
# E-Infrastructures
# H2020-EINFRA-2016-2017

# EINFRA-11-2016: Support to the next implementation phase of Pan-European High Performance Computing Infrastructure and Services (PRACE)

## PRACE-5IP

## PRACE Fifth Implementation Phase Project

**Grant Agreement Number: EINFRA-730913**

**D4.2**

# Final PRACE Training Report
***Final***

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## List of Acronyms and Abbreviations

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

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|---|---|
| Tier-0 | Denotes the apex of a conceptual pyramid of HPC systems. In this context, the Supercomputing Research Infrastructure would host the Tier-0 systems; national or topical HPC centres would constitute Tier-1 |
| UEABS | Unified European Application Benchmark Suite |

## List of Project Partner Acronyms

| | |
|---|---|
| BADW-LRZ | Leibniz-Rechenzentrum der Bayerischen Akademie der Wissenschaften, Germany (3rd Party to GCS) |
| BILKENT | Bilkent University, Turkey (3rd Party to UYBHM) |
| BSC | Barcelona Supercomputing Center - Centro Nacional de Supercomputacion, Spain |
| CaSToRC | Computation-based Science and Technology Research Center, Cyprus |
| CCSAS | Computing Centre of the Slovak Academy of Sciences, Slovakia |
| CEA | Commissariat à l'Energie Atomique et aux Energies Alternatives, France (3rd Party to GENCI) |
| CESGA | Fundacion Publica Gallega Centro Tecnológico de Supercomputación de Galicia, Spain, (3rd Party to BSC) |
| CINECA | CINECA Consorzio Interuniversitario, Italy |
| CINES | Centre Informatique National de l'Enseignement Supérieur, France (3rd Party to GENCI) |
| CNRS | Centre National de la Recherche Scientifique, France (3rd Party to GENCI) |
| CSC | CSC Scientific Computing Ltd., Finland |
| CSIC | Spanish Council for Scientific Research (3rd Party to BSC) |
| CYFRONET | Academic Computing Centre CYFRONET AGH, Poland (3rd party to PNSC) |
| EPCC | EPCC at The University of Edinburgh, UK |
| ETHZurich (CSCS) | Eidgenössische Technische Hochschule Zürich – CSCS, Switzerland |
| FIS | Faculty of Information Studies, Slovenia (3rd Party to ULFME) |
| GCS | Gauss Centre for Supercomputing e.V., Germany |
| GENCI | Grand Equipement National de Calcul Intensif, France |
| GRNET | Greek Research and Technology Network, Greece |
| ICHEC | Irish Centre for High-End Computing, hosted by NUI Galway |
| INRIA | Institut National de Recherche en Informatique et Automatique, France (3rd Party to GENCI) |
| IST | Instituto Superior Técnico, Portugal (3rd Party to UC-LCA) |
| IT4I | IT4Innovations, National supercomputing centre at VŠB-Technical University of Ostrava, Czech Republic |
| IUCC | Inter University Computation Centre, Israel |
| JUELICH | Forschungszentrum Juelich GmbH, Germany |
| KIFÜ (NIIFI) | Governmental Information Technology Development Agency, Hungary |
| KTH | Royal Institute of Technology, Sweden (3rd Party to SNIC) |
| LiU | Linkoping University, Sweden (3rd Party to SNIC) |
| NCSA | National Centre for Supercomputing Applications, Bulgaria |
| NTNU | The Norwegian University of Science and Technology, Norway (3rd Party to SIGMA) |

| | |
|---|---|
| NUI Galway | National University of Ireland Galway, Ireland |
| PRACE | Partnership for Advanced Computing in Europe aisbl, Belgium |
| PSNC | Poznan Supercomputing and Networking Center, Poland |
| RZG | Max Planck Gesellschaft zur Förderung der Wissenschaften e.V., Germany (3rd Party to GCS) |
| SIGMA2 | UNINETT Sigma2 AS, Norway |
| SNIC | Swedish National Infrastructure for Computing (within the Swedish Science Council), Sweden |
| STFC | Science and Technology Facilities Council, UK (3rd Party to EPSRC) |
| SURFsara | Dutch national high-performance computing and e-Science support center, part of the SURF cooperative, Netherlands |
| UC-LCA | Universidade de Coimbra, Labotatório de Computação Avançada, Portugal |
| UCPH | Københavns Universitet, Denmark |
| UHEM | Istanbul Technical University, Ayazaga Campus, Turkey |
| UiO | University of Oslo, Norway (3rd Party to SIGMA) |
| ULFME | Univerza V Ljubljani, Slovenia |
| UmU | Umea University, Sweden (3rd Party to SNIC) |
| UnivEvora | Universidade de Évora, Portugal (3rd Party to UC-LCA) |
| UPC | Universitat Politècnica de Catalunya, Spain (3rd Party to BSC) |
| UPM/CeSViMa | Madrid Supercomputing and Visualization Center, Spain (3rd Party to BSC) |
| USTUTT-HLRS | Universitaet Stuttgart – HLRS, Germany (3rd Party to GCS) |
| WCNS | Politechnika Wroclawska, Poland (3rd Party to PNSC) |

# Executive Summary

PRACE Training Work Package (WP4) of the PRACE Fifth Implementation Phase (PRACE-5IP) project is responsible for the training activities of PRACE. WP4 delivers an annually evaluated, extensive offering of face-to-face training from PRACE Training Centres (PTCs); on-demand training events; online training courses such as the Massive Open Online Courses (MOOCs); the training code repository (CodeVault) and the PRACE training portal itself. This deliverable is the final report of all the PRACE-5IP training activities during the project.

During the PRACE-5IP project, the six PRACE Advanced Training Centres were complemented by four PRACE Training Centres to the network, which have collectively been re-branded as a network of 10 PRACE Training Centres (PTCs). Together, the PTCs delivered 217 courses, 581 course-days with 5,221 participants. Overwhelmingly positive feedback was received from the participants. The jointly coordinated annual PTC programmes have seen new courses being introduced to the PTC programme on emerging fields such as Deep Learning and forward-looking workshops on future HPC technologies and Energy Efficiency. The PTCs have also devised the 2019-2020 programme, to be implemented in the next project, which includes new initiatives such as online PTC courses to complement the MOOCs and the continuation of collaboration with other parties.

All six PRACE Seasonal Schools in PRACE-5IP were selected via a formal selection process and organised as: the Autumn School 2017 in Gdańsk, Poland; the Spring Seasonal School 2018 in Bratislava, Slovak Republic; the Autumn School 2018 in Ljubljana Slovenia; the Winter School in Sofia, Bulgaria; the Winter School 2019 in Leuven, Belgium and Spring School in Stockholm, Sweden. The overall evaluation for the Seasonal Schools have been positive.

WP4 has continued the collaboration with the Centres of Excellence (CoEs) through jointly organised on-demand events and collaboration workshops. In October 2018 PRACE, EXDCI, CoEs, and FET projects jointly organised a collaboration workshop in Bruehl, Germany, during which the network of training coordinator contacts was formed, and the pursue towards common goal, collated HPC training offering in pan-European training portal, was established. The continuation of collaboration was further strengthened with FocusCoE project kick-off meeting in February 2019 in Frankfurt, Germany, where the mutual interest in deeper training offering and web portal development was addressed.

WP4 has co-organised the 2017 International Summer School on HPC Challenges in Computational Sciences in Boulder, Colorado, United States of America, from 25-30 June 2017. The 2018 International Summer School was held in Ostrava, Czech Republic 8-13 July 2018. In addition, PRACE organised three training workshops for student and other audiences during EHPCSW 2018 and planned five workshops for EHPCSW 2019.
All PRACE trainings are free of charge for both research and industry users. The success story of the PRACE training programmes hopefully continues and will continuously be further developed together with EuroHPC and other Research Infrastructure players, as well as CoEs to increase the accessibility and scope of HPC and future exascale computing community. This is possible with strong and continuous support and guidance from EC, both in philosophical and sufficient resource allocation level.

# 1 Introduction

PRACE Training remains as one of the core services delivered by PRACE, building the expertise of HPC users and application developers. Soon to be real Exascale HPC infrastructure, (Est.2022/2023) needs expertise that is built and developed on current HPC and applications. Europe´s massive investments in HPC infrastructure and its competitiveness means also investments in training programmes for both current and future experts. PRACE wants to be part of this development together with EuroHPC.

PRACE-5IP project has been training different user communities together with CoEs. Events have received very high feedback scores from the participants. At the same time the development of online training and new MOOC courses has been maintained with some delays. During PRACE-5IP, two new online courses were produced in addition to the existing ones.
PRACE CodeVault, was further developed as an open repository containing various HPC code samples serving self-education for learning HPC programming skills.

In this document, we describe the work carried out during the entire lifetime of the PRACE-5IP project, with a focus on the activities undertaken during the second year of the project (May 2018 – April 2019) by the Training Work Package (WP4), mainly face-to-face training events:

- PRACE Training Centres (Former PATC and PTC) Courses,
- PRACE Seasonal Schools and On-demand Events,
- International HPC Summer School,
- PRACE Summer of HPC.

The majority of events during the reporting period were organised by the PTCs operating in well-established supercomputing facilities. The Seasonal Schools organisation planning and selection follow the new selection scheme introduced in PRACE-4IP project. WP4 also co-organised the 2017 International Summer School on HPC Challenges in Computational Sciences in Boulder, Colorado, United States of America, 25-30 June 2017, in collaboration with XSEDE (USA), RIKEN (JAPAN) and Compute Canada. The 2018 International Summer School was held in Ostrava, Czech Republic. Finally, WP4 organised the PRACE Summer of HPC 2018 outreach and training programme for undergraduate students and early-stage post graduates.
This deliverable also presents the PRACE training strategy for supporting the needs of future HPC users, and a full list of courses provided in the project in the Annex.

The deliverable is organised as follows: Section 2 presents an overview of the PATC and PTC development and operation within the reporting period; Section 3 the relevant progress for Seasonal Schools; Section 4 and 5 the activities related to training collaboration related to On-demand events, the International HPC Summer School, and other projects as well as outreach to universities; Section 6 provides information on the PRACE Summer of HPC; Section 7 gives an update of the MOOC prepared by PRACE; Section 8 provides a report for the Training and Events portal of PRACE; and Section 9 gives an update of the PRACE CodeVault. The PRACE training strategy, and conclusions are provided in Section 10 and 11. Several annexes are also included: a list of all face-to-face training courses provided by PRACE during the reporting period, the reports from the Autumn 2017 and Spring 2018 Seasonal Schools that took place in Poland and Slovak Republic, respectively, and On-demand Events Templates and Reports as well as feedback reports from International Summer schools.

