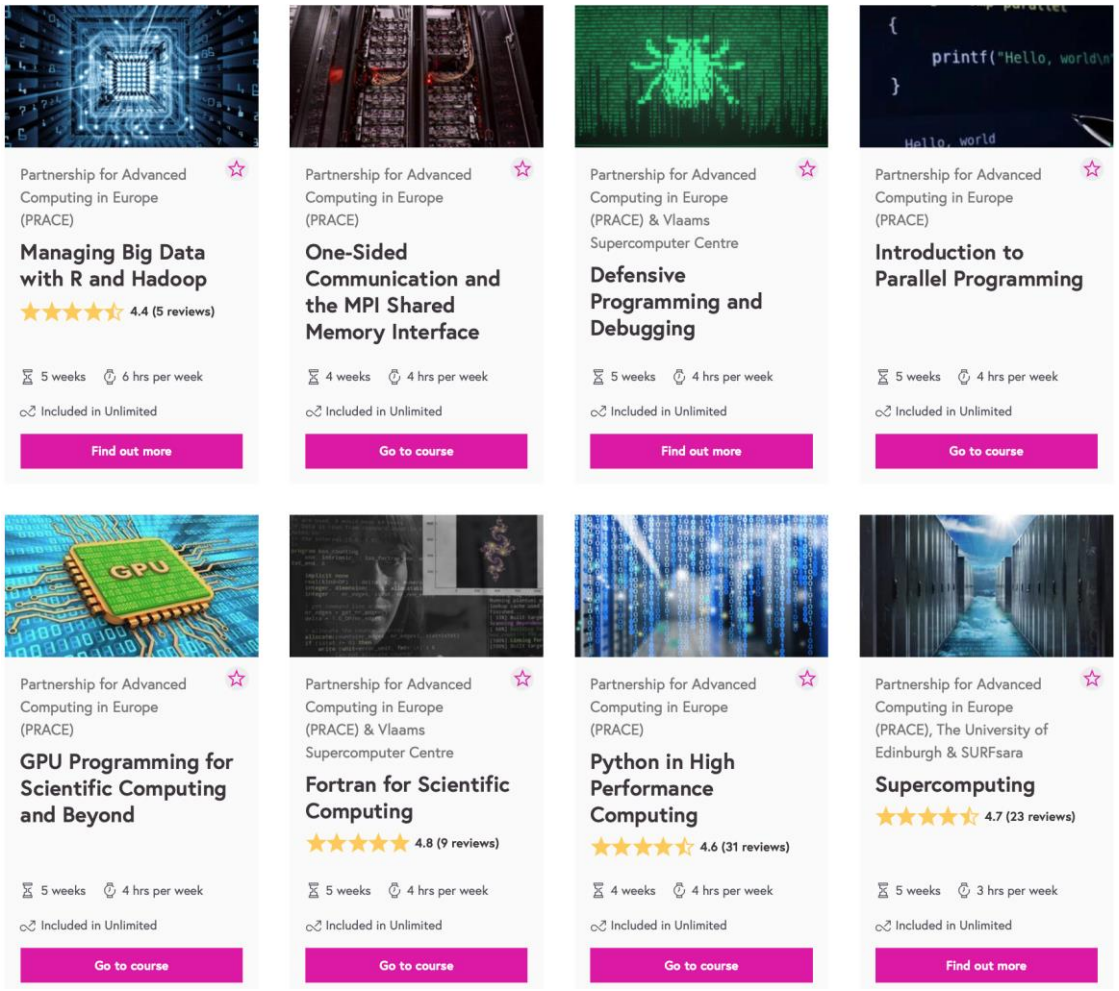


Figure 7: Dashboard of all PRACE MOOCs with trailer introductory videos

Some of the more established courses (e.g. managing Big Data, Python in HPC, Fortran for Scientific Computing, and Supercomputing) received more joiners than newly developed courses (e.g. one-sided communication and GPU programming.) that were introduced late 2021 and early 2022. A peak of interest for the courses was observed during the Covid-19 pandemics in 2020.

Course	Big Data	1Side MPI	Def. PrDe	Intro ParP	GPU f/ SC	Fortran for SC	Python HPC	Super Comp	Total
Joiners	4246	353	4401	830	375	866	6,843	4488	**22402**
Leavers	396	15	569	65	44	70	582	494	**2235**
Learners	2579	237	3034	707	279	737	4974	3385	**15932**
Active Learners	1265	111	1464	334	141	460	3254	2093	**9122**
Social Learners	452	28	316	75	25	166	714	653	**2429**
Learners with ≥50% steps	177	24	155	47	28	88	958	544	**2021**
Learners with ≥90% steps	78	18	61	29	21	53	656	319	**1235**
R-Index	0,236	0,334	0,197	0,261	0,256	0,250	0,327	0,331	

Table 7: Joiners and learners statistic of 8 MOOCs listed in Figure 7 during the PRACE-6IP (2019-2022).

From Table 7 we can see large number of learners with small numbers of leavers in total. The Course Retention Index (R-Index) show 20 % to 33 % of active learners who have completed an equivalent portion of the course. The span of R-Index differs from specialised (debugging, Fortran) to popular (Python, Supercomputing) topics. The topic on one-sided MPI with lowest number of learners got the highest R-Index because the topic attracted MPI specialists. The online nature of MOOCs leaves freedom to learners on what sections to complete and follow and they were able to attract a much larger, diverse audience compared to face-to-face courses.

9 Training and Events Portals

PRACE had launched and put into production a one stop shop for news and information of its training activities. The PRACE Training Portal [12] is tightly integrated with the PRACE Events Portal [13] which manages the information, registration and feedback collection of PRACE related events. These are complemented with the PRACE Material Portal [15] that serves as a repository for training materials.

9.1 Events Portal

The Indico software running the Events Portal has required constant maintenance and reaction to updates which often could have caused the site to change its behaviour which interfered with operation and needed to be fixed quickly. To avoid common errors during upgrades, a test infrastructure has also been maintained. These upgrades often introduced new and useful features requiring support of administrators, along with keeping the system secure. The latest version now supports tagging of registered users and offers global search functionality to enable easier access to events of specific topics.

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

The site functionality has been supported and integrated with PRACE Remote Platform pilot by using Single Sign On (SSO) method called ‘Edugain’. It has been developed and offered by GÉANT, and it 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 PRACE Remote Training 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 more easily. All of these new functions were developed with using proper edugain based access measures.

During the 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 [16], which has been 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.

The 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.

Finally, there was a concerted effort in the extension phase of the PRACE-6IP project to migrate some of the training materials that have been created or used during training events organised by PRACE. It is important to note that PRACE often do not have "ownership" of the materials at its training events, e.g. PTC courses are typically developed by the hosting institution, while PRACE supports their execution and delivery. Nevetheless, the latest, updated training materials from the PRACE events [13] and materials [15] portals have been migrated to the Zenodo repository [14]. This ensures future access to such materials beyond the end of the PRACE-6IP project.

Another point to note is that these materials are likely more useful for future trainers (e.g. those looking to develop or provide their own courses) and historians, rather than those who are learning HPC (though some might find certain materials useful regardless, or as a quick reference). For the latter audience the PRACE MOOCs should offer a more valuable learning resource. The materials on Zenodo should also offer a path towards their integration into a future HPC training materials portal.

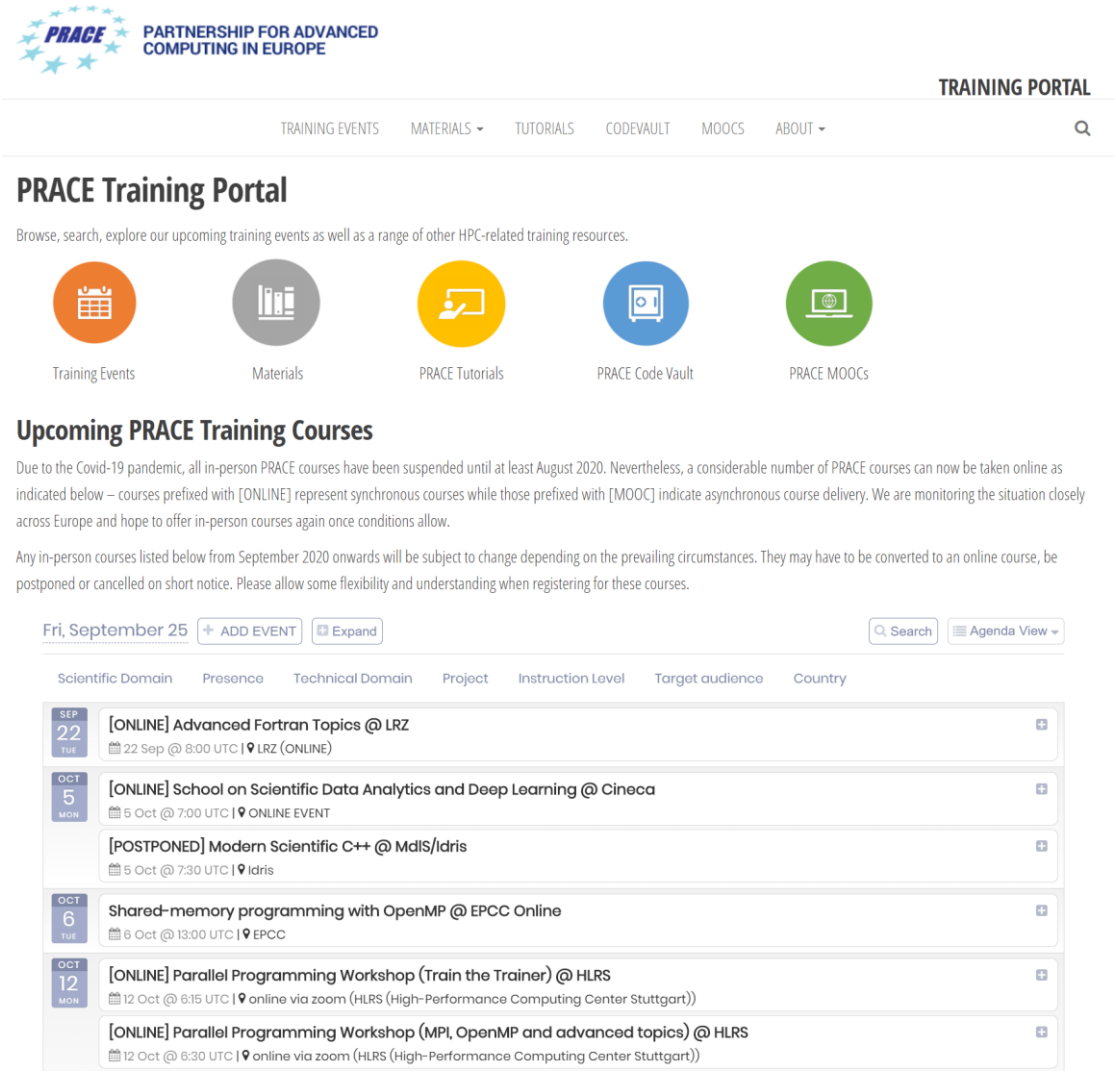


Figure 8: New PRACE Training Portal based on WordPress.

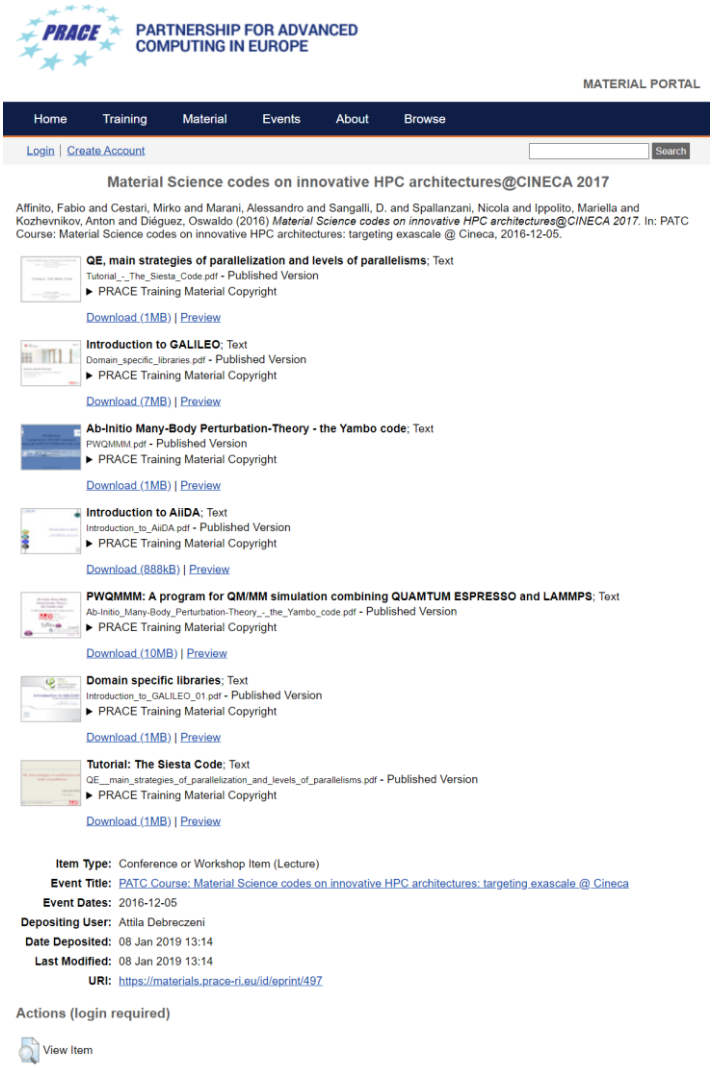


Figure 9: New PRACE material portal based on ePrints.

9.3 CodeVault

CodeVault [17] 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. The CodeVault was modified to be a repository of codes enriched with extra content so they have become self-contained lessons.

The UEABS suite was migrated to be stored on CodeVault in a hierarchically organized manner. CodeVault was also migrated to a cloud hosted gitlab from PRACE partners' server to be available for users in the future [18].

10 PRACE Training Collaboration

PRACE training has had natural collaboration areas with many international projects. The areas of collaboration include co-organising of training, joint workshops, participation in the portal development, course and MOOC development, sharing of best practices or joint ambition or desired outcome that led to different activities.

WP4 has always placed great emphasis on collaborating with other WPs within the project, as well as working with external projects and partners. The different modes for collaboration were typically dependent upon a joint ambition or desired outcome that led to different activities. The HPC in Europe portal development has been led by WP2 with WP6 assistance in technical solutions and training tools.

10.1 EuroHPC Summit Week – Hands-on Workshops and beyond

WP4 has worked with the 2019-2022 organising committees of the EuroHPC Summit Week (EHPCSW), in which PRACEdays has been a major component, to organise hands-on training workshops for students, training related panel discussions and workshops.

This has 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 five workshops, taught by PRACE trainers, were organised on the following topics in the 2019 EHPCSW:

- 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 five 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, due to COVID-19 considerations, WP4 considered to conduct similar workshops again for EHPCSW in 2021, 2022 even virtually, but the conclusion of the event organiser was that these online training workshops were not found beneficial as “co-located” with, presumably, a virtual EHPCSW.

The latest workshops, after the pandemic were organized during the EHPCSW 2022 in Paris on the industry day and addressed the HPC training and competence needs of industry. These topics were discussed in a panel discussion involving the training providers as well as industry representatives.

10.2 European and International Collaborations

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 included:

- Collaboration with ETP4HPC has been continuous since 2019 after the EU organised training discussion in Brussels and has been demonstrated especially by sharing the best practices related to industry engagement via training. The latest example of this collaboration was during EHPCSW 2022 [19], where PRACE & ETP4HPC organised a Workshop on HPC Education and Training - Industry Perspectives during the Industry Day of the EHPCSW2022 conference, as a natural continuation to the first online Industry training workshop in 2021 [20]. The workshops strengthened and demonstrated the willingness for continuing dialogue and developing the trainings and joint events together with the industry participants as well as involving both EuroHPC and ETP4HPC that have collected good experiences from the working training concepts as well as training models and future needs.
- Engagement with RedCLARA: A number of meetings have been held with representatives from the RedCLARA organisation, overseeing Latin America's academic computer networks, including some HPC skills. A joint workshop PRACE - RedCLARA - SCALAC Workshop on Online Teaching [21] was held which focused on topics common to all HPC trainers teaching online both in South America as well as in Europe.
- Talks on joint online training courses that could be arranged on areas such as scientific visualisation, parallel and GPU programming were continued. The PRACE GPU MOOC was launched since and serves as an example of trainer to trainer collaboration. RedClara was encouraged to make benefit from PRACE MOOC by translation and available course materials and established trainer contacts on an individual trainer level. The collaboration between RedClara and Spanish PTC were also continued and translation offer renewed. Further collaboration was not pursued in the extension periods after PRACE training policy change on the eligibility of non- European participants in the PRACE courses.
- Collaboration with Research Infrastructures: WP4 presented its activities at the recent CERN-GÉANT-PRACE-SKA kick-off workshop (online, 29 September 2020). There has 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. These discussions led to CERN's involvement in the SoHPC 2021 edition.
- WP4 looked into innovative approaches to developing training materials that are more accessible and easily maintained via collaborative efforts. The HPC Carpentry [22] approach has been identified to be a promising avenue. However, a level of internal upskilling was needed for many of the partners in order to adopt this approach to training development. While there were plans to deploy efforts towards this activity to develop a pool of training content in this style and format, unfortunately insufficient capacity was found to develop meaningful sets of materials; in part due to contention for additional

efforts being invested in online training courses. However, some PTCs have been leveraging the same style of content development and distribution for its courses [23].