# 2 PRACE Training Centres

As reported in earlier deliverables, the six PRACE Advanced Training Centres (established in 2012), and the four PRACE Training Centres (established in 2017), have a unified branding as PRACE Training Centres (PTCs) starting from the 2017-18 programme. The network of 10 PTCs continues to be a vehicle in providing a wide variety of high quality courses for a pan-European audience. They have an important role in the PRACE training strategy, responsible for delivering the bulk of PRACE HPC training focused mostly on intermediate to advanced topics, as envisaged in the PRACE-5IP D4.1 deliverable[2].
The PRACE-5IP project spans a period that covers partially the 2016-17 PTC programme, the entire 2017-18 programme and part of the 2018-19 programme. A full list of courses delivered by the PTCs during the reporting period can be found in Annex 12.1, and shown in Table 1 are the PTCs' annual statistics for each academic year since the network began in 2012. Specifically within the PRACE-5IP project, the 10 PTCs have collectively delivered 217 courses, representing 581 days of training with a total of 5,221 participants.

Reviewing the statistics on a year-on-year basis, the establishment of the additional 4 PTCs in the 2017-18 programme meant an increased number of courses to 93 courses for that year (instead of 70-80) and the number of participants has increased to over 2,000 which should become the new target for the 10 PTCs. The evaluation of the courses by participants continues to be consistently high (8.5 out of 10 in the overall score). The level of participation from non-host countries (i.e. those from institutions outside of the country where the PTC course was hosted) at 20.8% and from non-PTC countries at 15.8% are within the average range of past years, although the numbers do fluctuate from year to year.

| Programme | Pilot | 2012-13 | 2013-14 | 2014-15 | 2015-16 | 2016-17 | 2017-18 | 2018-19 |
|---|---|---|---|---|---|---|---|---|
| Date from… | Mar-2012 | Aug-2012 | Aug-2013 | Aug-2014 | Aug-2015 | Aug-2016 | Aug-2017 | Aug2018 |
| Date to… | Jul-2012 | Jul-2013 | Jul-2014 | Jul-2015 | Jul-2016 | Jul-2017 | Jul-2018 | Apr-2019 |
| Number of courses | 19 | 71 | 81 | 77 | 73 | 78 | 93 | 68 |
| Total duration (days) | 56 | 204 | 233 | 219 | 203 | 215 | 244 | 182 |
| Number of participants | 511 | 1,547 | 1,682 | 1,786 | 1,567 | 1,658 | 2,259 | 1,758 |
| Number of participant-days | 1,715 | 4,702 | 5,187 | 5,384 | 4,601 | 4,881 | 6,121 | 4,637 |
| | | | | | | | | |
| Female (%) | - | 12.9% | 14.4% | 16.3% | 17.6% | 19.3% | 21.0% | 20.5% |
| Non-academic (%) | - | 9.9% | 12.3% | 15.6% | 22.2% | 19.4% | 18.5% | 18.4% |
| Non-host country (%) | - | 20.6% | 25.4% | 29.5% | 16.3% | 16.2% | 20.8% | 19.6% |
| Non-PTC country (%) | - | 13.8% | 17.7% | 19.9% | 8.9% | 11.9% | 15.8% | 13.7% |
| | | | | | | | | |
| Feedback response rate (%) | - | 63% | 64% | 53% | 52% | 65% | 53% | 51% |
| Average overall rating (0 – waste of time; 10 - excellent) | - | 8.5 | 8.4 | 8.4 | 8.4 | 8.5 | 8.5 | 8.5 |

**Table 1. Statistics from the implementation of PATC and PTC programmes since 2012.**

During the reporting period, the PTCs have also put together a proposal for the 2019-2020 programme and submitted it for review by the PRACE Board of Directors (BoD), Scientific Steering Committee (SSC) and Industrial Advisory Committee (IAC). This programme consists of 104 courses that represent 265 days of training that will attract over 2,000 participants. While over half of the courses cover conventional HPC domains such as parallel programming and

performance engineering, the PTCs have increased coverage of in-demand topics such as data science, machine and deep learning. Some highlights of the 2019-2020 programme includes the following:

- Introduction of 20 new courses in the programme, including five in the area of Machine and Deep Learning, three domain-specific courses, three GPU courses and a new course on application containers. Six of the new courses are organised in collaboration with the CoEs or other projects.
- The pilot of two online courses, i.e. remote participation open to anyone, by the EPCC PTC to gauge interest in this type of teaching and expand the geographical reach of some PRACE training activities. One online course is on OpenMP which is delivered over four half-day sessions. The other is a rather specialised one-day course on non-volatile memory.
- BSC in Spain plans to organise one PTC training course that is targeted specifically at university teaching staff, e.g. professors, lecturers, so students get early exposure to basic HPC skills and concepts.
- The engagement with European HPC CoEs and other projects or initiative has strengthened. At least 18 proposed courses will involve collaboration with external projects. This includes at least 11-12 courses organised in collaboration with 8 CoEs (out of 10 existing ones); other collaborators include NEXGenIO, DEEP-EST, RRZE, etc. Hopefully this would go some way to address concerns from the PRACE-IP project reviewers related to the coordinated training effort with the CoEs.

# 3 Seasonal Schools

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

Since 2012, Seasonal Schools have run in parallel with the PRACE Training Centres offering training opportunities mainly in countries where PTCs are not in operation. In order to maximize PRACE training coverage across Europe, PTC hosting countries are not eligible to apply for hosting Seasonal Schools.

## 3.1 Selection Process

A Call for Seasonal Schools hosting was set up due to experiences in previous Seasonal Schools selection process, which resulted in six countries that hosted the Seasonal Schools for PRACE-5IP.

Table 2 summarises all Seasonal Schools dates, location and main topics. More details on the events are available in the relevant section of the PRACE Training Events portal [3].

| School | Location | Date | Main Subject | Overview |
|---|---|---|---|---|
| Autumn 2017 | Poland | 20-24 November 2017 | Computational Fluid-Structure Interaction | Sec. 3.2.1 |
| Spring 2018 | Slovakia | 23-26 April 2018 | PRACE Seasonal School on Bioinformatics | Sec. 3.2.2 |
| Autumn 2018 | Slovenia | 24-26 September 208 | HPC for engineering and Life sciences | Sec. 3.2.3 |
| Winter 2018 | Bulgaria | 26-29 November 2018 | Computational Chemistry, Biochemistry and Medicinal chemistry – Methods and Tools | Sec. 3.2.4 |
| Winter 2019 | Belgium | 4-8 March 2019 | Introduction to Machine Learning for scientists | Sec. 3.2.5 |
| Spring 2019 | Sweden | 10-13 June 2019 | HPC in the Life Sciences | Sec. 3.2.6 |

**Table 2. PRACE-5IP Seasonal School schedule**

## 3.2 Overview of accepted Seasonal Schools

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

### *3.2.1 Poland, Computational Fluid-Structure Interaction (Autumn 2017)*

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

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

### *3.2.2 Slovakia, PRACE Seasonal School on Bioinformatics (Spring 2018)*

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

There are a lot of tools available, that researchers working in this field can use, but most of them were developed for desktop applications. In this workshop, tools / frameworks that are designed towards parallel computer architectures were presented, thus suitable for running them on computer clusters or supercomputers. Participants learned not only about dedicated bioinformatics software, such as BLAST (Basic Local Alignment Search Tool), but also on

generally applicable tools, such as the R programming language or the Apache Spark framework, suitable for parallel (pre)processing of Big Data.

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

### *3.2.3 Slovenia, HPC for engineering and Life sciences (Autumn 2018)*

The aim of the Seasonal School was to increase the competencies of Slovenian academic and industrial researchers. A national HPC consortium founded in 2016 has set a strategic goal of giving training for industry personnel (trainees and interns) and university students and researchers. The call for PRACE Seasonal events was a good stimulus for progress in this direction. The proposed event had also some regional impact in the neighbouring countries. This event was also intended to increase the number of HPC users in the region, also among small and medium size enterprises (SMEs).

### *3.2.4 Bulgaria, Computational Chemistry, Biochemistry and Medicinal chemistry – Methods and Tools (Winter 2018)*

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

### *3.2.5 Belgium, Introduction to Machine Learning for scientist (Winter 2019)*

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

### *3.2.6 Sweden, HPC in the Life Sciences (Spring 2019)*

Life Science research has become increasingly digital, and this development is accelerating rapidly. Biomolecular modelling techniques such as homology modelling, docking, and molecular simulation have advanced tremendously due to world leading European research, resulting in extreme demands for better computational performance and throughput as these tools are used in applied research and industrial development. This research has direct influence on our daily life in areas such as health and medical applications, the development of new drugs, efficient drug delivery, biotechnology, environment, agriculture and food industry. Life Science is one of the largest and fastest growing communities in need of high-end computing, and it is a critically important industrial sector for Europe.

The dedicated CoE for Biomolecular Research (BioExcel) has been established in Sweden, Stockholm where KTH is the coordinating partner.

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

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

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

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

## 3.3 Results of PRACE-5IP Seasonal Schools

During the Project, all but one Seasonal Schools have taken place; The Spring 2019 Seasonal School will take place in Sweden from 10 to 13 June 2019.

### *3.3.1 Autumn 2017 Seasonal School, Poland*

The Autumn 2017 Seasonal School, named “PRACE Seasonal School on Computational Fluid-Structure Interaction”, took place in Gdańsk University of Technology, Poland from 20 to 24 November 2017. The programme included:

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

- Introduction to the Fluid-Structure Interaction

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

There were 32 participants to the Seasonal School, all from Poland. Most participants declared that they were satisfied with the course level and contents. The organisers declared that the organisation of the Seasonal School was a valuable experience, easier than they previously thought it would be. The official report of the Seasonal School can be found in Annex 12.2.1.

### *3.3.2 Winter 2017 Seasonal School, Slovakia*

The Winter Seasonal School, named "PRACE Seasonal School on Bioinformatics", was finally organised in Spring 2018, due to practical reasons. It took place in the Computing Centre of the Slovak Academy of Sciences in Bratislava, Slovak Republic from 23 to 26 April 2018.
The programme included:

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

There were 34 participants to the Seasonal School, most from Slovakia, one from Czech Republic and one from Germany. From the received evaluations, it can be extracted that the topic was relevant to the participants' research and inspiring. However, a rather significant number declared that the information provided was not good and they had problems comprehending the lectures and with the pace of teaching. The official report of the Seasonal School can be found in Annex 12.2.2.

### *3.3.3 Autumn 2018 Seasonal School, Slovenia*

The Autumn 2018 Seasonal School, named "HPC for engineering and Life sciences", took place at the University of Ljubljana, Slovenia, from 24 to 26 September 2018. The programme included:

- Introduction to HPC
- Parallel Computing
- OpenMP/ MPI
- Introduction to Finite Element, Boundary Element, and Meshless Methods – with applications in heat transfer and fluid flow
- Nanofluidics / Hands-on tutorial on Molecular dynamics and Computational fluid dynamics for nanofluidics
- Conjugate heat transfer and proper orthogonal decomposition

There were 31 participants to the Seasonal School, most from Slovenia (27), two from Romania, one from Iran and one from Spain. From the received evaluations, it can be concluded that the participants were satisfied with almost all elements of the School. More detailed information regarding the Autumn 2018 Seasonal School can be found in Annex 12.2.3.

### *3.3.4 Winter 2018 Seasonal School, Bulgaria*

The Winter 2018 Seasonal School, named "Computational Chemistry, Biochemistry and Medicinal chemistry – Methods and Tools", took place at the Institute of Information and

Communication Technologies, Bulgarian Academy of Sciences, Sofia, Bulgaria, from 26 to 29 November 2018. The programme included:

- Reaction mechanism in organic chemistry
- Case studies in drug design
- Computer modelling of π-hydrogen bonding in organic systems and grapheme
- Modelling of metal and metal oxides systems relevant for catalytic applications
- Introduction to DL_POLY and DL_MESO
- Introduction to DL_FIELD

There were 30 participants to the Seasonal School, most from Bulgaria (26), two from Italy, one from Czech Republic and one from Spain. Overall the School achieved very positive feedback which is evident from the average grades given in the feedback forms, both in terms of content of the training and overall organisation. More detailed information regarding the Winter 2018 Seasonal School can be found in in Annex 12.2.4.

### *3.3.5 Winter 2019 Seasonal School, Belgium*

The Winter 2019 Seasonal School, named "Introduction to Machine Learning for scientists", took place at KU Leuven, Belgium, from 04 to 08 March 2019. The programme included:

- Introduction to AI and applicability
- Linear regression
- Multilayer networks
- Frameworks and software ecosystem
- Supervised learning, CNN and RNN
- Unsupervised learning
- Reinforcement learning
- Scikit-learn pipelines
- AI Ethics
- AI at scale: using multiple GPUs

There were 27 participants from Belgium, seven from Germany, two from Portugal and one participant from each of the following countries: Portugal, UK, Cyprus, Netherlands and Iceland. The general evaluation of the school was very positive. More detailed information regarding the Winter 2019 Seasonal School can be found in Annex 12.2.5.

# 4 On demand events supporting collaboration

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

## 4.1. Selection Process for the on-demand events

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

The committee is responsible to respond within 20 calendar days with their position/recommendation regarding the organisation of the event, including any possible recommendations for the improvement of the event. The selection committee is comprised of five members: BoD representative, MB representative and three WP4 representatives. Task 4.1 leader coordinates and facilitates the process, without any power to influence the final decision.

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

## 4.2 Selection Criteria for the on-demand events

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

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

## 4.3 On-demand Events organised during PRACE-5IP

Table 3 presents the On-demand events schedule for the entire project lifetime of PRACE-5IP.

| Location | Date | Main Subject |
|---|---|---|
| Espoo, Finland | 7-9 June 2017 | E-CAM Workshop on Particle-Based Models and HPC |
| Barcelona, Spain | 21 November 2017 | Energy-aware application development for heterogeneous computing |
| Umeå, Sweden | 24-25 April 2018 | Programming and optimizing the Knights Landing |
| Barcelona, Spain | 3-5 October 2018 | Advanced CFD and Turbulence Modelling Targeting HPC |
| Ostrava, Czech Republic | 22-23 October 2018 | ANTAREX: Monitoring, Compilation and Autotuning Approach for Energy-Efficient HPC Systems |
| Stockholm, Sweden | 20-21 March 2019 | Workshop on Deep Learning |

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

The reader can find the corresponding reports for each of the organised On-demand event in Annex 12.3.3.

## 4.4 Results of PRACE-5IP on-demand Events

On-demand events have taken up their natural role in complementing the PRACE training portfolio offering with collaboration courses and events together with other projects and CoEs. This is the natural collaboration form between PRACE and CoEs. The on-demand event named "E-CAM Workshop on Particle-Based Models and HPC" took place in the CSC IT-Center for Science, in Aalto University, Espoo, Finland, from 07 to 09 June 2017. It attracted 21 participants, 17 from Finland, one from Estonia, Holland, Hungary and Germany, respectively. The small sample of evaluations gave an excellent grade to the event. The official report of this on-demand event can be found in Annex 12.3.1.

The event named "Energy-aware application development for heterogeneous computing" took place in the Barcelona Supercomputing Center in Barcelona, Spain, on 21 November 2017. The organisers aimed to present the TANGO toolbox, which provides a set of tools to simplify and optimise the usage of distributed heterogeneous computing environments. It attracted 15 participants overall, 13 from Spain and one from Brazil and Iran, respectively. The official report of this on-demand event can be found in Annex 12.3.2.

The event named "PRACE Workshop on Programming and Optimizing the Intel Knights Landing Manycore Processor" took place in HPC2N, Umeå University, Sweden, from 24-25 April 2018. It attracted 18 participants from various countries, including 10 participants from Sweden. The course focused on how to best use and efficiently program and optimize the Intel Manycore Processor codenamed "Knights Landing (KNL)". The official report of this on-demand event can be found in Annex 12.3.3.

The event named "Advanced CFD and Turbulence Modelling Targeting HPC" took place in BSC, Barcelona, Spain, from 03 to 05 October 2018. It attracted 18 participants from various

countries, including 10 participants from Spain. The course focused on advanced CFD and turbulence modelling targeting HPC. The official report of this on-demand event can be found in Annex 12.3.4.

The event named "ANTAREX: Monitoring, Compilation and Autotuning Approach for Energy-Efficient HPC Systems" took place in Technical University of Ostrava, Ostrava, Czech Republic, from 22 to 23 October 2018. It attracted 13 participants in total, 10 from whom from Czech Republic. The course focused on the main challenges of the ANTAREX project and the results of its research. The official report of this on-demand event can be found in Annex 12.3.5.
The event named "Workshop on Deep Learning" took place in Stockholm, Sweden, from 20 to 21 March 2019. It attracted 35 participants in total, 33 from whom came from Sweden and two from Finland. The course focused on deep learning, convolutional and recurrent neural networks, GPU computing, and tools to train and apply deep neural networks for natural language processing, images, and other applications. The official report of this on-demand event can be found in Annex 12.3.6.

# 5 International HPC Summer School

The PRACE-5IP project has supported the organisations of the 8th International HPC Summer School [32], which was held in Boulder, Colorado, USA on 25-30 June 2017 and the 9th International HPC Summer school 2018[33] held in Ostrava, Czech Republic. Some of the planning for the10th International Summer School[34] also took place within the PRACE-5IP project and the school will take place in Kobe, Japan on 7-12 July 2019. The collaboration in International Summer School 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) has proven hugely fruitful.

In 2017 the International Summer School edition in Boulder there were 342 applications in total, 136 applications from EU institutions. For the Summer school edition in Ostrava in 2018 there were 335 applications in total, of which 96 came from EU institutions.

For the PRACE-5IP International Summer schools in 2017 and 2018 there were 80 participants in total, of which 30 students came from EU/PRACE, 30 from US, 10 from Canada, and 10 from Japan. The participants were generally satisfied with the course organisation and particularly with their own involvement with other students. In the feedback most students stated that participants from other countries contributed to their learning and they were considering their participation in the Summer school as successful (mean of feedback responses 4.5/5).

The contents of each International Summer school were always focussed on HPC challenges by discipline (e.g, earth, life and materials sciences, physics), HPC programming proficiencies, performance analysis and profiling, algorithmic approaches and numerical libraries, data-intensive computing, scientific visualization and Canadian, European, Japanese and U.S. HPC-infrastructures.


**Figure 1. The 9th International HPC Summer School, Ostrava, Czech Republic, 8-13 July 2018 (80 participants)**

## 5.1. Outreach to Universities

*(Formerly a sub-task of WP3 and reported also in WP3)*

Outreach to universities has been seen as a pilot of voluntary best effort programme, and activities are only carried out when partners can voluntarily provide them. Simple activities such as a relative webpage, mailing list and sending of emails of relative content has been tried so far.

The Outreach to Universities webpage [41]was created and launched in 2017. The page acts as a one-stop shop for the latest student-centric information and educational opportunities PRACE has to offer.

During the reporting period, the webpage was updated and made clearer and more descriptive. The HPC Career Case studies created by the EXDCI project were incorporated, to provide the audience with real-life examples of people making a career in HPC.

For the Outreach to Universities a mailing list was created, and the following e-mails were sent to the subscribers during the reporting period:

- PRACE MOOCs – Managing Big Data with R and Hadoop, sent 23 May 2018
- Free "Supercomputing" MOOC starting on 24 September 2018, sent 11 September 2018

- Upcoming PRACE MOOC: Defensive programming and debugging, sent 15 October 2018
- STEM day at HiPEAC's Conference in Valencia, sent 20 December 2018
- PRACE Summer of HPC 2019 opens applications, sent 18 January 2019

Outreach to Universities Student Events, where PRACE staff present PRACE, its activities, and its student-centric opportunities, to students at a university, have taken place throughout the year. Eight such events were organised in Ireland by PRACE-5IP project partner ICHEC.

In the context of the PRACE Outreach to Universities task, WP3 was present at the HiPEAC Computing Systems Week, which took place in Edinburgh from 16 to 18 April 2019. Unoficial outreach to universities work have been done regularly in some centres but not as part of PRACE work but as part of their customer care and customer account managing processes. This pilot has shown that there is much customer potential in the universities and with increasing e-learning needs this can become more successful in the future by reaching out to the teachers in particular.

# 6 PRACE Summer of HPC

**Figure 2: PRACE Summer of HPC 2017 participants, training week 3-7 July, Ostrava, Czech Republic**

During the training week in 2017, participants learned about PRACE and the Summer of HPC program. As part of PRACE's outreach activities students studied about social media and its impact too. Summer of HPC blog was used for collecting students´ blog posts and teaching them how to share their posts using social media channels.

The Summer of HPC participants were also introduced to HPC topics at the hands-on sessions: how to access a HPC system, parallel programming and visualization. Various programming

subjects including an introduction to MPI, introduction to OpenMP, vectorization and parallel debugging were also shown to participants.

PRACE Summer of HPC (SoHPC) [6] outreach and training programme for undergraduate students and early stage post-graduates entered its sixth edition in 2018 (see timeline [20]). With 23 project proposals [38] the call for applications [35] was launched in January 2018 and closed with 58 registrants at the end of February 2018. Review and selection at consensus meeting allocated successful participants to projects. Immediately after invitations were accepted the site coordinators started preparations for travel to and from the training week together with selected participants. The training week was organised at the EPCC HPC centre in Edinburgh as a start of the students' summer project work. Each student had a mentor for their project and during the summer, weekly teleconferences were organised by SoHPC coordinating team to monitor the progress and advertise achievements on SoHPC Facebook [14] and Twitter [15] accounts.