- Training Portal development with FocusCoE and CASTIEL: There have been extensive engagements with FocusCoE and CASTIEL in looking towards a joint, pan-European HPC training course aggregating service/calendar which will disseminate all HPC courses in Europe, while maintaining the ability for individual projects to list and advertise its own events. One potential route to this goal is the development of the HPC in Europe portal [3] which was developed by PRACE to serve the European HPC community. One collaborative activity was with FocusCoE which developed technical solutions and standardised the metadata for the common portal, while PRACE maintains the HPC in Europe portal infrastructure. This had ultimately resulted in a MoU between PRACE, FocusCoE and CASTIEL in agreeing on a joint vision and understanding to work on a common portal for all their events.
- In order 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. A best practice workshop on online teaching was held in January 2021 [24].
- At ISC2021 WP4 partners along with UCL organised the first student BOF: "HPC and you". It was organised as an online event due to COVID-19 pandemic but the latest "HPC and you" edition took place in person on 1 June 2022 in Hamburg with WP4 members hosting the BOF. The idea behind these BOFs was to help students and early career HPC specialists to build a career and professional network for themselves and introduce them the PRACE training possibilities. The first successful BOF was given in ISC21 as online and the ISC22 organisers approached PRACE-6IP WP4 for the repetition of the BOF also this year.
- WP4 members organised a workshop to support the easy transition of the training activity to the EuroHPC era with detailed discussions and joint sessions with the EuroHPC Training representatives during the PRACE-6IP All-hand meeting in Vienna 5-6 May 2022.
- The collaboration with EuroHPC has covered also joint workshops and providing presentations in the area of sharing best practices and training for trainers together with CASTIEL.
- PRACE training collaboration with EuroHPC was also demonstrated on a course level. Two workshops were organised in Bulgaria during February-April 2022. "HPC Fundamentals for end-users introductory course" and "HPC - Intermediate Concepts for end-users" courses were held in spring 2022 on how to use the Discoverer supercomputer, one of the EuroHPC petascale systems. Altogether 99 participants attended these two events organised by NCSA Bulgaria and PetaSC/Sofia TechPark, Bulgaria, Center of Excellence in Combustion (CoEC), BioExcel Centre of Excellence, STFC Daresbury Laboratory, UK. Further report on these activities can be found in Annex 12.4.

11 Conclusions

The more than a decade long history of PRACE training will finish at the end of year 2022. The original goal of strengthening European competitiveness with HPC still remains. PRACE training has managed to establish, maintain and also develop new ways of delivering HPC training, which have been continued without a break for the participants over the years. The PRACE PTC training model of individuals, as well as centres working consistently together via the international training network, has remained strong and been committed to delivering the promised activities in a joint curriculum. There is no comparison to the scope and impact of this activity.

The international activities of Seasonal Schools organised around Europe in the English language, the global International HPC Summer Schools and Summer of HPC programmes supported by On-demand activities have provided a much appreciated and balanced set of training possibilities for users from different skill levels and nationalities.

WP4 has managed to tackle the COVID-19 pandemic by adapting and developing new courses to suit online training, developing many new practices and renewed old practices and tools to increase the quantity of participants. It has also retained the high quality as well as developed the understanding of training scope of HPC training in Europe via collaboration to many organisations and projects to strengthen the HPC training in the near future, in the exascale era.

12 Annex

12.1 List of online Training Tools used in PRACE Training

Tools	Purpose
LMS systems/ Moodle	Course discussion forum, course material and course structure and course video storage, Quizzes, Video quizzes, participant presence and progress monitoring
Mentimeter	Feedback collection
Slack channel	Internal and student communication
Video platforms	Storing course videos
Zoom breakout rooms	Facilitate pair and group work in exercises
GitHub	Offers possibility to use course material after the course has ended
White boards	Facilitating the drawing, demonstration and code training
Microsoft Teams,	Video meeting tool for delivering courses
Zoom video meeting tool	Video meeting tool used in many PTCs
Jupyter Notebooks	Platform for nodes, exercises, course material, offers possibility to use course material after the course has ended
Webex	Delivery of Online video courses
Mural	Enables teams to think and collaborate visually to solve problems.
BigBlueButton (https://bigbluebutton.org/)	Used instead of Zoom because it is really designed for lecturing, does not collect personal data
Godbolt (https://godbolt.org/)	For modern C++ lectures, we have used Godbolt (https://godbolt.org/)
Discord	Keep connection between lecturers and participants, especially when the same lecture was provided during few weeks. It was useful to help participants with their homeworks.

Some online training tool benefits mentioned often by the PTCs:

- **Big Blue Button (BBB)** intrinsic features of BBB for:
  1) whiteboards,
  2) polls: to check user knowledge and monitor user progress
  3) break out rooms: to solve individual problems for small groups of participants
  4) chat: for communication with and between participants

- **ZOOM** (@LRZ, @HLRS): very stable for all OS
  intrinsic features of ZOOM for
  1) polls to check user knowledge and scientific background
  2) break out rooms: exercises in small groups, to solve individual problems for small groups of participants
  3) chat: non-persistent chat with and between participants

Chat

- **Intrinsic Chat** of VC: non-persistent chat for easy communication
- **Slack**: persistent chat for easy communication also among participants, messages don't disappear after e.g. zoom meeting ends
- **RocketChat**: persistent chat for communication between participants, on-premise installation

Materials/Repositories

- **Jupyter NB**: offers possibility to use course material after course has ended)
- **GitHub /GitLab**: as repository and documentation, offers possibility to use course material after course has ended
- **Confluence**: to collect lecture notes and materials

Learning Platforms

- **MOOCs**
- **Moodle**

Surveys/Polls

- **Intrinsic Polls**: e.g. ZOOM Polls
- **Mentimeter:** to check user knowledge and scientific background
- **LimeSurvey**: for evaluation after the course

12.2 Report from PRACE Seasonal Schools

12.2.1 Autumn School 2019, Slovenia - Big data and HPC

- Dates: 17 – 20 September 2019
- Organizing sites: University of Ljubljana
- Venue: University of Ljubljana, Aškerčeva 6, Ljubljana, Slovenia
- Link: https://events.prace-ri.eu/event/896/
- 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.
HADOOP	A short introduction to Hadoop for the attendees. Later on hands-on tutorials on HADOOP were shown.
Introduction to Spark	Basic concepts of Apache Spark Data Analytic Framework were shown. Access to HPC available at UL where all necessary software was 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 Spark concepts by using the Python language	Hands-on approach using Apache Spark with implementation through Python programming language.
Big data analysis with RHadoop	Basic concepts of big data management and analysis using RHadoop was shown with explanation of how to create, store, load big data files and how to perform basic statistics above big data files.

Pre- and post-processing of scientific data with SALOME framework	Firstly, a general overview of SALOME has been presented. The usage of SALOME was shown through Shaper CAD modelling, meshing, visualization. Connection to solvers (MED coupling) and hands-on with ELMER multiphysics was showcased.
Introduction to TensorFlow	Introduction of TensorFlow to attendees through Keras and parallelization in TensorFlow through Horovod was showcased.
Applications of TensorFlow	Automatic differentiation and gradient descent was explained. Introduction to low-level TensorFlow API and built-in parallelism and GPU acceleration with TensorFlow was presented. Some use cases (clustering) were showcased.

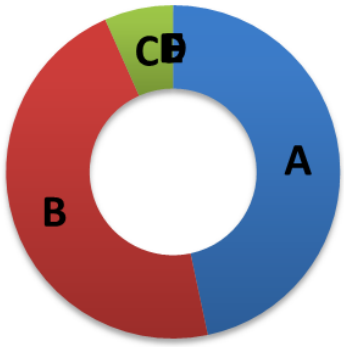
- Number of participants by country:

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

- Statistics of the feedback survey

Information about the school was... Answered: *15*

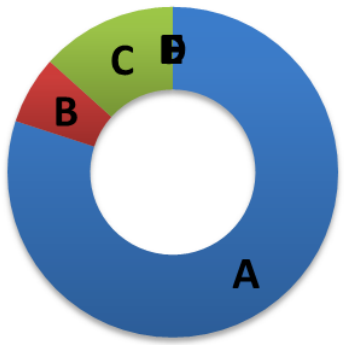
A	excellent	7	46,67%
B	good	7	46,67%
C	not good nor bad	1	6,67%
D	bad	0	0,00%
E	very bad	0	0,00%
F	don't know	0	0,00%



Registration was...

Answered: *15*

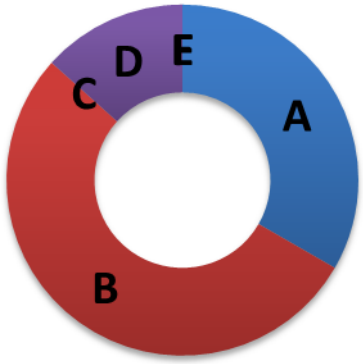
A	excellent	12	80,00%
B	good	1	6,67%
C	not good nor bad	2	13,33%
D	bad	0	0,00%
E	very bad	0	0,00%
F	don't know	0	0,00%



The venue was...

Answered: *15*

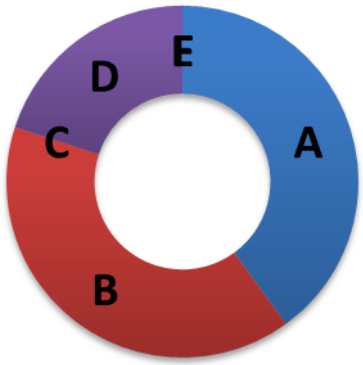
A	excellent	5	33,33%
B	good	8	53,33%
C	not good nor bad	0	0,00%
D	bad	2	13,33%
E	very bad	0	0,00%
F	don't know	0	0,00%



Catering was...

Answered: *15*

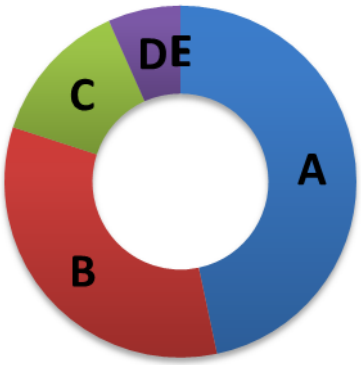
A	excellent	6	40,00%
B	good	6	40,00%
C	not good nor bad	0	0,00%
D	bad	3	20,00%
E	very bad	0	0,00%
F	don't know	0	0,00%



The overall organization was...

Answered: *15*

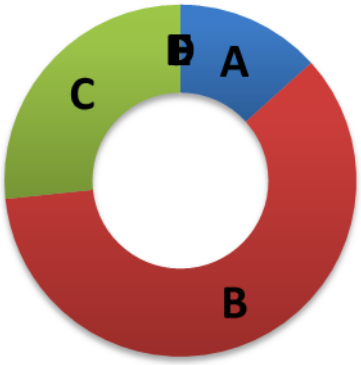
A	excellent	7	46,67%
B	good	5	33,33%
C	not good nor bad	2	13,33%
D	bad	1	6,67%
E	very bad	0	0,00%
F	don't know	0	0,00%



The topics were relevant for my work/research interests

Answered: *15*

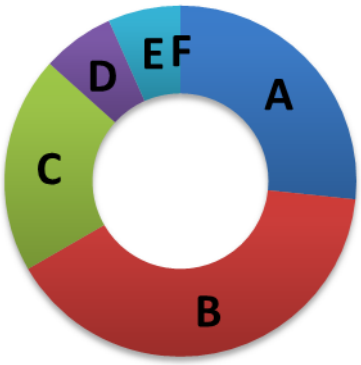
A	agree completely	2	13,33%
B	agree	9	60,00%
C	no strong feelings	4	26,67%
D	disagree	0	0,00%
E	disagree completely	0	0,00%
F	don't know	0	0,00%



I was inspired to new ways of thinking

Answered: *15*

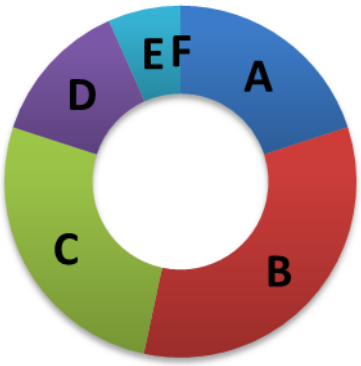
A	agree completely	4	26,67%
B	agree	6	40,00%
C	no strong feelings	3	20,00%
D	disagree	1	6,67%
E	disagree completely	1	6,67%
F	don't know	0	0,00%



The lectures were clearly presented and comprehensible

Answered: *15*

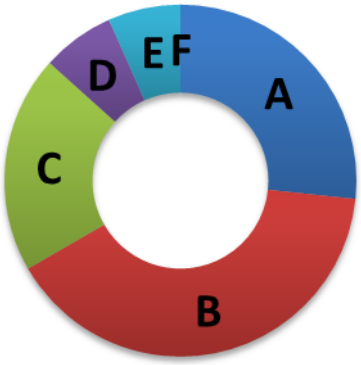
A	agree completely	3	20,00%
B	agree	5	33,33%
C	no strong feelings	4	26,67%
D	disagree	2	13,33%
E	disagree completely	1	6,67%
F	don't know	0	0,00%



The pace of teaching was right

Answered: *15*

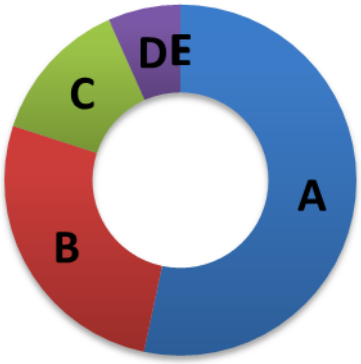
A	agree completely	4	26,67%
B	agree	6	40,00%
C	no strong feelings	3	20,00%
D	disagree	1	6,67%
E	disagree completely	1	6,67%
F	don't know	0	0,00%



Teaching aids used (e.g. slides) were well prepared

Answered: *15*

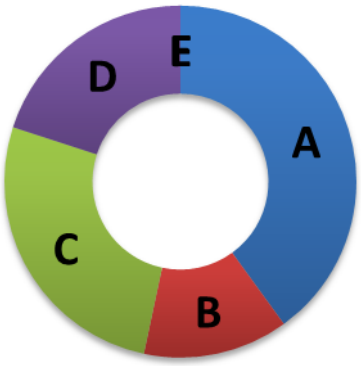
A	agree completely	8	53,33%
B	agree	4	26,67%
C	no strong feelings	2	13,33%
D	disagree	1	6,67%
E	disagree completely	0	0,00%
F	don't know	0	0,00%



Hands-on exercises and demonstrations were a valuable contribution to the school

Answered: *15*

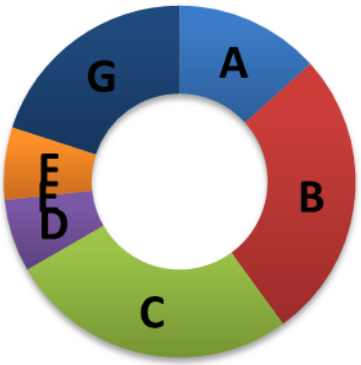
A	agree completely	6	40,00%
B	agree	2	13,33%
C	no strong feelings	4	26,67%
D	disagree	3	20,00%
E	disagree completely	0	0,00%
F	don't know	0	0,00%



Social event(s) were an enjoyable and important aspect of the school

Answered: *15*

A	agree completely	2	13,33%
B	agree	4	26,67%
C	no strong feelings	4	26,67%
D	disagree	1	6,67%
E	disagree completely	0	0,00%
F	don't know	1	6,67%
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.

Everything

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.

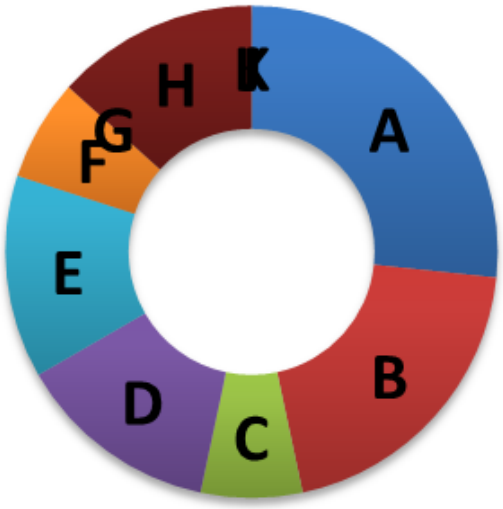
everything was excellent

Overall, how would you rate this school?