**Figure 3. PRACE Summer of HPC 2018 participants, training week in Edinburgh, UK 1-7 July 2018.**

During the summer, students wrote 76 blog posts [16] about their project and work at hosting sites. The programme finished at the end of August 2018 with project presentations uploaded on You Tube[17]. Students wrote popular scientific articles describing their achievements from the project work, which was used by PRACE dissemination team for outreach communication and PRACE Digest highlights. A SoHPC Awards selection panel was formed and selected the winners of the SoHPC 2018 HPC Ambassador and Best Performance Award. The award ceremony was held on 31 October 2018 in Juelich Supercomputing Centre[39].

Summer of HPC 2019 will be considered as a PRACE-6IP activity. Nevertheless, preparation work continued and the call for applications was launched in January 2019 with 25 project proposals and closed with 105 registrants at the end of February 2019. Review and selection at consensus meeting allocated successful participants to projects[40]. The programme starts in July 2019 with a training week in Bologna, organised by CINECA.

# 7 Massive Open Online Courses

PRACE piloted “Supercomputing” and “Managing Big Data with R and Hadoop” Massive Open Online Courses (MOOC) under PRACE-4IP as a different training method hosted on FutureLearn [21] platform. Each existing 5-weeks MOOC is offered twice a year with constant improvements by each MOOC team. “Supercomputing” MOOC with start dates 15 January 2018 and 24 September 2018 had 1825 and 1169 joiners respectively. “Managing Big Data with R and Hadoop” MOOC with start dates 7 Jan 2019 and 23 Apr 2018 had 951 and 2572 joiners respectively.

The plan in PRACE-5IP proposal was to develop two to three additional MOOCs. The “Defensive Programming and Debugging” course developed by CENAERO, KU Leuven started on 5 Nov 2018 with 1616 joiners. “Python in high performance computing” MOOC developed by CSC video and content material production is ready by April 2019 but the actual run will be delayed to August-September 2019. “The new MPI-3 Shared Memory Interface” MOOC course which was being prepared by HLRS, IUCC, and SURFsara was divided into two parts. First part is a two-week course, Mini MOOC, with new title “MPI: A Short Introduction to One-Sided Communication”. This course is being prepared to be run in 2 weeks, but it may also be used as part of longer, 5-week course “MPI-3: A Guide to the New Shared Memory Interface” in the future.

Overall, PRACE-5IP WP4 works in close contact with FutureLearn “partnership support” team with a mission on improving the impact of the courses. This means analysing and addressing week points in courses where substantial participants drop-off is observed. For “Defensive Programming and Debugging” that is planned for second run on 29 April 2019 the split into two parts is considered. For “Managing Big Data with R and Hadoop” we plan to introduce access to HPC cluster in week 1 already for planed start on 6 May 2019. This will increase access without established method of using virtual machine for the course. The MOOCs could be further used in *outreach to university programme* and offered as training material for universities in national level collaboration. The ownership of customer trainer contacts in each respective university around Europe remains in partner institutions and cannot be used for PRACE due to GDPR regulations.

# 8 Training and Events Portal

PRACE Events Portal manages all PRACE related events available at www.events.prace-ri.eu. The main focus was preparing the major version upgrade of PRACE Events portal [24] called Indico 2.0. This version was released early 2018, but preparatory work including installation of test systems, and testing migration itself was started at the beginning of PRACE-5IP. WP4 team worked closely together with Indico developers participating to conferences and solving issues together, as PRACE is hosting more events accommodating more users than typical Indico portals around the globe. After the test migrations and deep analysis of the upgrade problems together with the developers, 2.0 version was established and all content was migrated to production late 2018.

After the migration, some customization of the portal had been done, e.g, update of the PRACE banner, setup of a cookie warning popup, general GDPR coherence, insertion of Google Analytics tracking code, and modification of page templates to offer material style view of e.g. timetables.

## 8.1 Training portal overhaul

Training Portal is the portal system that aggregates Events information and Training materials, available at www.training.prace-ri.eu. Due to the security risk imposed by non-updated CMS, the previous operator stopped hosting TYPO-3 web content management system mid 2018. The content was migrated and a static version of training portal was further operated and manually updated occasionally to ensure safety. The training content was available through this static version, but the upgrade of Training Portal to restore previous functionality became urgent.

The current training portal [25] is to be changed into a completely new system due to its current limitations of lacking advanced search and proper categorisation of training materials. Initial findings supported using a repository system instead of a CMS for such a task, as it provides the desired features along with the capability of storing science related documents with metadata persistently (see Figure 4)

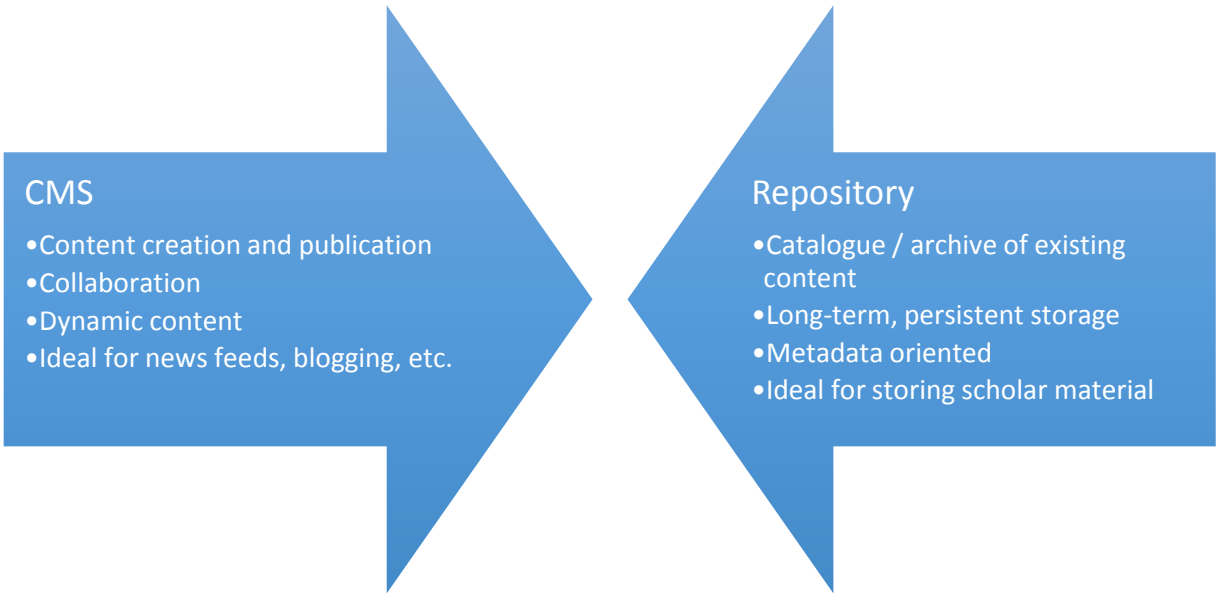


**Figure 4. Comparison between CMS and Repository systems.**

Expectations for the document repository:

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

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

Results showed that ePrints system was the one that satisfied all the requirements with its latest stable version to be further evaluated, however it lacked real graphic flexibility, and therefore decided to use also a Wordpress system as the front page of Training Portal and use ePrints for backend purposes offering materials.

Additionally, ePrints repository was tested and developed to include feed of events from Events Portal and a PRACE branded header. The structure and test data including playable video content was migrated. (see the test portal http://193.224.23.141)

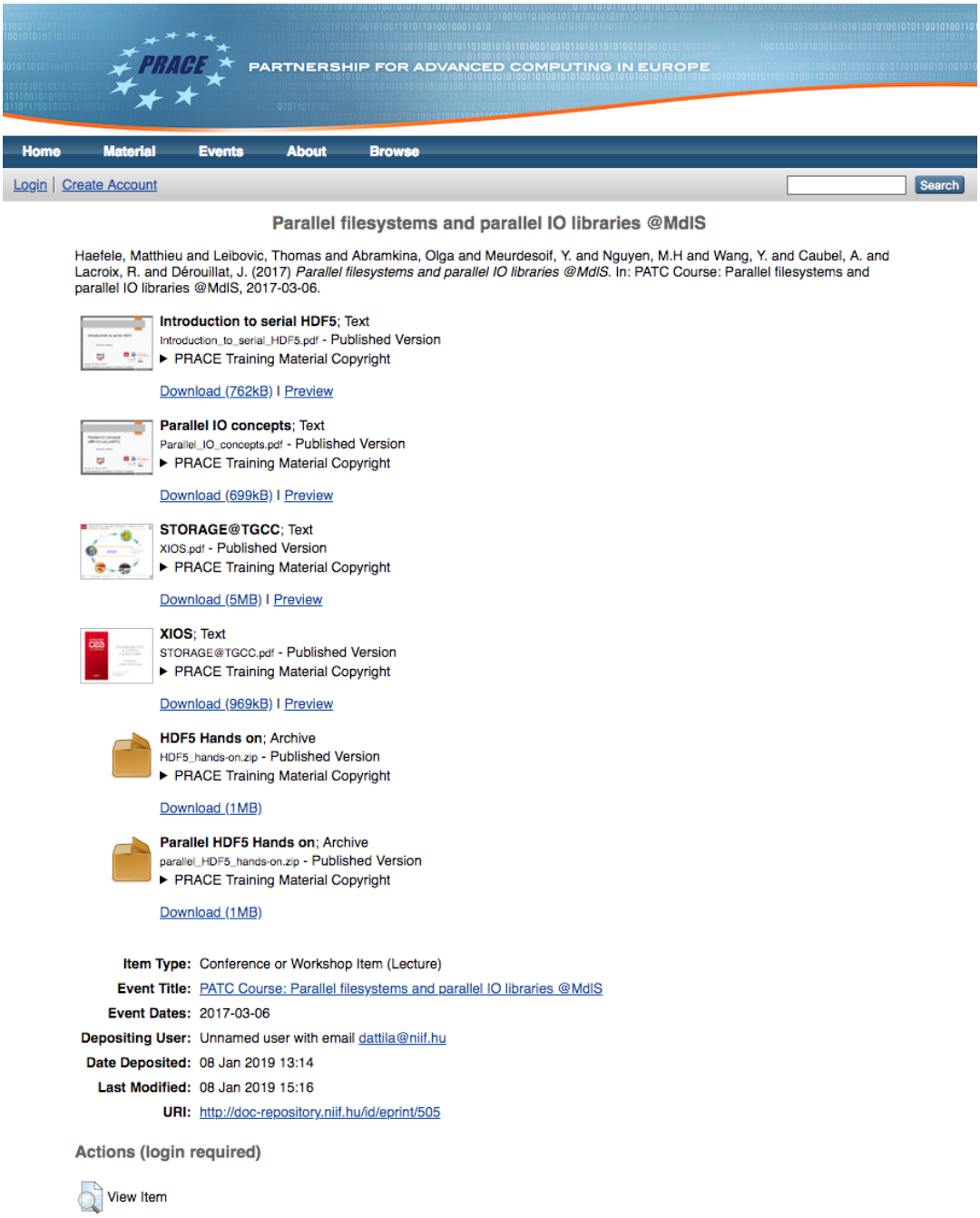


**Figure 5. New PRACE material portal based on ePrints.**

When the structure of the system was accepted, all documents and videos with metadata were migrated to the repository. Similar pages to the current portal were created with categories and menu items.