Answered: *15*

10 = excellent		0 = waste of time	
A	10	4	26,67%
B	9	3	20,00%
C	8	1	6,67%

D	7	2	13,33%
E	6	2	13,33%
F	5	1	6,67%
G	4	0	0,00%
H	3	2	13,33%
I	2	0	0,00%
J	1	0	0,00%
K	0	0	0,00%



In the future, I will need training in general HPC programming (MPI, OpenMP)...

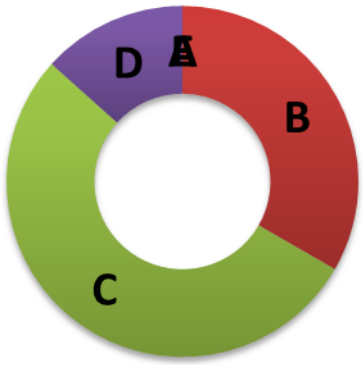
Answered: *15*

A	urgent need	0	0,00%
B	important need	7	46,67%
C	some need	6	40,00%
D	no need	2	13,33%
E	don't know	0	0,00%

In the future, I will need training in advanced HPC programming (Hybrid MPI-OpenMP; next-gen HPC languages e.g. PGAS; GPU computing e.g. CUDA)...

Answered: *15*

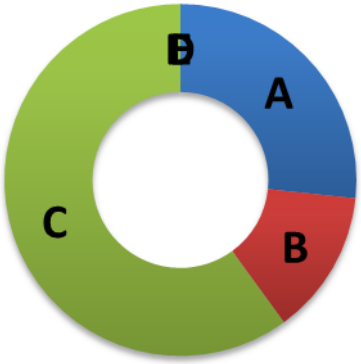
A	urgent need	0	0,00%
B	important need	5	33,33%
C	some need	8	53,33%
D	no need	2	13,33%
E	don't know	0	0,00%



In the future, I will need training in code optimisation and performance analysis...

Answered: *15*

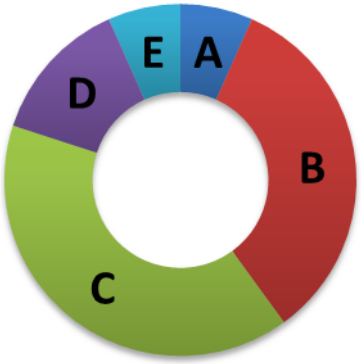
A	urgent need	4	26,67%
B	important need	2	13,33%
C	some need	9	60,00%
D	no need	0	0,00%
E	don't know	0	0,00%



In the future, I will need training in porting of existing codes to HPC architectures...

Answered: *15*

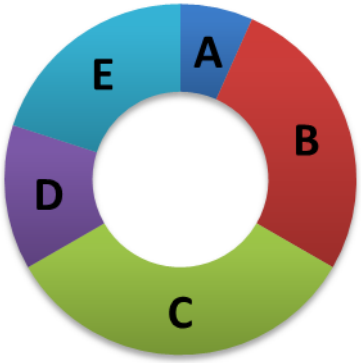
A	urgent need	1	6,67%
B	important need	5	33,33%
C	some need	6	40,00%
D	no need	2	13,33%
E	don't know	1	6,67%



In the future, I will need training in specific HPC application(s)...

Answered: *15*

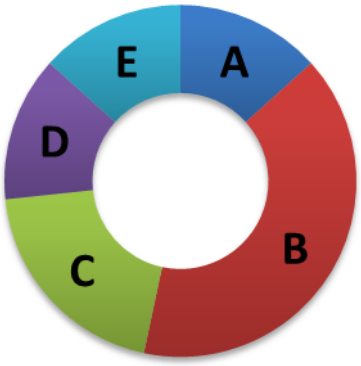
A	urgent need	1	6,67%
B	important need	4	26,67%
C	some need	5	33,33%
D	no need	2	13,33%
E	don't know	3	20,00%



In the future, I will need training in HPC programming and applications specific to my research community...

Answered: *15*

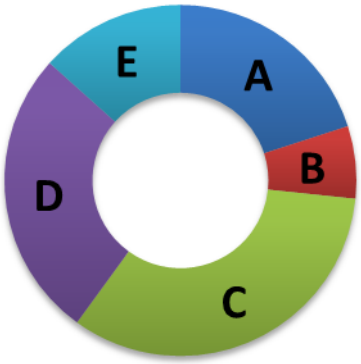
A	urgent need	2	13,33%
B	important need	6	40,00%
C	some need	3	20,00%
D	no need	2	13,33%
E	don't know	2	13,33%



In the future, I will need training in visualisation techniques...

Answered: *15*

A	urgent need	3	20,00%
B	important need	1	6,67%
C	some need	5	33,33%
D	no need	4	26,67%
E	don't know	2	13,33%



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.

Please give any other general comments about PRACE training activities.

Answered: *2*

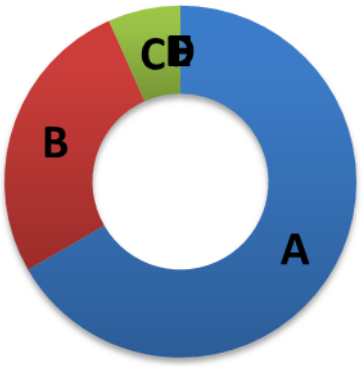
/

more practical examples.

The accessibility of venue (e.g. stairs, lifts, signage, facilites) was:

Answered: *15*

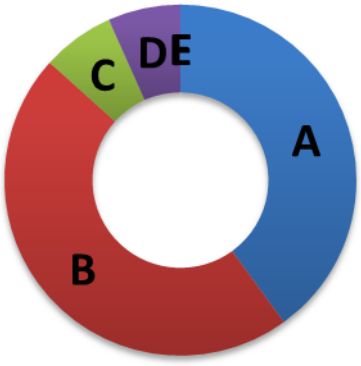
A	excellent	10	66,67%
B	good	4	26,67%
C	not good nor bad	1	6,67%
D	bad	0	0,00%
E	very bad	0	0,00%
F	don't know	0	0,00%



Teaching aids (e.g. slides, handouts, exercises) were clear and accessible

Answered: *15*

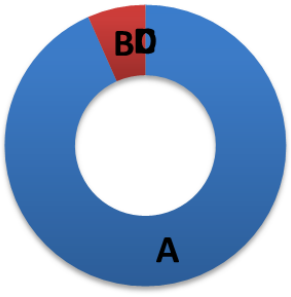
A	agree completely	6	40,00%
B	agree	7	46,67%
C	no strong feelings	1	6,67%
D	disagree	1	6,67%
E	disagree completely	0	0,00%
F	don't know	0	0,00%



Gender

Answered: *15*

A	male	14	93,33%
B	female	1	6,67%
C	prefer not to say	0	0,00%
D	other	0	0,00%



Job Title or Career Stage

Answered: *13*

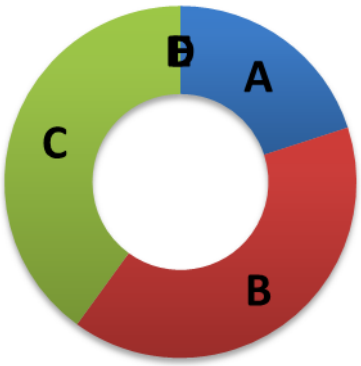
PhD student	Master's student
Researcher	Independent Expert at HPC
Data Scientist	MSc student

Research Fellow, Ph.D.	IT
Master's student	Student
Young researcher (PhD Candidate in Bioinformatics)	Researcher
Researcher	

How easy or hard did you find this course?

Answered: *15*

A	Very easy	3	20,00%
B	Quite easy	6	40,00%
C	Moderate	6	40,00%
D	Quite hard	0	0,00%
E	Very hard	0	0,00%



12.2.2 Spring School 2021, Belgium - Introduction to OpenFOAM

- Dates: 20-21 and 27-28 April 2021
- Organizing sites: Vlaams Super Computer Centrum (UGent and KU Leuven)
- Venue: online due to COVID-19 restrictions
- Link: https://events.prace-ri.eu/event/1196/
- Description of contents:

The sessions were a mix of lectures, examples and hands-on, with continuous opportunity for Q&A. Spread over three days of lecturing, in-depth program followed these subjects:

  - Introduction to OpenFOAM, example Pitz-Daily and Paraview
  - Mesh processing, elbow tutorial
  - Pressure-velocity coupling
  - Meshing in OpenFOAM, snappyHexMesh
  - Advanced post-processing
  - Turbulence and wall function
  - Dynamic code
  - Source terms in OpenFOAM
  - Bug reporting via GitLab

- Number of participants by country:

Country Institute	**count**
Belgium	**23**
KU Leuven	8
UA	1
UGent	8
ULB	4
VIB	1
VKI	1
Czech Republic	**1**
Czech Technical University Prague	1
Germany	**1**
N/A	1
Greece	**1**
National and Kapodistrian University of Athens	1
Spain	**1**
Jaume I University	1
Turkey	**3**
Middle East Technical University	2
Sivas University of Science and Technology	1
Total	**30**

- Statistics of the feedback survey:

General

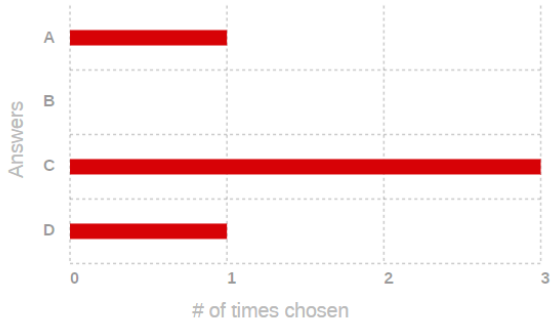
Where did you hear about the event — Answered: 5

A. from the Prace website: 1 (20.00%)

B. from a Prace newsletter: 0 (0.00%)

C. from a VSC communication: 3 (60.00%)

D. other: 1 (20.00%)



The event is open both to academic as industry users. To which of these categories do you consider yourself. — Answered: 5

A. Academic: 5 (100.00%)

B. Industry: 0 (0.00%)

Please rate your level of expertise in the science related to this course and expertise with other comparable software — Answered: 5

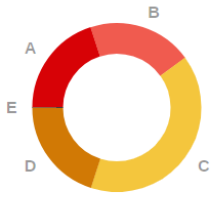
A. Novice: 1 (20.00%)

B. Advanced beginner: 1 (20.00%)

C. Competent: 2 (40.00%)

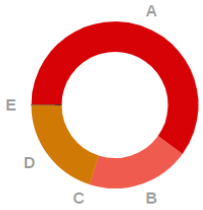
D. Proficient: 1 (20.00%)

E. Expert: 0 (0.00%)



Please rate your level of expertise as an OpenFOAM user before this course — Answered: 5

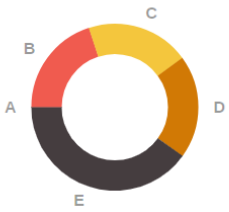
- A. Novice: 3 (60.00%)
- B. Advanced beginner: 1 (20.00%)
- C. Competent: 0 (0.00%)
- D. Proficient: 1 (20.00%)
- E. Expert: 0 (0.00%)



Course content

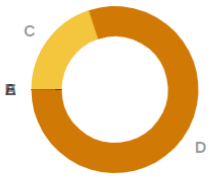
Course content matched the course description? — Answered: 5

- A. Disagree completely: 0 (0.00%)
- B. Disagree: 1 (20.00%)
- C. neutral: 1 (20.00%)
- D. Agree: 1 (20.00%)
- E. Agree completely: 2 (40.00%)



Prerequisities were well defined? — Answered: 5

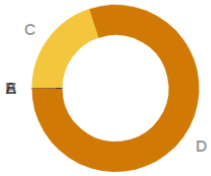
- A. Disagree completely: 0 (0.00%)
- B. Disagree: 0 (0.00%)
- C. neutral: 1 (20.00%)
- D. Agree: 4 (80.00%)
- E. Agree completely: 0 (0.00%)



I learned skills that are relevant to my work/research

Answered: 5

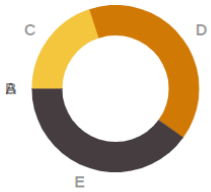
- A. Disagree completely: 0 (0.00%)
- B. Disagree: 0 (0.00%)
- C. neutral: 1 (20.00%)
- D. Agree: 4 (80.00%)
- E. Agree completely: 0 (0.00%)



The lectures were clearly presented and comprehensible:

Answered: 5

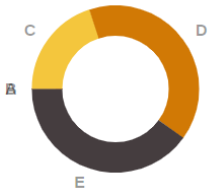
- A. Disagree completely: 0 (0.00%)
- B. Disagree: 0 (0.00%)
- C. neutral: 1 (20.00%)
- D. Agree: 2 (40.00%)
- E. Agree completely: 2 (40.00%)



Teaching aids used (e.g. slides) were well prepared:

Answered: 5

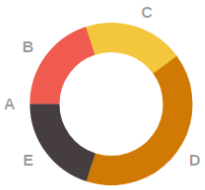
- A. Disagree completely: 0 (0.00%)
- B. Disagree: 0 (0.00%)
- C. neutral: 1 (20.00%)
- D. Agree: 2 (40.00%)
- E. Agree completely: 2 (40.00%)



The hands-on exercises and demonstrations were a valuable contribution to the event :

Answered: 5

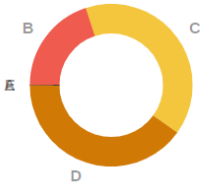
- **A. Disagree completely**: 0 (0.00%)
- **B. Disagree**: 1 (20.00%)
- **C. neutral**: 1 (20.00%)
- **D. Agree**: 2 (40.00%)
- **E. Agree completely**: 1 (20.00%)



The pace of teaching was

Answered: 5

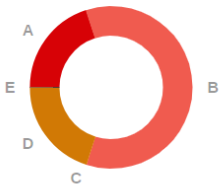
- **A. Way too slow for me**: 0 (0.00%)
- **B. A bit too slow for me**: 1 (20.00%)
- **C. About right for me**: 2 (40.00%)
- **D. A bit too fast**: 2 (40.00%)
- **E. Way too fast for me**: 0 (0.00%)



Please rate your level of expertise as an OpenFOAM user after this course

Answered: 5

- **A. Novice**: 1 (20.00%)
- **B. Advanced beginner**: 3 (60.00%)
- **C. Competent**: 0 (0.00%)
- **D. Proficient**: 1 (20.00%)
- **E. Expert**: 0 (0.00%)



Course organisation

What do you feel about online versus real-life for this specific event?

Answered: *5*

A. A real-life event would be better: 3 (60.00%)

B. An Online event is better: 2 (40.00%)

What are the reasons that you prefer one above the other, for this specific event.

Answered: *3*

I tend to fall asleep during online lecture no matter what it is about so I definitely prefer real-life event with a bit of peer pressure around.

Interaction is easier in a real life event.

there will be more interaction between lecturer and attendants, especially for an event with hands-on practice.

Do you have any suggestions how this event could be improved?

Answered: *2*

I saw this tutorial from H. Jasak at UGent on youtube and apart from saying and showing things, he also gave tasks to the students to first try to figure it out on their own before showing them the solution. Also he gave one easier and one complicated task for beginner and advanced users respectively.

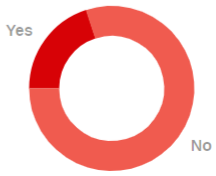
For me, the part where we divided into the code on the last day, went a bit over quick as I am not used to C++ nor OpenFOAM. Nonetheless, I found diving into the code very educational.

Did you have major technical problems which prevented you from following at least a substantial part of the event?

Answered: *5*

A. Yes: 1 (20.00%)

B. No: 4 (80.00%)



12.2.3 Spring School 2021, Slovakia - Modelling materials using HPC and AI/ML

- Dates: 15 – 18 June 2021
- Organizing sites: Centre of Operations – Computing Centre, Slovak Academy of Sciences (COO-CC SAS), Bratislava, Slovakia
- Venue: online due to COVID-19 restrictions
- Link: https://events.prace-ri.eu/event/1212/
- Description of contents:
    - *Brief introduction to HPC environment (Dr. Filip Holka):* A short overview of the resources allocated for the purposes of the spring school was given by the CC SAS staff, as well as the scheduler system used.
    - *OnDemand: How to & account activation (Dr. Michal Pitonak):* An interactive session introducing the participants to the OnDemand service that would be used later in the workshop. CC SAS staff helped all the participants to activate their account and gain access to the environment and workshop materials.
    - *Jupyter notebook interface and ML with Python (Miloslav Valco):* An interactive session covered briefly the specifics of working with Jupyter notebook interface and work with Python libraries required later during the workshop.
    - *Introduction to ML: Representations & Kernel methods (Prof. Milica Todorovic):* Lectures reviewed the workflows in classical machine learning applied to materials science, and in particular, to the structure and properties of molecules. The focus was on molecular representation for machine learning, as well as the widely-used kernel methods for machine learning molecular properties. The ensuing hands-on tutorial introduced descriptor building and simple machine learning applications.
    - *Chemical structure search using ML (Prof. Milica Todorovic):* The lecture compared active learning against classical machine learning, and considered how it could be applied to molecular conformer search. The accompanying tutorial served to gain practical experience with this application.
    - *Advanced applications of ML (Prof. Milica Todorovic):* The lecture described more complex ML applications to spectral properties of molecules and to molecular design. It served as a starting point for the participants for their further research and study in this area.
    - *Introduction to ab-initio simulation in VASP (Dr. Martijn Marsman):* Basic principles of DFT calculations, Kohn-Sham ground state, SCF scheme and basic algorithms implemented in VASP.
    - *Electronic convergence (Dr. Martijn Marsman):* Numerical determination of the ground state, algorithms for minimization of the functional, charge density mixing.
    - *Symmetry and sampling in reciprocal space (Dr. Martin Schlipf):* Introductiopn to simulations of condensed matter/surfaces: periodicity, boundary conditions, sampling of the Brillouin Zone, k-point generation.
    - *Introduction to molecular dynamics (Prof. Tomas Bucko):* Introduction to simulations of complex chemical systems modeled at an atomic level using quantum mechanics. The lecture covered energy terms and functions, steps in typical MD simulations.

- *Machine learning force fields (Prof. Georg Kresse):* The lecture covered novel approaches of using machine learning generated force fields on the basis of Bayesian inference during molecular dynamics simulations, and application to various chemical properties (ie. Melting points,…).
- *High performance computing with VASP (Dr. Martin Schlipf):* Parallel implementation and performance of VASP modules, advanced applications.

- Statistics of the feedback survey:

Organization:

Did you find the information about the event	
excellent	12
good	7
not good nor bad	1
bad	3
very bad	0
don't know	0

The Registration process was	
excellent	14
good	8
not good nor bad	0
bad	0
very bad	0
don't know	1

Online vs real-life format preference	
online format	10
no preference	6
face-to-face	7

Did you have any technical problems?	
no technical problems	15
minor issues	7
major problems	1
unable to follow event	0

Communication with the organizers was	
excellent	17
good	4
not good nor bad	2
bad	0
very bad	0
don't know	0

Overall, how would you rate the Spring school on Modelling materials using AI/ML?	
10	11
9	7
8	3
7	1
6	1
5 - 4	0

Lectures and exercises

The topics were relevant for my work/research interests	
agree completely:	16
agree:	6
no strong feelings:	1
disagree:	0
disagree completely:	0
don't know:	0

The lectures were clearly presented and comprehensible	
agree completely:	16
agree:	7
no strong feelings:	0
disagree:	0
disagree completely:	0
don't know:	0

Hands-on exercises and demonstrations were a valuable contribution to the school	
agree completely:	19
agree:	3
no strong feelings:	1
disagree:	0
disagree completely:	0
don't know:	0

The pace of teaching was right	
agree completely:	13
agree:	10
no strong feelings:	0
disagree:	0
disagree completely:	0
don't know:	0

Teaching aids used (e.g. slides) were well prepared	
agree completely:	17
agree:	6
no strong feelings:	0
disagree:	0
disagree completely:	0
don't know:	0

Additional information

Gender	
Female	10

Male	13
Other	0

12.2.4 Autumn School 2021, Bulgaria - Fundamentals of Bimolecular Simulations and Virtual Drug Development

- Dates: 20-24 September 2021
- Organizing sites: NCSA-Bulgaria, BioExcel Centre of Excellence, STFC Daresbury Laboratory, and Sofia University in partnership with AstraZeneca and NostrumBiodiscovery
- Venue: online due to COVID-19 restrictions
- Link: https://events.prace-ri.eu/event/1222/
- Description of contents:
    - **September 20, 2021: The school first lecture by Prof.** Irini Doychinova **introduced procedures for searching potential drug candidate via applying computational simulation.** Drug design is an ensemble of in silico methods and techniques for analyses and designing of novel molecules with desired properties and activities as potential drug candidates. It emerged in the early 1960s with studies on the relationships between chemical structure and bioactivity. Over the years, the drug design has been developed to comprise a wide range of methods for ligand-based and structure-based approaches for data analyses and visualization of ligand-macromolecule interactions. The present lecture describes the important place of drug design in the modern drug discovery and development, the major achievements in the field, the current state of the art and future expectations.
    - Centre of Excellence BioExcel was introduced by Dr. Rossen Apostolov. Over the last decades, Europe has invested heavily in the development of world-leading HPC infrastructure in particular the PRACE Tier-0 and Tier-1 machines. Much of the computational research communities, however, are not ready to make efficient use of the machines. Since 2015, BioExcel Centre of Excellence, one of the co-organizers of this school, has been developing key software applications, used extensively for computational biomolecular research, and preparing them for extreme-scale computing production operations. Most of those core applications have been covered in the program of the HPC school. The center is also developing workflow platforms and providing environments for much improved user-friendliness of the codes and opportunity to execute tailored runs.
    - The topic of parallel paradigms was presented by Dr. Valentin Pavlov – why are they needed, what are the different ways an HPC system can be used to carry out parallel work, tips for setting up and configuring each of the levels, basic introduction to what MPI and OpenMP is as well as advices for the end-users how to split their work. Following two lectures by Prof. Emanouil Atanassov and Prof. Ivan Dimov covered the way to gain access to HPC system and provided a brief tour of the newest supercomputing system in Bulgaria - Discoverer.
    - **September 21, 2021:** The classical computational method of molecular mechanics was introduced by Prof. Anela Ivanova, together with some elements from statistical thermodynamics and provided a general step-by-step scheme on how to conduct a biomolecular simulation. This included: how to choose the level of detail of molecular models, the appropriate force field and simulation method, the correct

thermodynamic ensemble. Then, the main part of the lecture was devoted to acquainting the audience with the fundament of the Molecular Dynamics method – presenting the equations of motion and the ways to integrate them, how to maintain constant temperature and pressure, how to calculate interaction forces efficiently and how to impose restraints and constraints. Finally, a note on the possible analysis of results was made, the advantages and drawbacks of the method were summarized, and its applicability discussed.

- Following the molecular dynamics introduction, Assoc. Prof. Peicho Petkov provided an overview of some basic functionalities of the GROMACS MD software package that enable the users to parametrize a molecule/s with a force field, set a box with optimal shape and dimensions, add solvent molecules and ions to the simulation box, equilibrate the resulting molecular system and finally run production MD simulations. Special attention is paid to the available algorithm and popular practices. During the practical session there was conducting MD simulation on a remote HPC system. The participants were briefly introduced how to connect to an HPC system and do file transfers between local and remote file system/s via SSH, how to prepare scripts for, submit and monitor SLURM jobs. An example of MD simulation protocol for peptide in water in physiological conditions was demonstrated mentioning different approaches for actions / manipulations to be done locally or remotely for preparing and running MD simulations on a remote HPC system.
- **September 22, 2021:** Biomolecular simulation based free energy calculations have become a standard technique in the field of computational chemistry. The method is frequently applied in drug discovery process to identify lead compounds or optimize already available ligands. Furthermore, the ability to accurately predict effects of amino acid mutations on protein stability and protein-protein interactions allows for an efficient rational protein engineering. In a talk Dr. Vytautas Gapsys provided a general overview of the molecular dynamics based free energy calculation methods. Subsequently, numerous applications were showcased to provide both theoretical and practical understanding of the introduced methods. The demonstrated applications highlighted amino acid mutations for protein folding free energy prediction and drug resistance studies, nucleotide mutations to probe for the changes in the protein-DNA binding, ligand modifications to predict protein-ligand binding affinities. In the subsequent practical session, open source Gromacs and PMX software packages were used to allow for a hands-on experience in predicting ligand-protein binding free energy change upon ligand modification. The participants were guided through a tutorial in which the essential steps for such an investigation step were performed.
- Molecular Dynamics simulations have matured to a level where they are routinely applied to address various problems in early drug discovery in the pharmaceutical industry. In his presentation, **Dr. Christian Margreitter from AstraZeneca** described key bottle-necks in the context of *de novo* generative design using state-of-the-art Deep Learning methods with a focus on how structural modelling in general and Molecular Dynamics in particular can close these gaps. Prominent

examples of use cases include the calculation of relative and absolute (binding) free energies and conformational sampling, both for small molecules and so-called "new modalities". We expect that the increase in computational resources, improved protocols and more accurate force fields together with automated, stable workflow execution will allow us to achieve even bigger impact on drug discovery projects in the near- to mid-term future.

- Prof. Alexandre Bonvin showed how one could credibly evaluate drug molecules interact with their target receptors in the body through the HADDOCK docking server. The prediction of the quaternary structure of biomolecular macromolecules is of paramount importance for fundamental understanding of cellular processes and drug design. In the era of integrative structural biology, one way of increasing the accuracy of modelling methods used to predict the structure of biomolecular complexes. We have developed for this purpose a versatile information-driven docking approach HADDOCK (http://www.bonvinlab.org/software). The lecture was followed by an online tutorial illustrating the use of the HADDOCK webportal (https://wenmr.science.uu.nl/haddock2.4) for the modelling of a protein-protein complex based on NMR chemical shift perturbation data small-angle, X-ray scattering and cryo-electron microscopy experiments. HADDOCK can integrate information derived from biochemical, biophysical or bioinformatics methods to enhance sampling, scoring, or both.
- **September 23, 2021:** During the fourth day, STFC Daresbury Laboratory team - Prof. Ilian Todorov, Dr. Tom Keal, Dr. Kakali Sen, and Dr. You Lu - demonstrated the capabilities of the ChemShell for designing the structure and properties of complex biomolecular complexes.
- **Introduction to ChemShell**
- The introductory lecture by Tom Keal covers the concepts of multiscale QM/MM modelling and gives an overview of the ChemShell package. The talk gives guidance on how to perform basic chemical tasks in ChemShell, including geometry optimisations using the DL-FIND optimisation library, for small molecule systems using both QM and QM/MM simulations. A live demo shows how ChemShell is compiled and run in practice using examples from the online tutorial.
- **Biomolecular modelling with QM/MM**
- This lecture takes an applicant's view on how to perform QM/MM calculations on biomolecular systems using Chemshell. Kakali Sen's lecture starts with a short introduction on the usefulness of QM/MM to study biomolecular systems with a focus on enzymes. It is then followed by a workflow that is necessary to prepare the system (enzyme) under investigation and the general considerations of key parameters involved in carrying out the QM/MM calculations. Finally, detailed case study of three applications showing the benefit of using QM/MM calculation is provided.
- **The Py-ChemShell biomolecular workflow**
- In this session You Lu explains the Py-ChemShell implementation of the biochemical simulation workflow. A real-life case study of the P450 enzyme is demonstrated with code running: from the crystal structure preparation to the whole

solvation procedure, and to the QM/MM setup and single-point/geometry-optimisation calculations.

- **September 24, 2021:** In the last day of the training, there were a number of illustrations of using HPC for biomolecular and applied research:
- In silico study of the anti-inflammatory action of heparin within the COVID-19 context
- We perform in silico study of the ability of low-molecular-weight heparin (LMWH) to inhibit both IFNγ and IL-6 signalling pathways. While heparin's binding affinity to these cytokines is well-known, the molecular mechanism of its impact on their biological activity has not been studied in detail. Our results show that LMWH is able to fully inhibit the interaction of IFNγ with its cellular receptor, thus blocking the IFNγ signalling pathway. It also influences the biological activity of IL-6 by preventing the formation of the IL-6/IL-6Rα/gp130 signalling complex. These findings shed light on the molecular mechanism of the anti-inflammatory action of LMWH, relating it to the impairment of the biological activity of these cytokines, and underpin heparin's ability to influence favourably conditions characterised by overexpression of the latter. Such conditions are associated with autoimmune diseases, but also with inflammatory processes, in particular with COVID-19. Our results put forward heparin as a promising means for prevention and suppression of the development of severe CRS in acute COVID-19 patients and encourage further investigations on its applicability as an anti-inflammatory agent.
- Different approaches for finding ligands inhibiting the NSP10/NSP16 complex of the SARS-CoV-2
- We reported our approach, focused on finding a ligand capable to competitively inhibit the NSP10/NSP16 of SARS-CoV-2 by blocking its SAM pocket. In this ambitious task we try to find such a ligand that can bind to SAM pocket from the existing pools of drugs, drugs candidates, metabolites or just commercially available compounds along with constructing new virtual compounds. We also demonstrate the process of optimizing methodology to evaluate binding energies good enough to distinguish the best ligands. To fulfill this task, we define the best working model of NSP10/NSP16 SAM pocket, to unify the optimal method for scoring of ligands-NSP16 interaction and after that we use several docking procedures for sieving existing pools of structures and several methods for generating the new ones. Emphasis is placed on relatively simple for synthesis compound with little or no asymmetric carbon atoms or which asymmetric carbon atoms are easily available fragments. The best ligands as a result of our workflow, are on the way of further refinement and we hope some of them will be helpful for further drug design as a CoViD drug.
- **Ligand- and structure-based studies of natural flavonoids from the plant Silybum marianum**
- Natural products have been a rich source for medical preparations since antiquity and nowadays they continue to provide inspiration for modern drug discovery. Such an example is the silymarin extract from the medical plant *Silybum marianum* (milk thistle), that is native to Bulgaria and is well-known for its favorable effect on liver,

cardio and biliary diseases. However, the ADMET (absorption, distribution, metabolism, excretion, toxicity) properties of flavonolignans, as well as their mechanisms of action, respectively a large part of their target proteins in the human body, are not completely defined. The presented case studies focused on prediction of gastrointestinal absorption and potential novel protein targets of flavonolignans from milk thistle, using ligand- and structure-based molecular modelling methods. According predictions performed using an in-house QSAR (quantitative structure activity relationship) model for PAMPA (parallel artificial membrane permeability assay) permeability, the main biologically active flavonolignans in milk thistle are highly permeable in the gastrointestinal tract, which is a good prerequisite for sufficient bioavailability. Docking stimulations in the ligand-binding domain of the human estrogen receptor alpha (ERα) showed that the main flavonolignans in milk thistle, silybins A and B, interact stereospecifically with the protein, which is consistent with and explains results from experimental studies of ERα-mediated activity of silymarin. The chemical similarity between flavonolignans and drugs with known mechanism of action was evaluated, and docking studies were performed to select potential common protein targets for the drugs and flavonolignans (BRAF kinase and Smoothened).

- **Could FE calculations with GROMACS be faster? NostrumBiodiscovery's attempt to achieve this goal**
- In this presentation we will introduce the development of a protocol to perform fast and accurate free energy calculations using GROMACS and PMX. This work was done in collaboration with BioExcel partners and pretends to create a workflow to accelerate the lead optimization stage of the drug discovery process, making it possible to easily calculate protein ligand relative binding affinities. The presentation pretends to explain the importance of the different steps of the workflow, its optimization and validation, and show the results.
- **Clustering of doxorubicin and its interaction with bio-polymers (alginates)**
- Doxorubicin is an anthracycline antibiotic derived from the acti-nobacteria Streptomyces peucetius var. caesius. The drug possesses a broad-spectrum of anticancer activity, including breast, ovarian, lung, bladder cancer etc. Chitosan/alginate nanoparticles are attractive platform for doxor-ubicin loading since both polysaccharides are biocompatible, biode-gradable and non-toxic. In order to clarify the interactions between the drug and sodium alginate we performed series of classical molecular dynamic simulations using various ratios between the two components in water environment. Classical molecular dynamic simulations, performed here, revealed that the high encapsulation efficiency (above 90%) of doxorubicin in alginate/chitosan nanoparticles was mainly due to electrostatic interaction between doxorubicin and sodium alginate, although dipole-dipole and hydrophobic interactions might also contribute.
- **Selectivity of binding of vector molecules to the folate receptor-alpha observed by molecular dynamics**
- The lecture illustrated the application of atomistic molecular dynamics simulations on the example of studying the process of binding of folic acid and several of its

bioactive derivatives to their target folate receptor-α. The construction of the models of the ligands and of a receptor-embedded lipid bilayer (modelling a cancer cell membrane) and the protocol for running MD simulations for these models were explained. The most important results obtained for the unbound systems were summarized. Then, outcome from MD simulations revealing the mechanism of binding of the ligands to the receptor was presented and discussed, rationalizing the differences between the molecules. Both data for free ligands and for such carrying a bioactive drug cargo were shown.

- **Molecular dynamics simulations of fenofibrata solubilization into bile salt and fatty acids micelles**
- In the presented study, atomistic molecular dynamic simulations of taurodeoxycholate micelle formation (TDC) and solubilization of fenofibrate (FFB) in the resulting micelles are performed in the absence and presence of sodium salts of fatty acids (myristic, oleic acid and stearic). The systems are modeled under conditions as close as possible to the experimental ones in terms of electrolyte concentration, temperature and ratio between different types of molecules, as their concentration is increased 5 times. For each system, trajectories with length of 300 ns are generated, which are analyzed in terms of micelle formation kinetics. From the last 150 ns, the size of the obtained micelles is estimated, the percentage of different types of molecules in the case of mixed micelles of bile and fatty acids and the solubilization capacity for the FFT drug. Theurodeoxycholate is found to form secondary micelles (over 9 molecules in size) with an average aggregation number (N_{agg}) of 19, which is in full agreement with the experimental data N_{agg} (TDC) = 18. When monomers of the sodium salt of fatty acids are added to the TDC micelles, one part of them associates with the TDC micelles to form mixed micelles and another part assemble to form pure micelles. Regarding the solubilization of fenofibrate, it is found that it is higher in the presence of oleic and myristic acids and the effect is greater with oleic than myristic acid, and there is no effect of the stearic acid. The obtained results are in full agreement with the experimental data.