To offer a more user-friendly experience for those who want to find out about PRACE Training offerings, a landing page / front page to the Training Portal Wordpress was installed. It supports a calendar plugin able to aggregate events from Events Portal with all required information along with external training event feeds e.g. HPC FETs or CoEs. Existing content was migrated and new content was uploaded to offer more visually inviting structure.

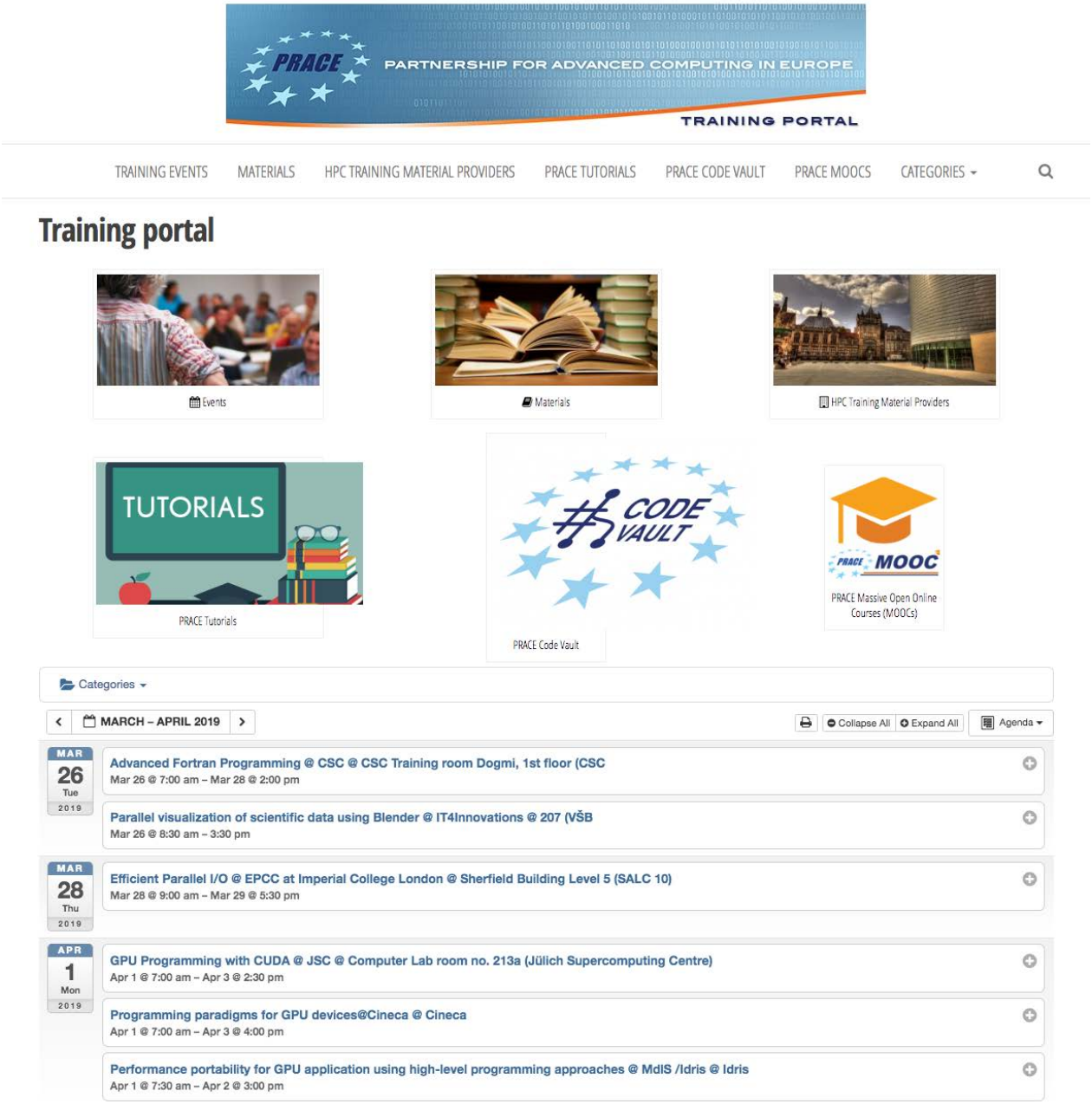


**Figure 6. New PRACE Training Portal based on Wordpress.**

## 8.2 European HPC Training Portal development

PRACE has started building also a Pan-European HPC Training Portal, which would include training events and training material from CoEs, FETs and Exascale Projects. Furthermore, it should provide a roadmap of training material users should follow based on their level of competence, their background (e.g. whether they are from academia or industry) and their requirements (what they want to learn). A demonstration webpage was set up to be further developed based on the comments of the reviewers and other actors of HPC.

This portal contains a map of HPC centers, aggregated data of available computational and training resources of Europe. ( http://82.116.198.186:8080/HPC_in_Europe) The development work continues together with EC, EuroHPC and CoEs as well as HPC actors in the coming 6IP project. This demonstration web concept page is created to facilitate the multilateral discussions and will be produced by an external company when parties have given their respective comments.


**Figure 7. European HPC Portal concept.**

# 9 CodeVault

CodeVault is a repository/storage facility for the needs of PRACE. Apart from WP4 Training, other WPs also need repository facilities for storing content in an organised way. However, in this particular section, we focus on the CodeVault aspect concerning WP4.
All decisions regarding CodeVault that were taken during the first year of the project, have been implemented. First, CodeVault repository was re-instantiated into PRACE-owned infrastructure under the **`prace-ri.eu`** domain. CodeVault can be accessed via the following url: https://repository.prace-ri.eu/git/CodeVault (see Figure 8). The new repository infrastructure is based on the gitlab open source software.

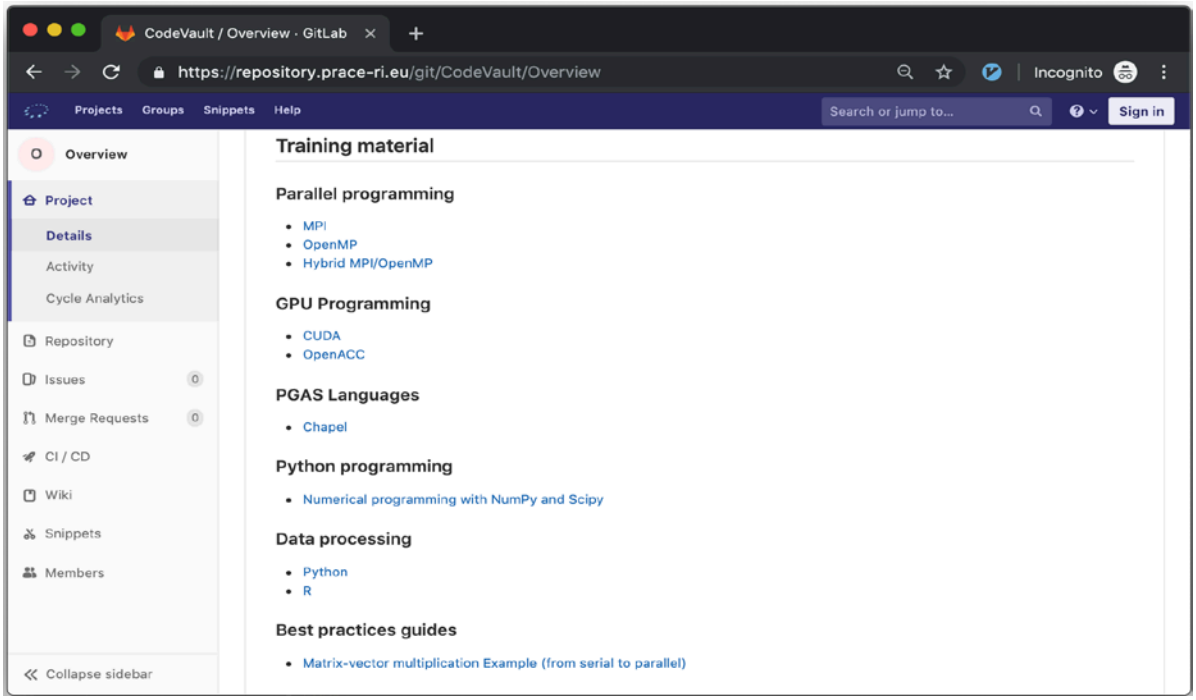


**Figure 8. CodeVault in its current form at gitlab.com facility.**

Second, the training section of the CodeVault is not a single repository any more. It is a set of groups, each of which contains several projects. Each project is essentially a git repository, which can be handled separately from the others. This means that each project can be git cloned separately, which results in a more fine-grained handling of the various HPC interest fields.
The current structure of CodeVault training sections can be seen above. The main categories have been created as groups, while all subcategories have been created as projects/git repositories. For example, in the current structure, the category “Parallel Programming” is a gitlab group, while the category “MPI” is a gitlab project/git repository.

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

A drawback of the gitlab's group notion is the fact that a group lacks the landing page. While, on the contrary, each git project is a git repository, which has a landing page, like all git repos do, a README.md file. This disadvantage can be overcome with the convention of accommodating a "dummy" project for each group, just to use its README.md page for general information about each group. An example of this convention can be seen in the topmost CodeVault group, which makes use of the `Overview` project just as a landing page, in order to present general information about CodeVault. Access has been provided to all interested PRACE parties and several categories of the new CodeVault have been populated with training material.

# 10 Developing the PRACE Training Strategy

The PRACE Training Strategy was first highlighted in the deliverable PRACE-5IP D4.1: "Interim Training Report"[2] and summarised below, including an important section on the target audience and relative investment. While this strategy is evolving in the context of other entities in the training landscape, e.g. CoEs, EuroHPC and the upcoming HPC Competence Centres, plans have been put in place for better communication and coordination amongst the different actors to propose a European HPC training strategy, which should help focus the PRACE Training Strategy in future. It is equally important to coordinate and integrate the target audiences discussion with the coming PRACE dissemination strategy, based on our existing target contact information and results of the strategic discussions with the projects to form a full map of potential audiences.

## Target audience of PRACE Training

The PRACE model of current HPC user base in Europe consists of a large group of users with a basic knowledge of HPC, followed by a smaller group of "intermediate level" users, and finally an even smaller group of advanced users, as shown in Figure 9.

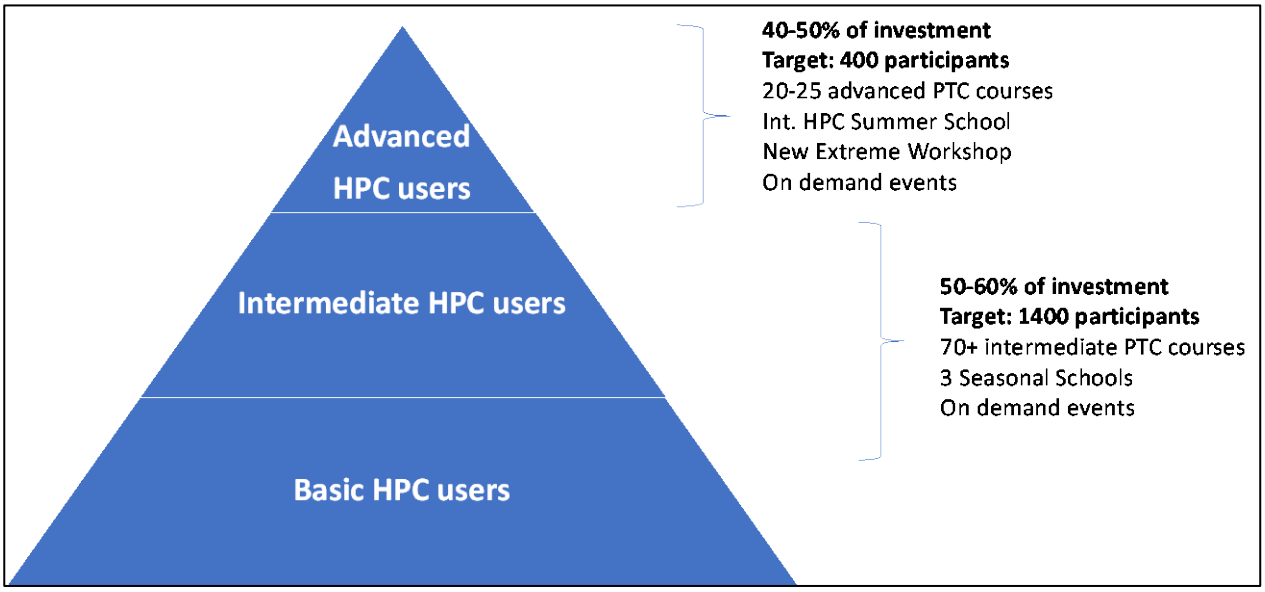


**Figure 9. The HPC user pyramid, in context of HPC training.**

PRACE alone cannot provide the necessary training for the entire European HPC user base. Collaboration and coordination is needed with different HPC players (CoEs, EuroHPC, etc.) especially in training.

Therefore, the strategy of PRACE is to:

- Focus its resources mainly on face-to-face training services that grow the community of advanced users who would gain the prerequisite experience and know-how to exploit pre-exascale and EuroHPC infrastructure. This investment is targeted towards a relatively small audience of 400 participants per year. It will also organise advanced training that no individual HPC centre can provide by pooling European HPC expertise.
- Dedicate its remaining resources to enable a diverse range of intermediate level HPC courses across Europe, the stepping stones to more advanced courses. Some effort is put also into training that brings new user groups (SMEs, new scientific disciplines) into HPC. This investment is more diffused relative to that for advanced users because the target audience is 1,400 participants per year but it is a necessary and cost-effective investment by PRACE (in terms of cost per participant) to ensure continued accessibility and dissemination of such courses to all European researchers.

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

## Summary of PRACE Training strategy

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

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

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

Apart from face-to-face training events, PRACE will maintain and develop online resources that will provide pan-European information on face-to-face courses, training material, sample codes, online tutorials, etc. The cornerstones will be the PRACE Training Portal (http://193.224.23.141 ) and the hpc-in Europe portal (http://82.116.198.186:8080/HPC_in_Europe ) to facilitate users. There is also tremendous potential for PRACE partners to pool their training expertise to develop MOOCs to attract a global audience for its training offerings. Finally, PRACE will continue its outreach programme to universities to stimulate interest in HPC training among undergraduate students and develops training for trainers opportunities for university trainers providing material and e-learning material for use.

## Training role in context of the European HPC CoEs

With the establishment of the European HPC CoEs, each having its own training activity, it raises the question of how do all the training activities fit in the overall landscape. Empirical data suggest that PRACE training activities are often focused on more transversal subjects (e.g. how to program in parallel, improve performance and scaling of codes, how to take advantage of new HPC tools and technologies), whereas CoEs typically focus on more domain oriented topics (e.g. how to solve a particular problem in a scientific domain using HPC).However, there is some overlap between the training activities of PRACE and the CoEs. Even from the early establishment of the CoEs, PRACE has organised joint events with the CoEs and
Table 4 provides a list of all the past and planned PRACE-CoE joint courses, with the planned collaborations being included in the proposed PTC 2019-2020 programme.

| CoE | Date | Duration | Course Title | Location | PRACE partner |
|---|---|---|---|---|---|
| E-CAM | 16/05/2016 | 5 | PRACE Spring School 2016 & E-CAM Tutorial on Molecular and Atomistic Modelling | Dublin, IE | ICHEC |
| CoeGSS | 17/10/2016 | 2 | Parallel Programming with MPI and OpenMP | Stuttgart, DE | HLRS |
| MaX | 05/12/2016 | 3 | Material Science codes on innovative HPC architectures: targeting exascale | Bologna, IT | CINECA |
| POP | 14/12/2016 | 2 | Performance and Productivity Tutorial with POP CoE | Ostrava, CZ | IT4I |
| POP | 08/02/2017 | 3 | 24th VI-HPS Tuning Workshop | Southampton, UK | EPCC |
| BioExcel | 10/04/2017 | 4 | PRACE Spring School 2017 - HPC in Life Sciences | Stockholm, SE | KTH |
| EoCoE, POP | 24/04/2017 | 3 | Third Training Workshop EoCoE-POP | Barcelona, ES | BSC |
| E-CAM | 07/06/2017 | 3 | E-CAM Workshop on Particle-Based Models in HPC | Espoo, FI | CSC |
| BioExcel | 29/11/2017 | 3 | Hands-on Introduction to HPC for Life Scientists | Edinburgh, UK | EPCC |
| EoCoE, POP | 11/12/2017 | 4 | EoCoE-POP Performance Evaluation Workshop | Saclay, FR | MdlS |
| MaX | 30/05/2018 | 3 | PRACE-MaX Tutorial on high-throughput computations | Bologna, IT | CINECA |
| E-CAM | 13/06/2018 | 3 | HPC in Molecular and Atomistic Simulations | Dublin, IE | ICHEC |
| CompBioMed | 13/02/2019 | 3 | Short course on HPC-based Computational Bio-Medicine | Barcelona, ES | BSC |
| E-CAM | Oct-19 | 2 | GPU Programming with OpenACC | FI | CSC |
| E-CAM | Oct-19 | 3 | Introduction to Parallel Programming | FI | CSC |
| BioExcel | Oct-19 | 3 | Hands-on Intro to HPC for Life Scientists | UK | EPCC |
| ChEESE | Dec-19 | 4 | HPC and natural hazards: modelling tsunamis and volcanic plumes using European flagship codes | ES | BSC |
| EXCELLERAT | Dec-19 | 5 | School on Numerical Methods for Parallel CFD | IT | CINECA |
| E-CAM | Jan-20 | 4 | PRACE & E-CAM Tutorial on Deep Learning for Simulations | IE | ICHEC |
| CompBioMed | Feb-20 | 2 | Short course on HPC-based Computational Bio-Medicine @ BSC | ES | BSC |
| EoCoE | Mar-20 | 3 | Parallel I/O and Portable Data Formats | DE | GCS |
| POP | Mar-20 | 2 | Performance Analysis of CPU and GPU enabled HPC applications | CZ | IT4I |

| CoE | Date | Duration | Course Title | Location | PRACE partner |
|---|---|---|---|---|---|
| ChEESE | Apr-20 | 3 | Preparing HPC Application for Exascale: the ChEESE Metodology. | IT | CINECA |
| MaX | May-20 | 5 | Tutorial on writing reproducible workflows for Computational Materials Science with AiiDA | IT | CINECA |
| E-CAM | Jun-20 | 3 | High-performance scientific computing in C++ | DE | GCS |

Table 4. Past and planned PRACE collaborations with the European HPC CoEs.

Finally, further effort is under way that will provide more clarity to the training roles of PRACE and CoEs. Planning is already progressing when PRACE, CoEs, as well as other European HPC training stakeholders agreed to engage in a workshop later in 2019 to develop a future European HPC training strategy. This will continue the good collaboration possibilities recognised in a Collaboration workshop organised in Bruehl in October 2018. The HPC ecosystem summit already taking place 14 May 2019 in Poznan, during the EuroHPC summit week (13-17 May) week aims to create a coherent HPC landscape including access to HPC resources, services for users and research. This summit will help to clarify the future roles of each actor in the field.

# 11 Conclusion

PRACE-5IP, WP4 has continued to provide world-class training in high-performance and scientific computing. There were over 5221 participants in face-to-face courses and workshops, and over 4500 people registered for PRACE MOOCs. PRACE has also strengthened the on-line training offering by developing the PRACE Training portal and the CodeVault repository of code samples. User satisfaction has been extremely high with an overall score of 8.5 (on a scale of 0-10) for PRACE courses.
In order to ensure continued high-impact training for the European HPC ecosystem in the future, WP4 has refined the strategy of PRACE training. The user perspective of PRACE training has also been streamlined by rebranding the previously distinct PATCs and PTCs under a common PRACE Training Centre brand. The training strategy work will be further continued when PRACE and EuroHPC have had a chance to work together on their training strategy, in particularly how they will organise together their training services production and collaboration models, and work division.

Currently, online learning is a hugely growing trend that should be followed. PRACE is developing three new MOOCs and more online offering. However, face-to-face events still hold a very strong position in PRACE training.

PRACE has continued and intensified training collaborations with CoEs and the Focus CoE after the Bruehl collaboration workshop. Joint agreement of common goals were identified, training counterpart colleagues identified with appropriate mailing list. Joint meeting opportunities have been created, both in WP4 level as well as strategic level dialog with other European Union funded projects and infrastructures: these will continue firstly already in EHPCSW in Poznan 13-17 May 2019 and at WP level meetings planned in autumn 2019. Participation in further international collaboration such as contributing to HPC Carpentry and providing HPC trainers in the universities with more online training material, suggested by the project reviewers, are a feasible roadmap to follow and expand the offering with sufficient funding and work division. Together with EuroHPC, PRACE continues to be a key player in HPC training at a global level.