- Number of participants by country:

Country	Count
Armenia	3
Belgium	3
Bulgaria	21
Cyprus	2
Czech Republic	4
Denmark	2
Estonia	1
Finland	2
France	1

Country	Count
Germany	29
Greece	10
Hungary	3
Israel	3
Italy	1
Latvia	4
Netherlands	2
Poland	10
Romania	2
Slovakia	6
Spain	10
Sweden	14
Switzerland	1
Turkey	20
Ukraine	5
United Kingdom	6
Total	**165**

- Statistics of the feedback survey:

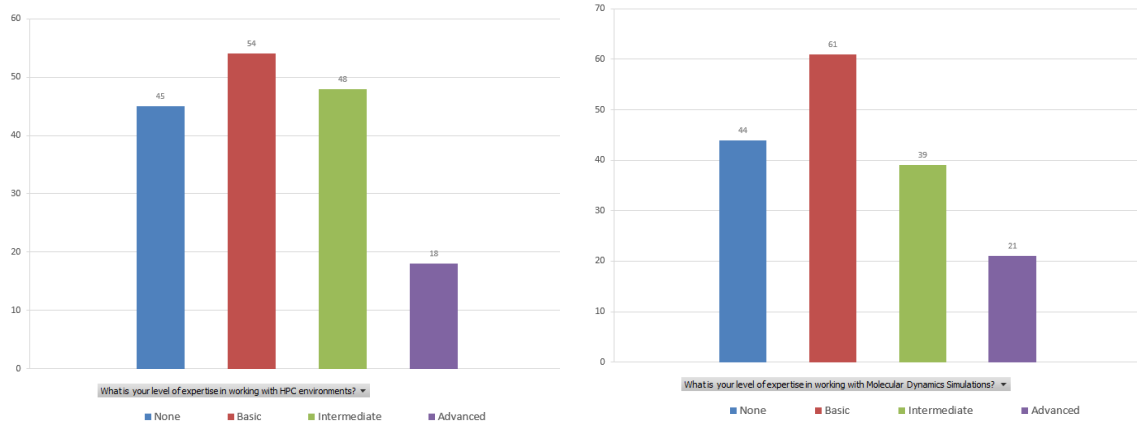


Figure 1: Expertise in HPC and Molecular Dynamics

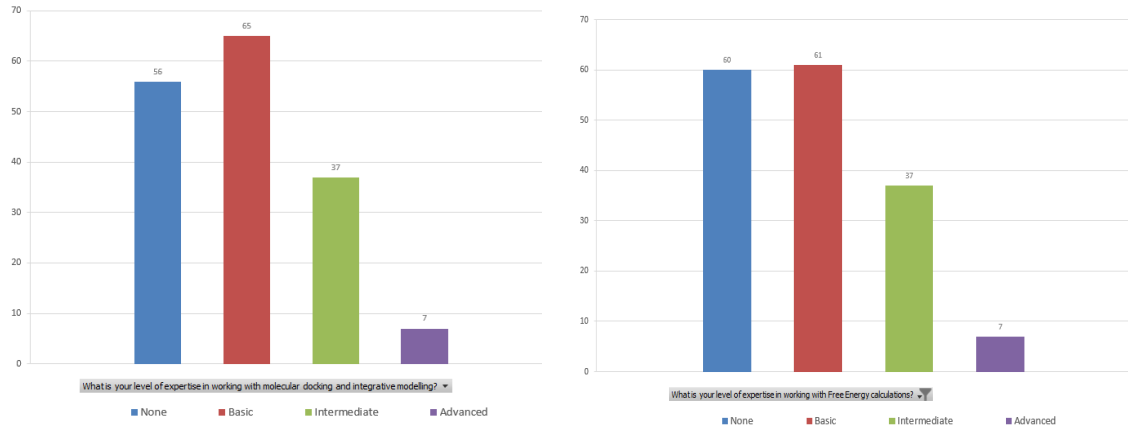


Figure 2: Expertise in Molecular docking and integrative modelling / Free Energy calculations

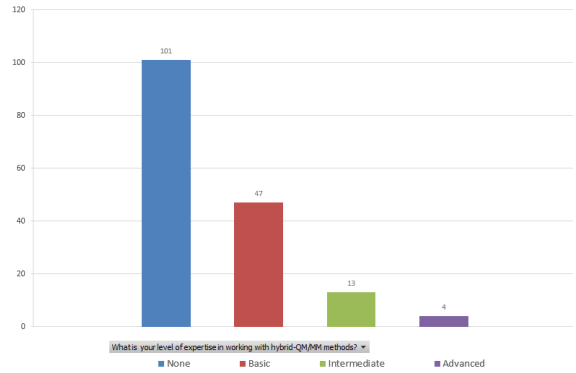


Figure 3: Expertise in Hybrid QM/MM methods

12.2.5 Autumn School 2021, Slovenia - Big Data with Hadoop and Keras

- Dates: 27 – 30 September 2021
- Organizing sites: University of Ljubljana – Faculty for mechanical engineering, Aškerčeva 6, Ljubljana, Slovenia
- Venue: online due to COVID-19 restrictions
- Link: https://events.prace-ri.eu/event/1226/
- Description of contents:
  The target group of training event in Autumn of 2021 were:
  - 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.
  - Engineers from SMEs and business experts that will find this course of professional 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 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 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.
Parallelization with R	Focus of the session is on parallelization using available libraries.
Big data analysis with RHadoop	Basic concepts of big data management and analysis using RHadoop.
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.
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.

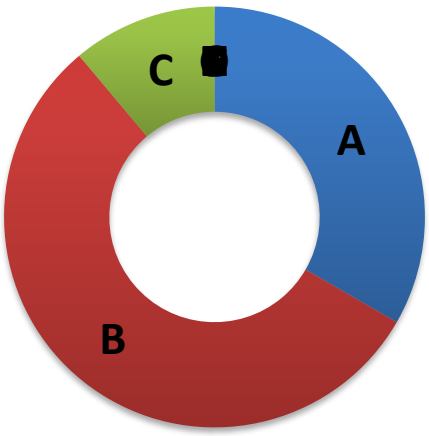
- Number of participants by country:

Country	No. of participants		Country	No. of participants
Austria	1		Ireland	1
Croatia	1		Italy	4
Czech Republic	1		Netherlands	1
Denmark	2		Nigeria	1
France	2		Slovenia	1
Germany	1		Sweden	1
India	1		Turkey	4
			Not specified	0
Suma:	**22**			

- Statistics of the feedback survey:

Overall, how would you rate this training event? Answered: 9

A	10 - excellent	3	33,33%
B	9	5	55,56%
C	8	1	11,11%
D	7	0	0,00%
E	6	0	0,00%
F	5	0	0,00%
G	4	0	0,00%
H	3	0	0,00%
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: 9

It's incredibly well, the transition to an online format is fantastic.

It was quite good, the lectures and the topics were interesting

I am looking forward to onsite events, but it was good!

In-person is better because of more informal interactions, but overall it was ok and I very much appreciated the effort to increase participation even remotely

Although online format has not the same effectiveness of an in-person course (being physically in a classroom and having the chance of interacting with others cannot be covered by online communication tools in all aspects), the format demonstrated to be very useful and provided lot of knowledge to me.

I like it, it is flexible.

For me it is an excellent format with plenty of advantages, it should be always an option

Offline learning with interaction and networking would be great idea for learning. However, the event was awesome.

I liked it for the opportunity to attend from another country and for the overall management of the course

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

Answered: *9*

I enjoyed the contents of the materials and the nature of the training.

The Material was adequate, Best: The step by step execution of the exercises

Everything was well-paced and good, to me

Working on exercises together was really helpful in grasping concepts, thus I particularly liked interactive colaboratory notebooks

The structure of the course and the provided material were enough for understanding well the topic

I liked deep learning the most.

Topic

Every thing was good

Competence and clearly explanation by the panellists, topics, materials and structure.

Where should we improve?

Answered: 6

The program is designed well even in this pace.

The duration of the sessions was sometimes too long, it is better to make shorter sessions with short breaks, and more in number to compensate,, this apply only in virtual mode.

Actually there is very few to be improved ... I would like to start again to have the chance of attending in person such kind of courses

exercises

I was getting more disturbance in sound during the course. I am not sure it is due to the problem in my system or host.

Maybe providing more practical sessions related to real world problem and/or use cases would be helpful to clarify some specific concepts in particular for the deep learning part.

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

Answered: 6

Training on Linux, and Matlab.

I am not in position to decide that

python (maybe with a focus on advanced programming techniques) for scientific applications; GPU programming (also looking at AMD tools, not only to Nvidia/CUDA); FPGA programming (this kind of devices are becoming more and more present in HPC systems, so OpenCL based programming could be of interest); advanced C/C++ programming for scientific applications.

Bioinformatics and deep learning

more about deep learning and Big data

HPC and deep learning applied to Earth observation and to medical images

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

Answered: 6

I think the training should continue online and at this pace.

"The fast response was the best. To improve, not that long lectures, but more short with small breaks if is virtual"

Availability of all materials was super. Communications have been maybe a bit too scarce (e.g. about news on how the school would be run). But it might also be a problem with my spam filter...

I think that the current system of using a mailing list for announcing the courses is fine

see #1

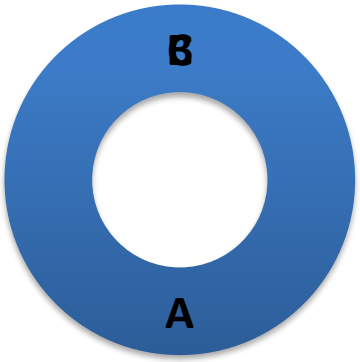
I think everything was good

The organization and the communication in preparation of the course were clear and in time.

Would you recommend this training event to others?

Answered: 9

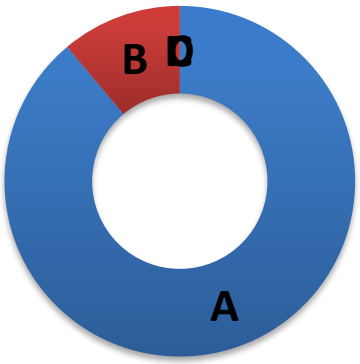
A	Yes	9	100,00%
B	No	0	0,00%
C	No selection	0	0,00%



Subject of course for me was

Answered: 9

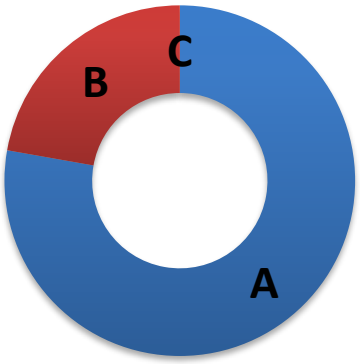
A	important	8	88,89%
B	minor	1	11,11%
C	not relevant	0	0,00%
D	no selection	0	0,00%



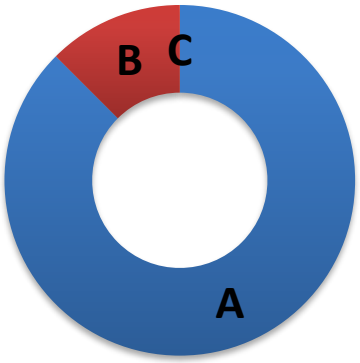
I was inspired to new ways of thinking

Answered: 9

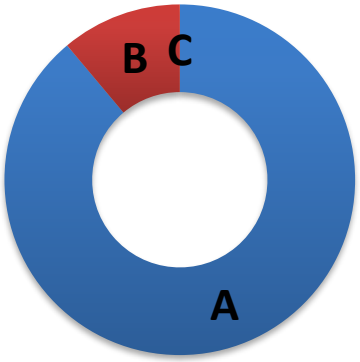
A	yes	7	77,78%
B	partially	2	22,22%
C	no	0	0,00%



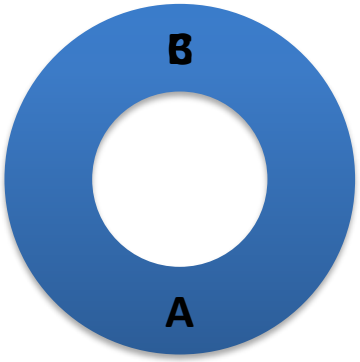
Length of course was				Answered: 8
A	adequate	7	87,50%	
B	too short	1	12,50%	
C	too long	0	0,00%	



Depth of content was				Answered: 9
A	adequate	8	88,89%	
B	too superficial	1	11,11%	
C	too profound	0	0,00%	



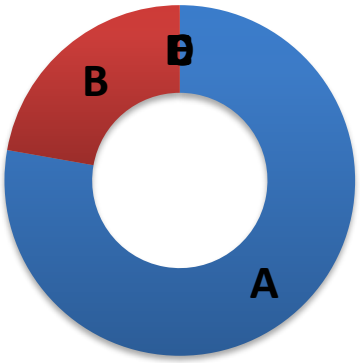
The pace of teaching was				Answered: 9
A	adequate	9	100,00%	
B	too slow	0	0,00%	
C	too fast	0	0,00%	



Teaching aids used (e.g. slides) were well prepared

Answered: 9

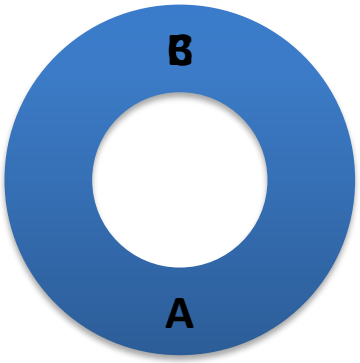
A	agree completely	7	77,78%
B	agree	2	22,22%
C	no strong feelings	0	0,00%
D	disagree	0	0,00%
E	disagree completely	0	0,00%



Hands-on exercises and demonstrations were

Answered: 9

A	adequate	9	100,00%
B	too few	0	0,00%
C	too many	0	0,00%



12.2.6 Autumn School 2021, Austria - GPU programming with CUDA

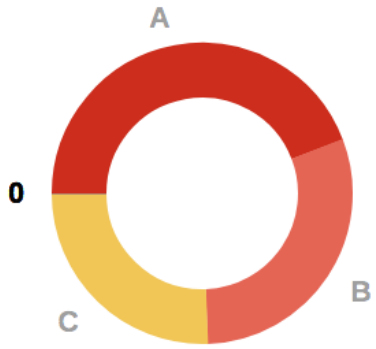
- Dates: 4 – 7 October 2021
- Organizing sites: University of Innsbruck (UIBK) and VSC (Vienna Scientific Cluster) Research Center of TU Wien, Austria (PRACE-6IP partner TU WIEN and its linked 3rd party UIBK)
- Venue: hybrid in-person (Campus Technik of the University of Innsbruck, Austria) & online format
- Link: https://events.prace-ri.eu/event/1154
- Description of contents:

Session	Description
Introduction to GPU Computing with CUDA	Necessary knowledge on how GPU hardware operates. How GPUs are different from multi-core systems. Basic features of the CUDA programming language.
Memory Hierarchies in CPU/GPU Architectures	Memory management on CPU and GPU. Performance implications. Unified Memory.
CUDA SDK – Basic Concepts	Synchronization of the work in CUDA kernels. Performance implications.
CUDA SDK – Libraries, Numerical Accuracy	Introduction to linear algebra libraries.
Best practice: How to write correct CUDA programs	Discussion of pitfalls that lead to incorrect programs. Patterns that avoid common issues.
Best practice: How to write efficient CUDA programs	How to reason about performance on GPUs. Common patterns that lead to good performance.
Using the CUDA debugger	Using the CUDA debugger to identify bugs in the code.
Using multiple GPUs & Advanced CUDA topics	A selection of advanced topics in CUDA (programming multiple GPUs, interleaving work on CPU and GPU, etc.).
Containerization of GPU applications with Singularity	Building a Singularity container for GPU applications and running this container in a job script on an HPC cluster.
Native GPU computing in Julia	Lecture and demo on native GPU computing in Julia.
GPU programming in practice I-III	Invited speakers discuss how GPU computing is used in practice, what difficulties had to be overcome, etc. for AMBER (I+II) and FELTOR (III)

- Statistics of the feedback survey:

1. Overall, how would you rate this training event? Answered: 43

		online listening		online + hands-on		no info		in-person		**total**	
	average rating	9.67		9.33		9.50		9.04		**9.19**	
	feedback rate	75+%		43+%		← ? →		82+%		**83%**	
	# feedback	3	(of 4)	6	(of 14)	6	(← ? →)	28	(of 34)	**43**	**(of 52)**
A	**10 - excellent**	2	66.67%	3	50.00%	4	66.67%	10	35.71%	**19**	**44.19%**
B	**9**	1	33.33%	2	33.33%	1	16.67%	9	32.14%	**13**	**30.23%**
C	**8**	0	0%	1	16.67%	1	16.67%	9	32.14%	**11**	**25.58%**
D	**7**									**0**	**0%**
E	**6**									**0**	**0%**
F	**5**									**0**	**0%**
G	**4**									**0**	**0%**
H	**3**									**0**	**0%**
I	**2**									**0**	**0%**
J	**1**									**0**	**0%**
K	**0 - bad**									**0**	**0%**



– Please indicate your mode of participation: in-person, online+hands-on, online-listening
– How did you like the hybrid format?

Answered: 37

28 times: *in-person* *(here omitting 21 answers without further comments)*

in-person - I don't think I would have followed otherwise.

in-person - I would have not learnt as much as I did when I would have participated online.

in-person - The event felt like a "normal" in-person event.

in-person - I am not sure the hybrid format really had a close effect as attending in person though.

in-person - Sometimes hard to follow/ask questions in RR14, otherwise excellent.

In-person - I'd suggest to improve a bit the structure of the streaming if there are multiple rooms, so that really everybody can participate actively.

in-person - I did not really like the bbb lectures.

6 times: *online+hands-on* *(here omitting 3 answers without further comments)*

online + hands-on. The experience was perfect, and well organized.

online + hands-on: It was great experience other than some hiccups on the last day of online presentation. The content was good enough to introduce basics followed by hands-on sessions.

I participated in the online+hands-on format. I enjoyed the hybrid format although it was difficult to follow the lecture when there were questions from the audience, since I couldn't hear the questions and follow the discussion.

3 times: *online-listening* *(here omitting 1 answer without further comments)*

I participated via online-listening. I liked the hybrid format very much. The course was very interesting and otherwise I wouldn't have been able to participate.

online listening (with interruptions due to other obligations on my side) - It allowed me to follow at least some parts of the course which I would have missed completely in a presence-only format.

6 times: *no answer given*

2. Training event content and feedback to lecturers (e.g. topic, materials, exercises, structure): – What did you like best? Answered: 34

Learning about the importance that memory allocation and management has on the computational time.

I liked the rooms for the hands-on

It was a great mix. I really liked that we had exactly the right amount of time to solve the exercises.

topic materials

Content of Monday and Thursday was most useful to me.

Materials, Exercises, Structure I like the best.

The best practices and tips

It is difficult to say what the outcome should have been because it seemed like the talks were pretty high-level and over most people's heads. Should participant have had any GPU programming experience? Programming? C/C++?

materials and topic

variety of topics

Hands-on, materials, structure. Well organized.

I really liked the structure of the course (explanation + hands on) and also the fact that all the material is available for future reference and to study on my own. Moreover, it was very helpful to have a separated room for the hands on part where the lecturers could help with configuration problems on the VSC and could give clarifications on the exercises. I would have liked the possibility to access the VSC platform for a few more days, but I understand that this is not feasible.

The training was well structured, in the sense that the topics had the right progression in terms of difficulty

Being basically a CUDA beginner, I liked all the lectures and the structure of the school in general

Generally excellent, although a little bit more time to do the exercises would have been nice.

I really liked the provided mixture in terms of topics and materials. I think the course was well thought out and I especially liked the inclusion of non-pure-cuda topics (containers, Feltor, ...).

I liked how for each topic there was a dedicated segment for exercises.

I think it would be even better, if we could work on one code example successively. That decreases the time we spent on understanding the overall purpose of the code and exercises would be much faster.

topic

The level and speed of the lectures and exercises was very good

All presentations were clear and it was easy to follow them, even though some content was quite advanced and I did not have much prior knowledge. The speakers made a very professional impression, not only during their talks but also when answering questions from the audience.

As online-listener, topic and materials were really good

The slides where very well prepared and understandable. It would have been very interesting to pinpoint the problem with wrong debugger output.

coffee breaks ;) and also the lectures were very good!

Topics and structure

The coding-problems where a bit hard for me.

I like that it was focused to concepts and not just on programming. Shipping exercise solution was also helpful for feedback.

Overall structure and hardworking of management and teachers

Hands-on is very important. Nice that we had enough hardware for everyone!

The topic

that there were so many different topics.

Really liked the performance lectures by Lukas Einkemmer.

advanced memory management

Some lecturers weren't the best, i.e. their mode of teaching was too slow, at times hard to understand what they were saying or what they meant. Lukas and Phillip were excellent! The rest were so and so.

– Where should we improve?	Answered: 25

-

As an intro course there is nothing to improve here.

some parallel courses for begineers

The parts I could attend are hard to be improved.

This is the best you have, Keep up your good work.

It may be limiting the scope, but it probably should try to teach a particular item of knowledge and ensuring that participants really get a good grasp of it.

exercise

A little more time for hands-on exercises

To improve the experience of online participants I would suggest to repeat all the questions coming from the audience, so that everyone can follow the discussion. Some of the lecturers did this (I really appreciated it) but some others were difficult to follow mainly for this reason.

- some arguments should be dropped, like Julia, or other too specific applications, like Amber or Feltor, which may be interesting only for a selected audience - the hands-on time should be longer, with more excercises - the solution of the exercises should be given only after the hands-on time - the exercises should be more on-point: after a given topic, the given task should be mostly on that topic and should require some reasoning for solving real-world problems regarding that topic. Instead, most of the exercises contained somewhat unrelated software-engineering problems or with purposely wrong solutions

--

A little bit more time for the exercises

I think a depper dive into what is actually happening on the GPU in terms of memory etc. could be interesting, however, I do understand that these topics might not be interesting for all, be out of scope or even partly non disclosed information by NVIDIA.

.

part of the MD code was not interesting

I do not see a need nor an obvious possibility for improvement.

It could be interesting to choose a project from a list of projects and implement this on our own (with a short presentation in the end) to apply the learned subjects on your own. This of course is only possible with a longer school.

explaining the first login, maybe do that together a little bit slower. I would have needed more time for the exercises, but this way there was more content and I can practice at home

/

Lab sessions

Some lectures were a bit fuzzy, e.g. Julia and Introduction (CUDA is very easy, you only have to do those three things ...)

more time for the exercises / shorter.

For me the content could have been more advanced.

Have longer hands on sessions and maybe provide a set of problems for students to solve as practice. We cant immediately start using these concepts in our research

Could potentially invited better lecturers!

3. Which future training topics would you like to be provided by PRACE or the training host? Answered: 24

Since this was a GPU parallelization topic, MPI parallelization would also be of great interest for those who can only afford a central processing unit.

Machine learning , Reinforcement learning

AI in CUA

I would really like a hackathon-like event where teams can focus on their own code / problems while being supported during the attempts. Minimal examples as presented during the course often do not give one the tools to address real-world problems. Topics: CFD, GPU, Profiling.

Working on CUDA GPU with FORTRAN language.

Deep learning

Robotic simulations with GPU programming

MPI, OpenMP, OpenCL

some C/C++ CUDA abstractions, like thrust

An MPI course would be really interesting to me

** Distributed memory parallelisation (MPI) * Modern C++*

While the training host provides excellent advanced programming language courses, including external lecturers, I believe some people might benefit from basic programming courses, especially when coming from the domain sciences (C++, Fortran, ...).

MPI, and again CUDA

CUDA + MPI, OpenACC+MPI

Workflow for writing and running code on HPC systems

-

CUDA on Jetson Modules and there pitfalls CUDA for realtime data processing How to optimize CUDA code (more indepth)

Profiling and debugging when MPI, CUDA, OpenMP and so on is used.

Quantum-computig, maybe it is a little early, but better to early than to late.

Heterogeneous computing (GPU+FPGA+CPU)

Accelerator abstraction frameworks? How to get away from CUDA and NVidia vendor lock-in.

(Many) (much) more advanced cuda courses.

more CUDA!!! <3

Numerical methods in physics and astrophysics

4. Training event organisation (e.g. announcement, registration, changes due to COVID-19): – What did you like best? – Where should we improve? Answered: 24

Keine Ahnung! Alles waren gut!

It was lla okay.

Very kind and responsive, despite of trouble with e-mail communication (cause possibly on my side)

The smooth organising of hybrid event is not easy, and you have pulled it off with ease. It's really great experience to attend these sessions and hands-on exercises.

The time table was well managed. Pretty organised school.

Everything was well organized. Nothing to complain here.

Everything perfect

All perfect

No comments on that, everything was always up to date

Organization was generally really good. The only thing, that was somewhat less nice (although probably not avoidable due to covid), was, that a third of the audience had to take part in RR14 via live stream. But the organization of the streaming setup could be improved a little bit and it would have been nice if the speakers had repeated questions from the audience, so that the people attending via stream could also her them and not only the answers.

I again want to underline the excellent organisation of the event, considering it's hybrid nature, the ongoing pandemic and the added complexity of having two different lecture rooms on premise! Mr. Eduard Reiter along with the rest of the organisation team really did a great job!

It was great.

organization was perfect

I was satisfied with all organisational aspects of the event. I only got one minor suggestion: Maybe one could label food in the coffee breaks (what is vegetarian/vegan/lactose free?)

A recomondation for a hotel or even a contigent of rooms at a hotel would have been helpful.

organisation was great!

Everything was organized very well

Free coffee, snacks and meals

The separated room for on-side people was unfortunately and should be avoid next time. It does not make sense to be on-place and watch stream at the same time. Otherwise organization was great. I appreciate the tour and dinner.

Accommodation was much expensive, it should be arranged by the org

Well organised. Not much to improve.

the get together could be on the first day, in order to get to know each other immediately.

All perfect - thanks!

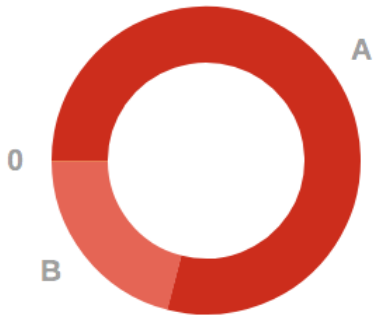
Reasonably well done

5. Would you recommend this training event to others? Answered: 43

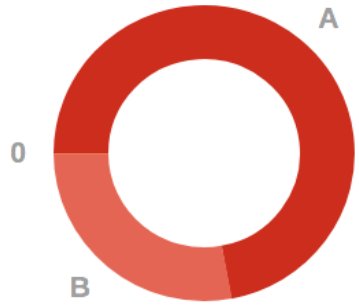
A	yes:	43	100.00%
B	no:	0	0%

6. Subject of course for me was Answered: 43

A	important:	34	79.09%
B	minor:	9	20.93%
C	not relevant:	0	0%



7. I was inspired to new ways of thinking			Answered: 43
A	yes:	31	72.09%
B	partially:	12	27.91%
C	no:	0	0%

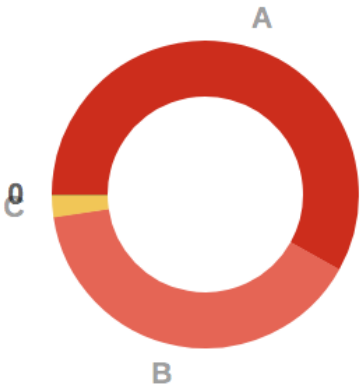


8. Length of course was			Answered: 43
A	adequate:	40	93.02%
B	too short:	2	4.65%
C	too too long:	1	2.33%

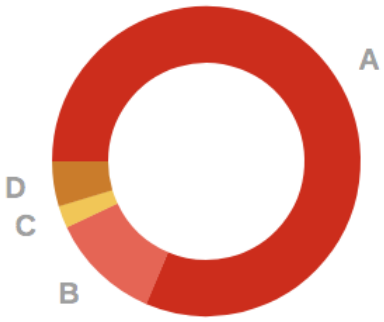
9. Depth of content was			Answered: 43
A	adequate:	39	90.70%
B	too superficial:	3	6.98%
C	too profound:	1	2.33%

10. The pace of teaching was			Answered: 43
A	adequate:	39	90.70%
B	too slow:	1	2.33%
C	too fast:	3	6.98%

11. Teaching aids used (e.g. slides) were well prepared			Answered: 43
A	agree completely:	25	58.14%
B	agree:	17	39.53%
C	no strong feelings:	1	2.33%
D	disagree:	0	0%
E	disagree completely:	0	0%



12. Hands-on exercises and demonstrations were			Answered: 43
A	adequate:	35	81.40%
B	too few:	5	11.63%
C	too many:	1	2.33%
D	No selection:	2	4.65%



12.2.7 Autumn School 2021, Finland - Harnessing the EuroHPC Flagship Supercomputers

- Dates: 11 - 15 October 2021
- Organizing sites: CSC – IT Center for Science Ltd.
- Venue: Vuokatti Sport Resort, Sotkamo Finland
- Link: https://events.prace-ri.eu/event/1188/
- Description of contents:

There were three parallel hands-on tracks in the school. The actual content of hands-on tracks consisted of the following topics.

- Introduction to Deep Learning - Dr. Markus Koskela & Dr. Mats Sjöberg, CSC
  - Introduction to deep learning
  - Multi-layer perceptron networks
  - Images and convolutional neural networks
  - Text data, embeddings, recurrent neural networks
  - Attention models
  - GPUs and batch jobs (LUMI or Puhti)
  - Using multiple GPUs
  - Exercises in the cluster

- Introduction to GPU Programming with OpenMP - Dr. Jussi Enkovaara, Dr. Pekka Manninen, CSC & Dr. Alfio Lazzaro, HPE HPC/AI Research Lab, HPE Switzerland
  - Introduction to GPUs
  - OpenMP programming model for GPUs
  - Execution controls
  - Data transfers
  - Performance analysis
  - Using multiple GPUs

- Hackathon: Optimizing GPU applications on LUMI supercomputer - Dr. Fredrik Robertsen, CSC, Dr. George S. Markomanolis, CSC & Dr. Michael Klemm, AMD
  - The participants are expected to bring a code that they expect to port or optimize for GPUs. Some instructors were available to help the participants of this hands-on track.

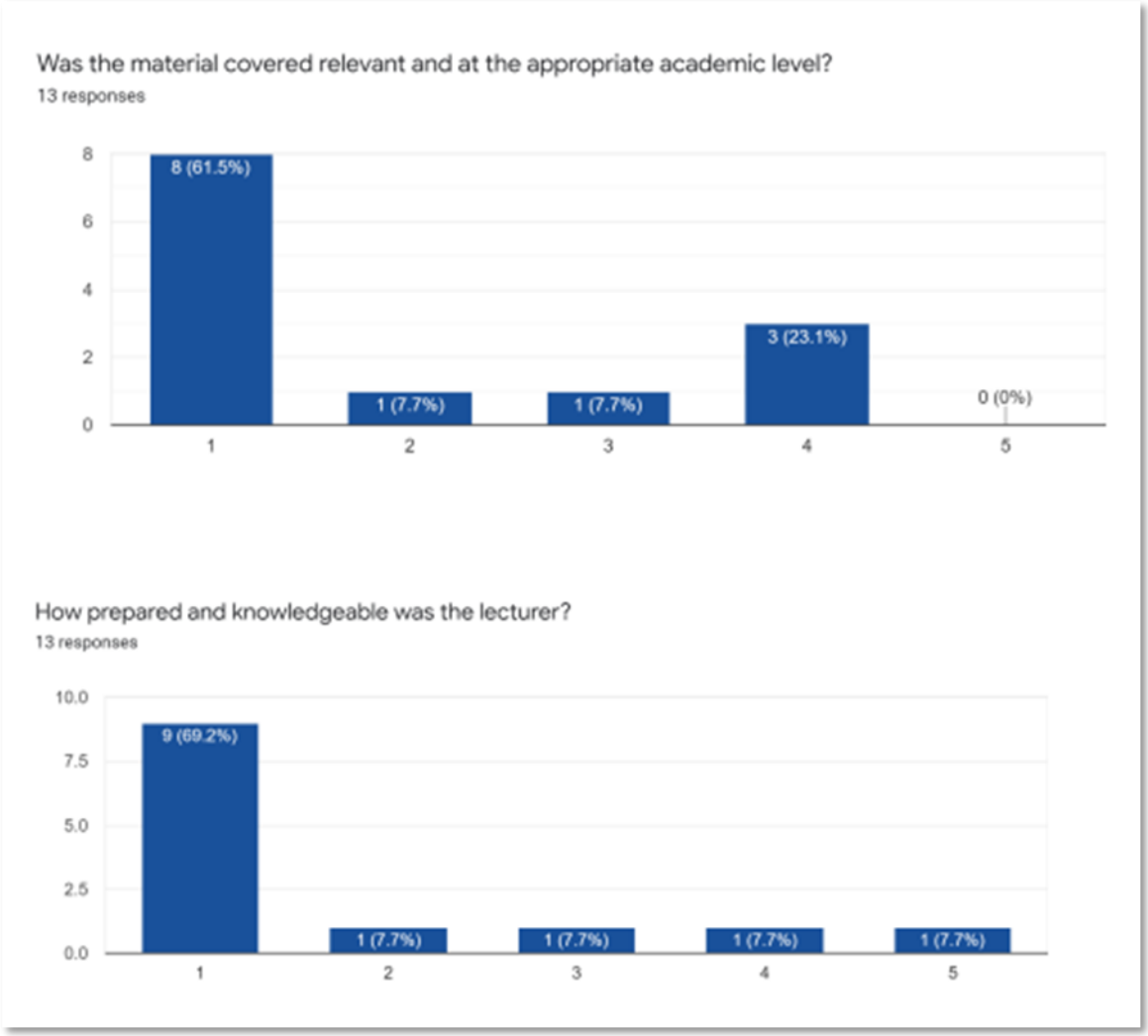
In addition to the parallel tracks, there were a keynote speech and science cases on utilization of simulation, AI and HPDA methods by eminent researchers (see the final agenda on the appendix 1). The third day (Thursday 14th of October 2021) featured a visit to LUMI data center including lectures on the system architecture as well as on how supercomputers are operated