# 12 Annex

This section contains supplementary material and references for the main text of the deliverable.

## 12.1 PRACE Training Centre events during PRACE-5IP project

The following lists all the PTC courses that have been carried out during the PRACE-5IP project.

| Programme | Course title | PTC | Location | Start Date | Duration (days) |
|---|---|---|---|---|---|
| 2018-19 | Performance Analysis Workshop | EPCC | Bristol, UK | 2019-04-24 | 3 |
| 2018-19 | Data science with R and Python | IT4I | Ostrava, CZ | 2019-04-24 | 2 |
| 2018-19 | Modern C++ for Computational Scientists | EPCC | Cambridge, UK | 2019-04-16 | 2 |
| 2018-19 | Meteorological and climate modelling | GRNET | Athens, Greece | 2019-04-16 | 1 |
| 2018-19 | Interactive High-Performance Computing | GCS | Juelich, DE | 2019-04-09 | 2 |
| 2018-19 | Introduction to CUDA Programming | BSC | Barcelona, ES | 2019-04-08 | 4 |
| 2018-19 | Introduction to OpenACC | BSC | Barcelona, ES | 2019-04-04 | 2 |
| 2018-19 | Performance portability for GPU application using high-level programming approaches | MdlS | Orsay, FR | 2019-04-01 | 2 |
| 2018-19 | Programming paradigms for GPU devices | CINECA | Rome, IT | 2019-04-01 | 3 |
| 2018-19 | GPU Programming with CUDA | GCS | Juelich, DE | 2019-04-01 | 3 |
| 2018-19 | Efficient Parallel I/O | EPCC | London, UK | 2019-03-28 | 2 |
| 2018-19 | Parallel visualization of scientific data using Blender | IT4I | Ostrava, CZ | 2019-03-26 | 1 |
| 2018-19 | Advanced Fortran Programming | CSC | Espoo, FI | 2019-03-26 | 3 |
| 2018-19 | Petaflop System Administration - Marenostrum 4 | BSC | Barcelona, ES | 2019-03-20 | 2 |
| 2018-19 | Spring School in Computational Chemistry 2019 | CSC | Espoo, FI | 2019-03-19 | 4 |
| 2018-19 | Advanced Topics in High Performance Computing | GCS | Garching, DE | 2019-03-18 | 4 |

| Programme | Course title | PTC | Location | Start Date | Duration (days) |
|---|---|---|---|---|---|
| 2018-19 | Introduction for Simulation Environments for Life Sciences | BSC | Barcelona, ES | 2019-03-14 | 2 |
| 2018-19 | Accelerator Programming | GRNET | Athens, Greece | 2019-03-13 | 2 |
| 2018-19 | High Performance Parallel IO and post-processing | MdlS | Saclay, FR | 2019-03-11 | 3 |
| 2018-19 | Systems Workshop: Programming MareNostrum 4 | BSC | Barcelona, ES | 2019-02-27 | 2 |
| 2018-19 | Advanced Parallel Programming | CSC | Espoo, FI | 2019-02-27 | 3 |
| 2018-19 | Introduction to Heterogeneous Memory Usage | BSC | Barcelona, ES | 2019-02-26 | 1 |
| 2018-19 | Parallel and Scalable Machine Learning | JSC | Juelich, DE | 2019-02-25 | 3 |
| 2018-19 | Energy Efficency in HPC | CINECA | Bologna, IT | 2019-02-21 | 2 |
| 2018-19 | Node-Level Performance Engineering | LRZ | Garching, DE | 2019-02-20 | 2 |
| 2018-19 | High Performance Molecular Dynamics | CINECA | Bologna, IT | 2019-02-18 | 3 |
| 2018-19 | Short course on HPC-based Computational Bio-Medicine | BSC | Barcelona, ES | 2019-02-13 | 3 |
| 2018-19 | Practical Deep Learning | CSC | Espoo, FI | 2019-02-13 | 2 |
| 2018-19 | 15th Advanced School on Parallel Computing | CINECA | Bologna, IT | 2019-02-11 | 5 |
| 2018-19 | Data Management Plan | MdlS | Montpellier, FR | 2019-02-06 | 3 |
| 2018-19 | Big Data Analytics | BSC | Barcelona, ES | 2019-02-05 | 4 |
| 2018-19 | Introduction to Molecular Modelling (materials and bio) and Molecular dynamics in HPC | GRNET | Athens, GR | 2019-02-04 | 2 |
| 2018-19 | Programming Distributed Computing Platforms with COMPSs | BSC | Barcelona, ES | 2019-01-29 | 2 |
| 2018-19 | Introduction to Hybrid Programming in HPC | LRZ | Garching, DE | 2019-01-28 | 2 |
| 2018-19 | Python in High-Performance Computing | CSC | Espoo, FI | 2019-01-23 | 3 |
| 2018-19 | 30th VI-HPS Tuning Workshop | BSC | Barcelona, ES | 2019-01-21 | 5 |
| 2018-19 | Hands-on Introduction to HPC for Life Scientists | EPCC | Edinburgh, UK | 2019-01-17 | 2 |
| 2018-19 | Developing efficient HPC applications for the latest CPU architectures with C++ and Fortran | IT4I | Ostrava, CZ | 2019-01-14 | 2 |
| 2018-19 | Introduction to Spark for Data Scientists | EPCC | Edinburgh, UK | 2019-01-10 | 2 |
| 2018-19 | OpenMP | SURFsara | Leuven, BE | 2018-12-13 | 1 |
| 2018-19 | Efficient Use of HPC Systems | GRNET | Athens, GR | 2018-12-11 | 2 |

| Programme | Course title | PTC | Location | Start Date | Duration (days) |
|---|---|---|---|---|---|
| 2018-19 | High Performance Bioinformatics | CINECA | Rome, IT | 2018-12-10 | 3 |
| 2018-19 | Parallel and GPU Programming in Python | SURFsara | Amsterdam, NL | 2018-12-10 | 2 |
| 2018-19 | Programming the ARM64 Processor | EPCC | Edinburgh, UK | 2018-12-03 | 2 |
| 2018-19 | Debugging & Optimization | MdS | Montpellier, FR | 2018-12-03 | 4 |
| 2018-19 | HPC methods for Computational Fluid Dynamics and Astrophysics | CINECA | Rome, IT | 2018-12-03 | 3 |
| 2018-19 | Data science with R | CINECA | Milan, IT | 2018-11-28 | 3 |
| 2018-19 | Data, lights, camera, action! Scientific visualization done beautifully | SURFsara | Amsterdam, NL | 2018-11-28 | 1 |
| 2018-19 | Earth Sciences Simulation Environments | BSC | Barcelona, ES | 2018-11-27 | 3 |
| 2018-19 | MPI | SURFsara | Leuven, BE | 2018-11-27 | 4 |
| 2018-19 | GPU Programming with CUDA | EPCC | London, UK | 2018-11-26 | 2 |
| 2018-19 | Fortran modernization workshop | MdS | Saclay, FR | 2018-11-26 | 2 |
| 2018-19 | Introduction to Parallel Programming | GRNET | Athens, GR | 2018-11-20 | 3 |
| 2018-19 | Debugging and Optimization of Scientific Application | CINECA | Bologna, IT | 2018-11-19 | 3 |
| 2018-19 | Analysing large datasets with Apache Spark | CSC | Espoo, FI | 2018-11-19 | 2 |
| 2018-19 | Parallel Design Patterns | EPCC | Oxford, UK | 2018-11-06 | 3 |
| 2018-19 | Productivity tools for High Performance Computing | IT4I | Ostrava, CZ | 2018-10-24 | 2 |
| 2018-19 | Parallel Programming Workshop | BSC | Barcelona, ES | 2018-10-15 | 5 |
| 2018-19 | 29th VI-HPS Tuning Workshop | MdS | Reims, FR | 2018-10-15 | 5 |
| 2018-19 | Parallel Programming Workshop (MPI, OpenMP and advanced topics) | GCS | Stuttgart, DE | 2018-10-15 | 5 |
| 2018-19 | Parallel Programming Workshop (Train the Trainer) | GCS | Stuttgart, DE | 2018-10-15 | 5 |
| 2018-19 | Advanced usage on Irene Joliot-Curie supercomputer: Architecture & Best practices | MdS | Bruyères-le-Châtel, FR | 2018-10-10 | 3 |
| 2018-19 | Introduction to Parallel Programming | CSC | Espoo, FI | 2018-10-03 | 3 |
| 2018-19 | Data Carpentry | EPCC | Swansea, UK | 2018-09-20 | 1 |
| 2018-19 | Scientific Programming with Python | EPCC | Durham, UK | 2018-09-17 | 2 |
| 2018-19 | Advanced Fortran Topics | GCS | Garching, DE | 2018-09-17 | 5 |
| 2018-19 | Fortran Programming for Scientific Computing | CSC | Espoo, FI | 2018-09-13 | 2 |
| 2018-19 | Data management with iRODS and Compute | SURFsara | Amsterdam, NL | 2018-09-06 | 1 |