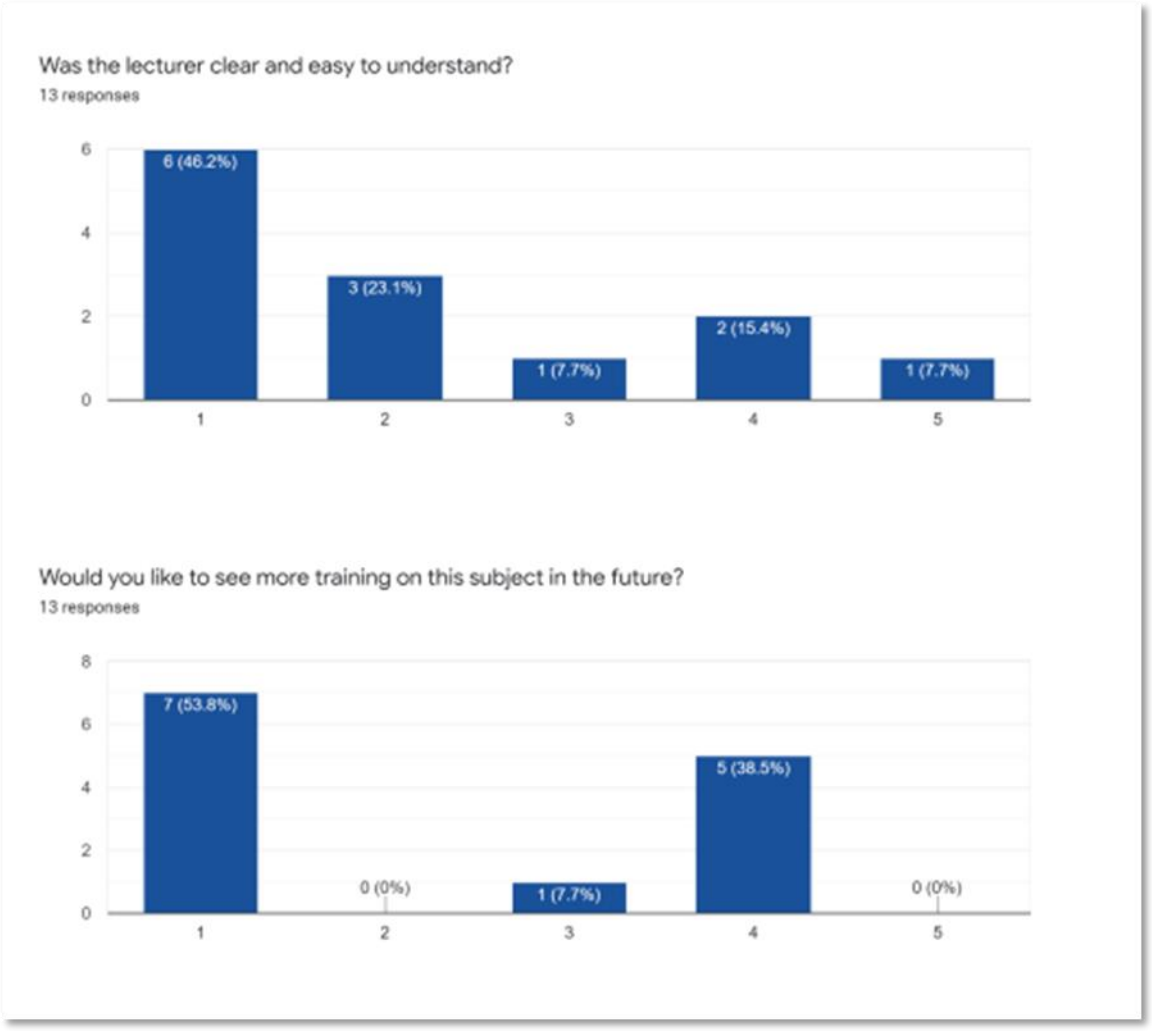
12.2.8 Winter School 2021, Israel - Converging HPC Infrastructure & Methodologies

- Dates: 7-9 December 2021
- Organizing sites: Inter-University Computation Center (IUCC)
- Venue:online due to COVID-19 restrictions
- Link: https://events.prace-ri.eu/event/1215/
- Description of contents:
  - HPC Visualizations: HPC Visualization for atoms and continuum, including installation of AViz codes and examples with wrappers tied to LAMMPS/QUANTUM ESPRESSO/VASP for atomistic and general datafiles for continuum.
  - MPI, OpenMP, and Profiling: General introduction to Parallel Processing, the Message Passing Interface (MPI), OpenMP, profiling parallel programs and hands-on practice of each.
  - Scientific Computing with EC2 and S3 on AWS, hands-on practice: Introduction to cloud for scientific computing. The goal is to give students the skills to use AWS for scientific computing inspired by genomics use cases.
  - HPC on AWS: set up and configuration, hands-on practice: Setting up HPC compute on AWS using open source tools to stand up a HPC cluster in an AWS account, allowing scaling up HPC applications to 1000s of cores.
  - Heterogeneous HPC and remote visualisation on AWS, hands-on practice: Demonstration of Heterogeneous (CPU, GPU, Graviton, etc) HPC infrastructure for performance optimization demonstrated with common applications, including remote visualization.
  - Running large-scale OpenFOAM simulations on AWS: Demonstration of large-scale OpenFOAM simulation on AWS, including tooling for data visualization.
  - Large-scale GROMACS biomolecular simulations using AWS Batch: How biomolecular simulations scale on AWS CPU and GPU instances across regions using GROMACS through AWS Batch.
  - Event-driven Simulation at scale using EFISPEC3D on AWS: Setting up event-driven workflows on AWS to perform realistic earthquake ground-motion simulations using EFISPEC3D.
  - Kubernetes and docker for massive AI workloads.

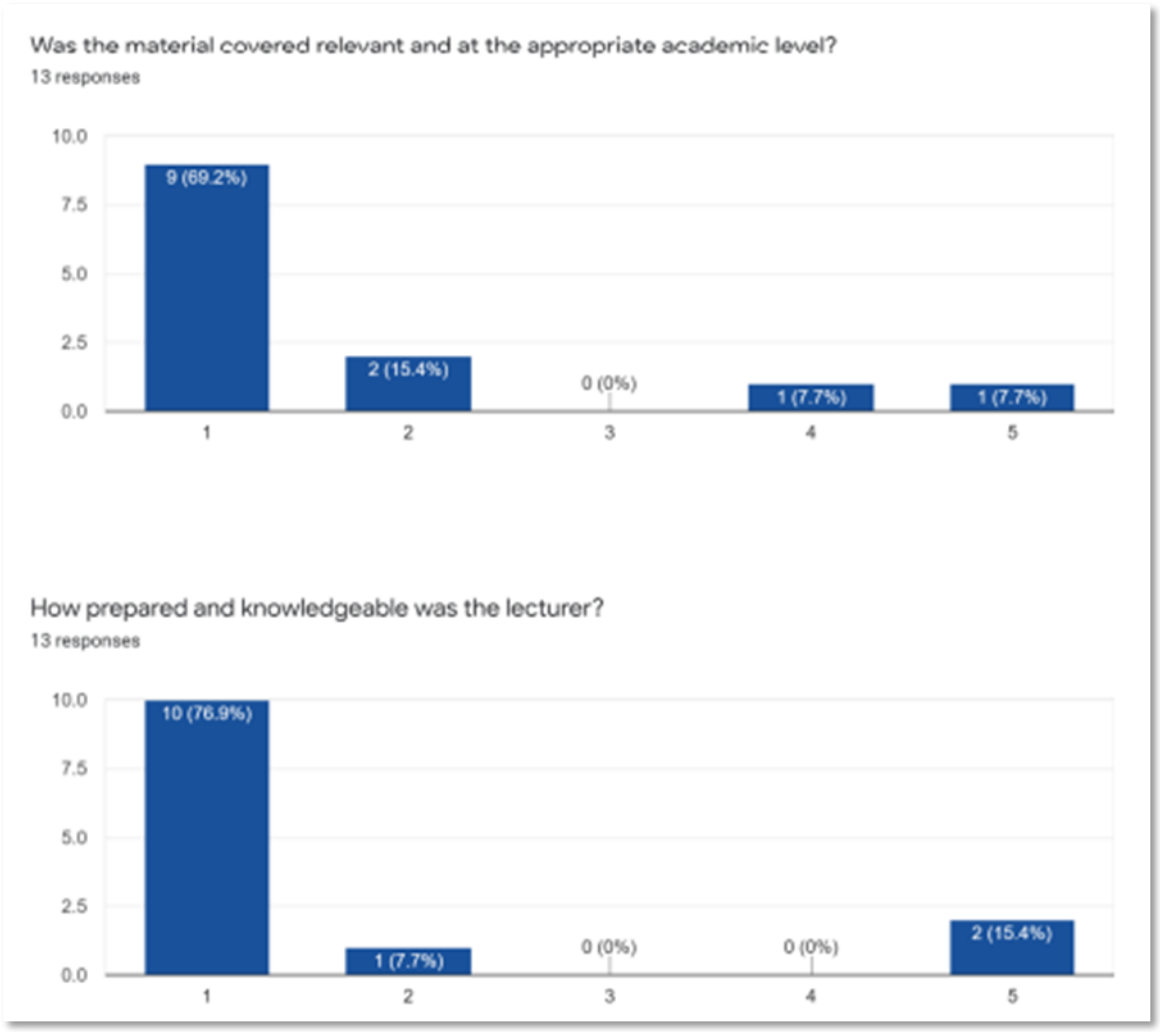
- Statistics of the feedback survey:

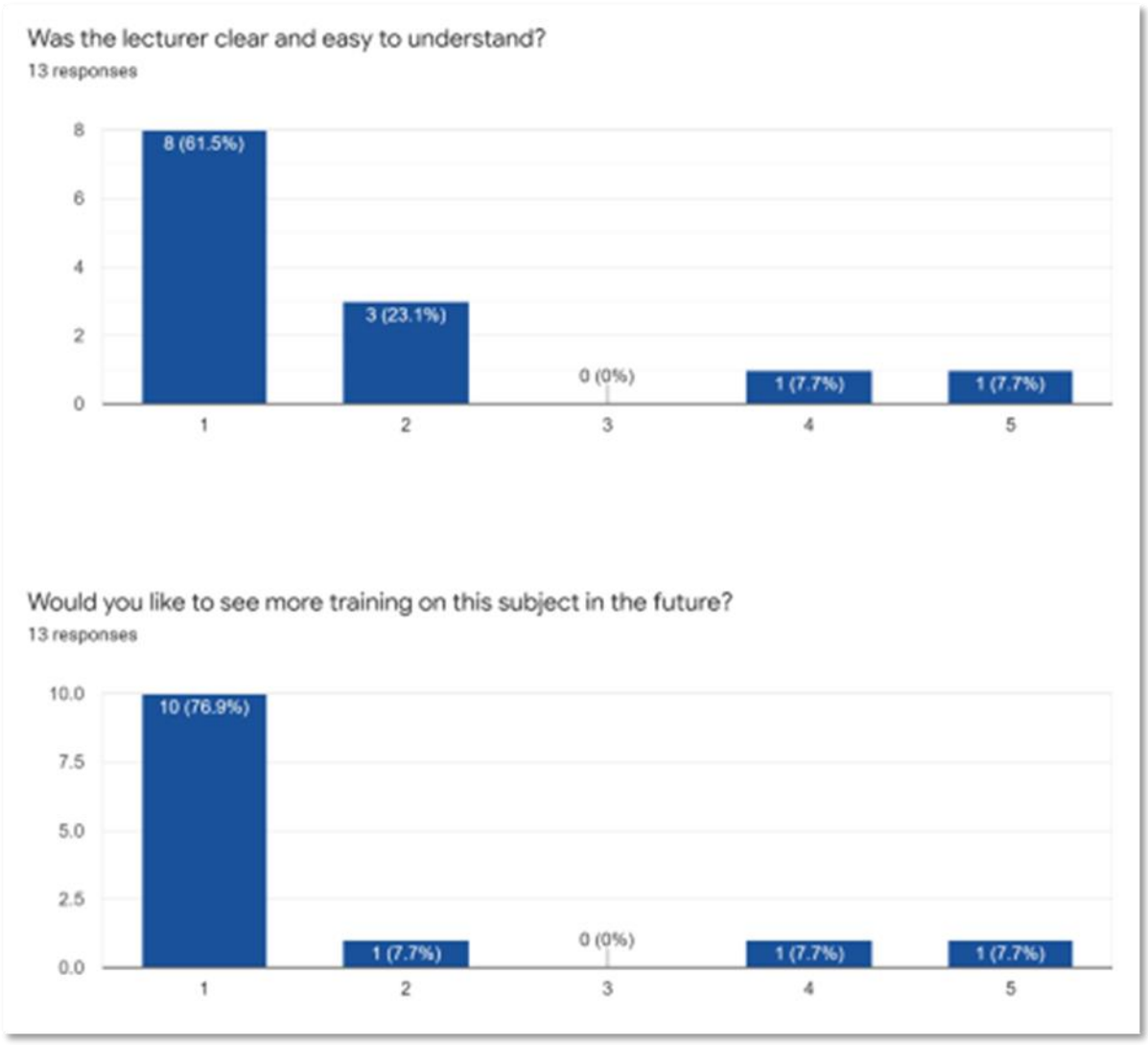
HPC Visualizations, Dr. Joan Adler



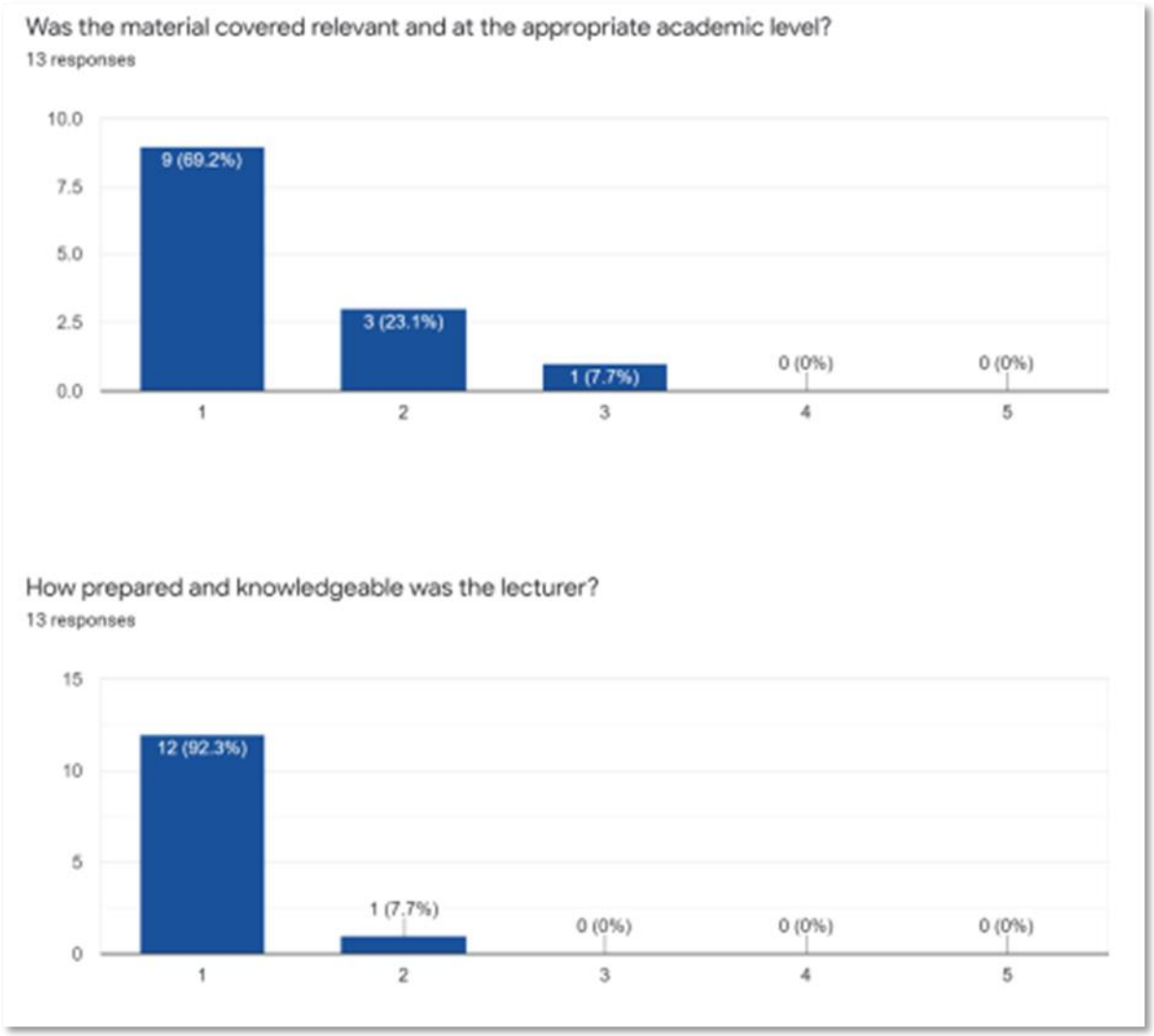


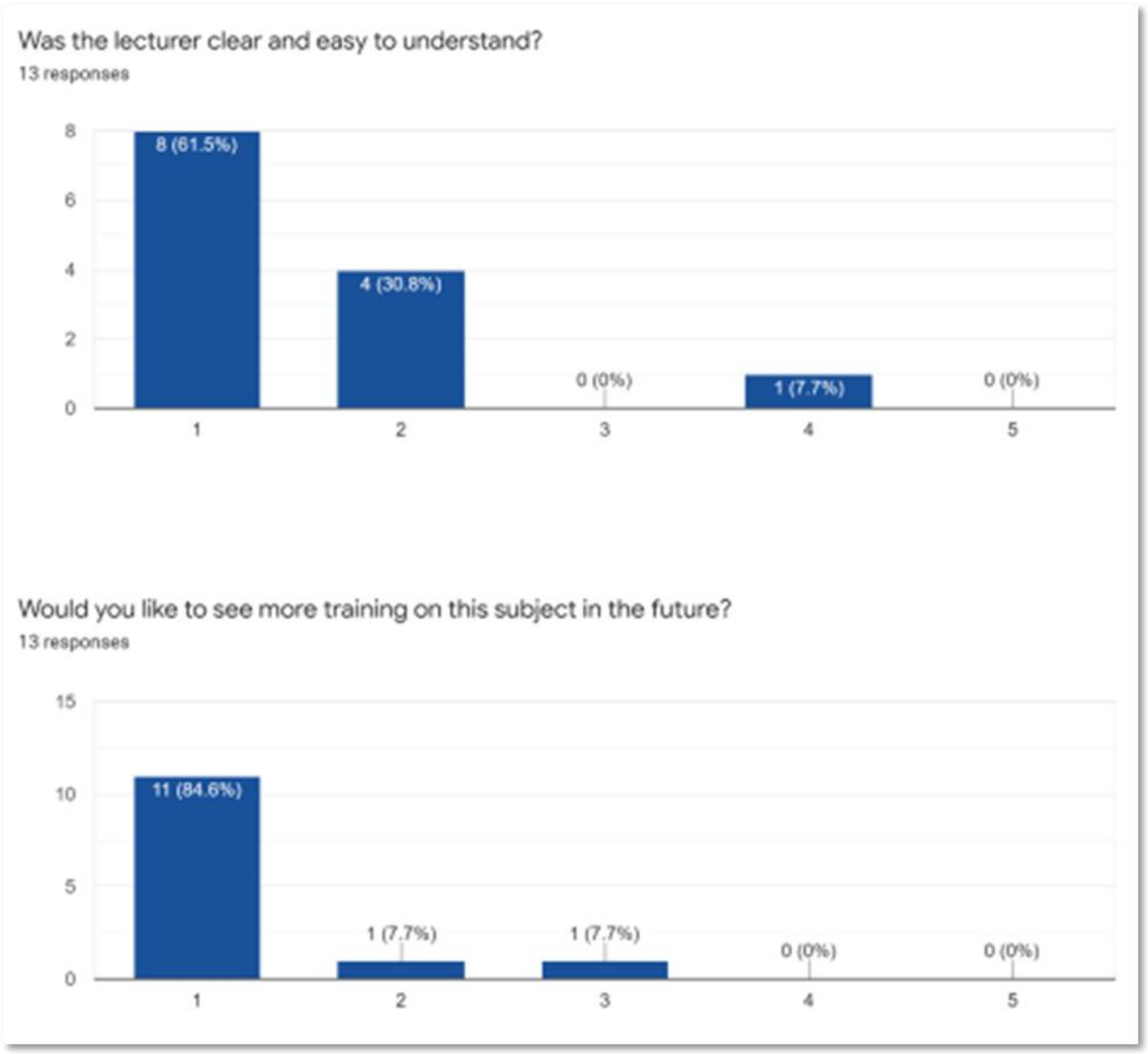
Suggestions for improvement: Clearer presentation as needed for people not coming with relevant background. The subject matter was very good. Self-practice tasks may be assigned to participants so that learning level can be time bound and more productive.


Was the material covered relevant and at the appropriate academic level?
13 responses
10.0
7.5
5.0
2.5
0.0
9 (69.2%)
2 (15.4%)
0 (0%)
1 (7.7%)
1 (7.7%)
1
2
3
4
5
How prepared and knowledgeable was the lecturer?
13 responses
10.0
7.5
5.0
2.5
0.0
10 (76.9%)
1 (7.7%)
0 (0%)
0 (0%)
2 (15.4%)
1
2
3
4
5



Suggestions for improvement: It was excellent. Lecture session was enriched and ideal for the limited time bound session. Wish more time was allotted. The course ranged from the very basics to an advanced level, which is always challenging since beginners need to introduction at the beginning, and experienced users do not find this useful, and vice versa.


Was the material covered relevant and at the appropriate academic level?
13 responses
10.0
7.5
5.0
2.5
0.0
9 (69.2%)
3 (23.1%)
1 (7.7%)
0 (0%)
0 (0%)
1
2
3
4
5
How prepared and knowledgeable was the lecturer?
13 responses
15
10
5
0
12 (92.3%)
1 (7.7%)
0 (0%)
0 (0%)
0 (0%)
1
2
3
4
5



Suggestions for improvement: The tasks should have been more detailed enough. There where parts where one got stuck and could not continue because of errors and there was no solutions in the task documentation. It would have been helpful to demonstrate the full the solution after each task. This step is important as it aligns students to the same line after each task and is especially crucial when the tasks are dependent on one another. Kubernetes and docker on the same day was a bit too hard and perhaps should be split. More training for beginners would be welcome.

12.3 Reports from the International HPC Summer Schools

12.3.1 International HPC Summer School 2019

- Dates: 7-12 July 2019
- Venue: RIKEN Center for Computational Science, Kobe, Japan
- Participants: 81
- Content and Programme: https://ss19.ihpcss.org/agenda/

Evaluation:

The feedback from participants were overwhelmingly positive. The following scores were obtained from 70 survey responses (Scale 1: strongly disagree – 5: strongly agree).

Question	N	M	SD
b) The summer school was well organized	70	4.73	0.50
c) I am satisfied with the delivery format of the summer school	70	4.41	0.64
d) I am satisfied with the amount of hands-on activities	70	3.84	0.92
f) I am satisfied with the technical assistance available during the summer school (i.e. mentors, session facilitators, extra help sessions, etc)	70	4.57	0.57
m) The knowledge/skills I gained during this summer school will significantly contribute to my work/research	70	4.51	0.63
n) I know the next step for me to build on what I learned at this summer school	70	4.40	0.62
p) I plan on obtaining (or currently have) access to SciNet, PRACE, RIKEN, or XSEDE resources	70	4.30	0.82

12.3.2 International HPC Summer School 2021

- Dates: 18-30 July 2021
- Venue: Online (dual sessions for two time zones)
- Participants: 64
- Content and Programme: https://ss21.ihpcss.org/agenda/

Evaluation:

On the last day of the Summer School, students were asked to complete an online survey asking them to evaluation their experience. Sixty percent of students responded. Results were quite positive:

- 91% of participants reported that their goals for IHPCSS were achieved.
- 97% felt that the Summer School was well organized.
- 97% believed that the Code of Conduct was effective at setting expectations.
- 81% were satisfied with their mentor interactions.
- 87% were satisfied with technical assistance and support they received during the hands-on and extra help sessions.

- 91% reported that the skills/knowledge gained in the Summer School would significantly contribute to their research.
- 94% would rate their Summer School experience as successful.
- Students requested even more hands-on exercises.
- While most students were not significantly disadvantaged with the online format, they felt that it was difficult to connect student to student, especially with students that they did not know already.
- Additional topics suggested for future Summer Schools include I/O optimization, quantum computing, Python parallel computing, alternative to OpenACC, how HPC is applied in different fields, cloud computing, and task-based parallelism.
- 88% would return as mentors.

12.3.3 International HPC Summer School 2022

- Dates: 19-24 July 2022
- Venue: Athens, Greece
- Participants: 76
- Content and Programme: https://ss22.ihpcss.org/agenda/

Evaluation:

On the last day of the Summer School, students were asked to complete an online survey asking them to evaluate their experience. Nearly 80% of students responded. Results were mostly very positive.

- 98.2% would rate their Summer School experience as successful.
- 94.4% reported that the skills/knowledge gained in the Summer School would
- significantly contribute to their research.
- 92.7% reported that their goals for IHPCSS were achieved.
- 90.9% felt that the Summer School was well organized.
- 90.6% would return as mentors.
- 88.9% felt the Code of Conduct was effective in setting expectations.
- 85.5% were satisfied with technical assistance and support they received during the hands-on and extra help sessions.
- 72.7% were satisfied with their mentor interactions.
- 69.0% of respondents felt the health and safety precautions (i.e., testing, single rooms, masks, etc.) were sufficient. The rest were neutral (14.5%) or felt the precautions were not sufficient (16.4%).
- Half of participants found the Summer School to be of neutral challenge; one third found it difficult or very difficult.
- Additional topics suggested for future Summer Schools include computer architecture and system design, OpenMP, OpenMPI, numerical libraries, parallel debugging, HPC for mathematical optimization, and GPU parallelization techniques.
- Students requested more time for hands-on exercises.

12.4 Reports from PRACE Training courses in Bulgaria

I. Event title: PRACE Course: HPC Fundamentals for end-users, February 1-4, 2022

Venue: Online via Zoom

Organizing sites

NCSA Bulgaria and PetaSC/Sofia TechPark, Bulgaria, Center of Excellence in Combustion (CoEC), BioExcel Centre of Excellence, STFC Daresbury Laboratory, UK.

Description

HPC Fundamentals for end-users was an introductory course on how to use Discoverer supercomputer, a EuroHPC petascale system capable of executing more than 4.2 Petaflops Rmax and over 6 petaFLOPS Rpeak, by users with no prior exposure to supercomputing systems. This was the first training course in a series of two courses for beginner and intermediate HPC users that allowed them to master their skills, knowledge and confidence to work with supercomputing environments. The course started with introduction to the Discoverer systems and computing architecture including storage subsystem and computer network infrastructure. During the four days training, there were a number of hands-on exercises so that attendees gained immediate experience on working in typical user environment by building and running state of the art parallel codes on Discoverer supercomputing system. Practical sessions covered examples from different research fields such as Life Sciences, Material Science and Multiphysics simulations. Sofia TechPark graciously provided Discoverer compute resources for the hands-on sessions.

List of Speakers / Lectures

Dr. Valentin Pavlov, NCSA, Bulgaria / Introduction to Parallelization Paradigms - usage of MPI, OpenMP, Vectorization

Dr. Veselin Kolev, PetaSC, Sofia Tech Park, Bulgaria / Introduction to modern HPC architectures and Hierarchical optimization of Parallel processes/processing with focus on Discover

Dr. Arno Proeme, EPCC, UK & BioExcel Centre of Excellence / Hands-on quantum chemistry with CP2K on Discoverer: running efficient jobs and building CP2K from source

Dr. Eduardo J. Pérez Sánchez and Dr. Anurag Surapaneni, Barcelona Supercomputing Centre, Spain / Introduction to CFD from Fundamentals to Applications: Hands on examples with Alya

Dr. Ricard Borrell, Barcelona Supercomputing Centre, Spain / High-Performance Computing applied to CFD. Hands on examples with Alya.

Dr. Guillaume Houzeaux, Barcelona Supercomputing Centre, Spain / Parallel algorithms for Computational Mechanics

Dr. Stephen Farr, EPCC, UK & BioExcel Centre of Excellence / Hands-on Molecular Dynamics with GROMACS on Discoverer: running efficient jobs and building GROMACS from source

Prof. Dr. Ilian Todorov, STFC Daresbury Laboratory, UK / Molecular Modelling on the atomistic scale with DL_POLY

Dr. Alin Elena, STFC Daresbury Laboratory, UK / Molecular Modelling on the atomistic scale with DL_POLY – Hands-on

Dr. Michael Seaton, STFC Daresbury Laboratory, UK / Molecular Mesoscale modelling on HPC with DL_MESO and Compiling and running DL_MESO – Hands-on

Dr. Chin W Yong, STFC Daresbury Laboratory, UK / DL_FIELD: A force field setup tool for DL_POLY Introduction and demonstrations

Number of participants by country

A total of 58 participants from 5 countries registered in the PRACE Course: HPC Fundamentals for end-users with an average participation rate of 33 students per day over the span of the course. The course achieved an overall rating of 8.6 (1: worst, 10: excellent).

Country	Count
Bulgaria	44
Croatia	1
Greece	6
Romania	1
Turkey	6
Total	**58**

II. Event title: PRACE course: HPC - Intermediate Concepts for end-users, April 11-14, 2022

Venue: Online via Zoom

Organizing sites

NCSA Bulgaria and PetaSC/Sofia TechPark, Bulgaria

Description

The PRACE Course: "HPC - Intermediate concepts for end-users" is intended for researchers and IT specialists having basic knowledge of HPC usage wishing to advance in the field. It builds on the top of the first PRACE Course HPC Fundamentals for end-users, February 1-4, 2022 and extends it by discussing the profiling and scaling of parallel applications, which is extremely important for efficiently running simulations on Petascale systems. The course starts with an introduction to modern build tools and parallel frameworks including TBB, OpenACC and DC++. It then proceeds to present the concept of profiling parallel applications, techniques and important metrics, demonstrated with an example of a simple implementation of the Conjugate Gradient algorithm. The third day is dedicated to weak and strong scaling procedures, demonstrated on a state-of-the-art scientific parallel application. The last day is fully dedicated to the versatile use of Python in HPC. PetaSC/Sofia TechPark will graciously provide Discoverer compute resources for the hands-on sessions.

List of Speakers

Assoc. Prof. Peicho Petkov, NCSA, Bulgaria

Dr. Valentin Pavlov, NCSA, Bulgaria

Dr. Veselin Kolev, PetaSC, Sofia Tech Park, Bulgaria

Number of participants by country

A total of 41 students from 9 European countries registered in the event with an average participation rate of 19 students per day over the span of the course. Out of all attended students, 8 people answered the survey. The course achieved an overall rating of 9.5 (1: worst, 10: excellent).

Country	Count
Bulgaria	28
Greece	1
Croatia	1
Germany	1
France	1
Romania	1
Serbia	3
Turkey	4
Ukraine	1
Total	**41**

12.5 Reports from On-demand events in PRACE-6IP

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

- Event date: 23-27 September 2019
- Event venue: Trieste, Italy
- Participants: 26 from 19 countries

Content and Comments:

The EUDAT-PRACE Summer School on managing scientific data from analysis to long term archiving, kindly hosted by the the International Centre for Theoretical Physics (ICTP) of Trieste (Italy), welcomed a total of 26 Masters and PhD students and researchers from all over the world from diverse disciplines, such as computer & information sciences, earth and environmental sciences, HPC, biological sciences, chemical sciences, the clinical medicine field and many others.

Experienced and motivated trainers guided the students on a 5-day journey through a typical research data lifecycle (data discovery; data processing; data analysis; data preservation and publishing) combining traditional theoretical lessons with hands-on sessions. Event was found useful by the participants and increased fruitful collaboration between the participants and trainers from EUDAT and PPRACE.

12.5.2 Advanced Gromacs, HADDOCK + PMXWorkshop

- Event date: 9-11 October 2019
- Event venue: CSC, Espoo, Finland
- Participants: 24 on-site + 10 on-line

Content and Comments:

The workshop introduced participants withHADDOCK (High Ambiguity Driven protein-protein DOCKing), information-driven flexible docking approach for the modeling of biomolecular complexes, and PMX, service for users who need to do free energy calculations. PMX utilizes the Gromacs classical molecular dynamics simulation engine to perform calculations at the background. The workshop also covered advanced usage of Gromacs itself in particular on HPC environment. The event was found well organized and useful by the participants and generated fruitful and needed interaction between BioExcel CoE.

12.5.3 HPC Workshop on Containers and Unikernels

- Event date: 5-9 July 2021
- Event venue: University of Ljubljana, Slovenia
- Participants: 46 participants from 17 countries

Content and Comments:

This online workshop introduced participants with several container platforms (Docker, Singularity, Sarus, Charliecloud) and provided hands-on MPI and GPU examples. In addition, with a demo on Unikernels. The Piz-Daint Supercomputer was used in the hands on excercises. The participants found the event useful, appreciated the trainers expertise on the topics chosen and found the event in general as a well organised online event.