| Programme | Course title | PTC | Location | Start Date | Duration (days) |
|---|---|---|---|---|---|
| 2017-18 | Advanced MPI | EPCC | Edinburgh, UK | 2018-07-30 | 2 |
| 2017-18 | Parallel Programming Workshop | BSC | Barcelona, ES | 2018-07-26 | 5 |
| 2017-18 | Advanced OpenMP | EPCC | Edinburgh, UK | 2018-07-17 | 3 |
| 2017-18 | 9th Programming and Tuning Massively Parallel Systems summer schoo l (PUMPS) | BSC | Barcelona, ES | 2018-07-16 | 5 |
| 2017-18 | Intel Manycore Programming Workshop | GCS | Garching, DE | 2018-07-16 | 3 |
| 2017-18 | Parallel Programming with MPI and OpenMP | SURFsara | Amsterdam, NL | 2018-07-05 | 3 |
| 2017-18 | Introduction to Unified Parallel C (UPC) and Co-array Fortran (CAF) | GCS | Stuttgart, DE | 2018-07-05 | 2 |
| 2017-18 | Message-passing Programming with MPI | EPCC | Edinburgh, UK | 2018-07-04 | 3 |
| 2017-18 | Meteorological and climate modelling | GRNET | Athens, GR | 2018-07-04 | 1 |
| 2017-18 | Parallel Programming Workshop | ICHEC | Dublin, IE | 2018-07-02 | 5 |
| 2017-18 | Concepts of GASPI and interoperability with other communication AP Is | GCS | Stuttgart, DE | 2018-07-02 | 2 |
| 2017-18 | Introduction to PETSc | MdS | Orsay, FR | 2018-06-25 | 2 |
| 2017-18 | HPC code optimization workshop | GCS | Garching, DE | 2018-06-21 | 2 |
| 2017-18 | Data Analytics with HPC | EPCC | Edinburgh, UK | 2018-06-20 | 2 |
| 2017-18 | CP2K Summer School | EPCC | Edinburgh, UK | 2018-06-19 | 4 |
| 2017-18 | Performance Analysis Workshop | EPCC | Edinburgh, UK | 2018-06-19 | 3 |
| 2017-18 | HPC Methods for Engineering Applications | CINECA | Bologna, IT | 2018-06-18 | 3 |
| 2017-18 | High-performance computing with Python | GCS | Juelich, DE | 2018-06-18 | 2 |
| 2017-18 | Node-Level Performance Engineering | GCS | Stuttgart, DE | 2018-06-14 | 2 |
| 2017-18 | HPC in Molecular and Atomistic Simulations | ICHEC | Dublin, IE | 2018-06-13 | 3 |
| 2017-18 | School on Scientific Data Analytics and Visualization | CINECA | Bologna, IT | 2018-06-11 | 5 |
| 2017-18 | High-performance scientific computing in C++ | GCS | Juelich, DE | 2018-06-11 | 3 |
| 2017-18 | Runtime systems for heterogeneous platform programming | MdS | Saclay, FR | 2018-06-04 | 2 |
| 2017-18 | Performance portability for GPU application using high-level progr amming approaches | MdS | Orsay, FR | 2018-05-31 | 2 |
| 2017-18 | PRACE-MaX Tutorial on high-throughput computations: general method s and applications using AiiDA | CINECA | Bologna, IT | 2018-05-30 | 3 |
| 2017-18 | Introduction to Python programming | CINECA | Bologna, IT | 2018-05-28 | 2 |
| 2017-18 | Accelerator Programming | GRNET | Athens, GR | 2018-05-22 | 2 |
| 2017-18 | Uncertainty quantification | MdS | Orsay, FR | 2018-05-16 | 3 |
| 2017-18 | Systems Workshop: Programming ARM based prototypes | BSC | Barcelona, ES | 2018-05-11 | 1 |
| 2017-18 | PETSc Basic & Advanced Tutorial | IT4I | Ostrava, CZ | 2018-05-10 | 2 |
| 2017-18 | Performance Analysis and Tools | BSC | Barcelona, ES | 2018-05-07 | 2 |
| 2017-18 | Data, lights, camera, action! Scientific visualization done beautifully | SURFsara | Amsterdam, NL | 2018-04-24 | 1 |
| 2017-18 | VI-HPS Tuning Workshop | GCS | Garching, DE | 2018-04-23 | 5 |
| 2017-18 | GPU Programming with CUDA | GCS | Juelich, DE | 2018-04-23 | 3 |
| 2017-18 | Parallel filesystems and parallel IO libraries | MdS | Saclay, FR | 2018-04-23 | 2 |
| 2017-18 | Introduction to Biomolecular modelling and Molecular dynamics in HPC | GRNET | Athens, GR | 2018-04-23 | 1 |
| 2017-18 | Programming paradigms for GPU devices | CINECA | Bologna, IT | 2018-04-18 | 3 |
| 2017-18 | Introduction to CUDA Programming | BSC | Barcelona, ES | 2018-04-16 | 5 |
| 2017-18 | Introduction to the DAVIDE OpenPower GPU cluster | CINECA | Bologna, IT | 2018-04-16 | 2 |
| 2017-18 | Introduction to OpenACC | BSC | Barcelona, ES | 2018-04-12 | 2 |
| 2017-18 | Fortran for Scientific Computing | GCS | Stuttgart, DE | 2018-04-09 | 5 |

| Programme | Course title | PTC | Location | Start Date | Duration (days) |
|---|---|---|---|---|---|
| 2017-18 | Systems Workshop: Programming MareNostrum 4 | BSC | Barcelona, ES | 2018-04-09 | 2 |
| 2017-18 | Advanced Threading and Optimization | CSC | Espoo, FI | 2018-04-04 | 3 |
| 2017-18 | Advanced Topics in High Performance Computing | GCS | Garching, DE | 2018-03-26 | 4 |
| 2017-18 | High Performance Molecular Dynamics | CINECA | Rome, IT | 2018-03-26 | 3 |
| 2017-18 | Advanced Fortran Programming | CSC | Espoo, FI | 2018-03-26 | 3 |
| 2017-18 | Petaflop System Administration\; Marenostrum 4 | BSC | Barcelona, ES | 2018-03-22 | 2 |
| 2017-18 | Parallel I/O & Libraries | GCS | Ostrava, CZ | 2018-03-22 | 2 |
| 2017-18 | Efficient Parallel IO on ARCHER | EPCC | Cambridge, UK | 2018-03-20 | 2 |
| 2017-18 | Simulation Environments for Life Sciences | BSC | Barcelona, ES | 2018-03-14 | 2 |
| 2017-18 | Spring School in Computational Chemistry 2018 | CSC | Espoo, FI | 2018-03-13 | 4 |
| 2017-18 | Parallel I/O and Portable Data Formats | GCS | Juelich, DE | 2018-03-12 | 3 |
| 2017-18 | OpenMP GPU Directives for Parallel Accelerated Supercomputers - an alternative to CUDA from Cray perspective | GCS | Stuttgart, DE | 2018-03-12 | 2 |
| 2017-18 | Hands-on Porting and Optimisation Workshop: Making the most of ARC HER | EPCC | Oxford, UK | 2018-03-08 | 1 |
| 2017-18 | Intel Xeon Phi Programming | IT4I | Ostrava, CZ | 2018-03-01 | 2 |
| 2017-18 | Object-Oriented Programming with Fortran | EPCC | Daresbury, UK | 2018-02-27 | 2 |
| 2017-18 | HPC-based simulations\, Engineering and Environment with Applicati ons in Bioengineering | BSC | Barcelona, ES | 2018-02-14 | 3 |
| 2017-18 | Introduction to High-Performance Machine Learning | SURFsara | Amsterdam, NL | 2018-02-14 | 1 |
| 2017-18 | Efficient Use of HPC Systems | GRNET | Athens, GR | 2018-02-13 | 2 |
| 2017-18 | Machine Learning with Apache Spark | SURFsara | Amsterdam, NL | 2018-02-13 | 1 |
| 2017-18 | 14th Advanced School on Parallel Computing | CINECA | Bologna, IT | 2018-02-12 | 5 |
| 2017-18 | Advanced Parallel Programming | CSC | Espoo, FI | 2018-02-12 | 3 |

| Programme | Course title | PTC | Location | Start Date | Duration (days) |
|---|---|---|---|---|---|
| 2017-18 | Big Data Analytics | BSC | Barcelona, ES | 2018-02-06 | 4 |
| 2017-18 | Programming Distributed Computing Platforms with COMPSs | BSC | Barcelona, ES | 2018-01-30 | 1 |
| 2017-18 | Python in High-Performance Computing | CSC | Espoo, FI | 2018-01-29 | 3 |
| 2017-18 | Introduction to hybrid programming in HPC | GCS | Garching, DE | 2018-01-18 | 1 |
| 2017-18 | Parallel and Scalable Machine Learning | GCS | Juelich, DE | 2018-01-15 | 3 |
| 2017-18 | CFD Simulations using OpenFOAM | IT4I | Ostrava, CZ | 2017-12-14 | 2 |
| 2017-18 | High Performance Bioinformatics | CINECA | Rome, IT | 2017-12-13 | 3 |
| 2017-18 | Advanced OpenMP | EPCC | London, UK | 2017-12-12 | 3 |
| 2017-18 | EoCoE-POP Performance Evaluation Workshop | MdS | Saclay, FR | 2017-12-11 | 4 |
| 2017-18 | Parallel and GPU Programming in Python | SURFsara | Amsterdam, NL | 2017-12-06 | 2 |
| 2017-18 | Debugging & Optimization | MdS | Montpellier, FR | 2017-12-04 | 5 |
| 2017-18 | GPU Programming with OpenACC | CSC | Espoo, FI | 2017-12-04 | 2 |
| 2017-18 | Node-Level Performance Engineering | GCS | Garching, DE | 2017-11-30 | 2 |
| 2017-18 | Earth Sciences Simulation Environments | BSC | Barcelona, ES | 2017-11-29 | 3 |
| 2017-18 | Hands-on Introduction to HPC for Life Scientists | EPCC | Edinburgh, UK | 2017-11-29 | 3 |
| 2017-18 | Introduction in Parallel Programming | GRNET | Athens, GR | 2017-11-29 | 3 |
| 2017-18 | Debugging and Optimization of Scientific Applications | CINECA | Bologna, IT | 2017-11-27 | 3 |
| 2017-18 | Productivity Tools for High Performance Computing | IT4I | Ostrava, CZ | 2017-11-27 | 2 |
| 2017-18 | GPU Programming with CUDA | EPCC | Daresbury, UK | 2017-11-21 | 2 |
| 2017-18 | Analysing large datasets with Apache Spark | CSC | Espoo, FI | 2017-11-16 | 2 |
| 2017-18 | HPC methods for Computational Fluid Dynamics and Astrophysics | CINECA | Bologna, IT | 2017-11-13 | 3 |
| 2017-18 | Single Node Performance Optimisation | EPCC | Edinburgh, UK | 2017-11-06 | 2 |
| 2017-18 | Programming the Manycore Knights Landing Processor | EPCC | Cambridge, UK | 2017-10-31 | 2 |
| 2017-18 | Mastering GPU-Acceleration on OpenPOWER Platform for Optimal Appli cation Performance | MdS | Orsay, FR | 2017-10-24 | 3 |
| 2017-18 | Parallel Programming Workshop | BSC | Barcelona, ES | 2017-10-23 | 5 |
| 2017-18 | Introduction to Marconi KNL Cluster, for users and developers | CINECA | Rome, IT | 2017-10-23 | 1 |
| 2017-18 | Parallel Programming Workshop (Train the Trainer) | GCS | Stuttgart, DE | 2017-10-16 | 5 |
| 2017-18 | Parallel Programming Workshop (MPI, OpenMP and advanced topics) | GCS | Stuttgart, DE | 2017-10-16 | 5 |
| 2017-18 | Introduction to Parallel Programming | CSC | Espoo, FI | 2017-10-09 | 3 |
| 2017-18 | Systems Workshop: Programming MareNostrum 4 | BSC | Barcelona, ES | 2017-09-26 | 2 |
| 2017-18 | Data Management with iRODS | SURFsara | Amsterdam, NL | 2017-09-25 | 1 |
| 2017-18 | Fortran Programming for Scientific Computing | CSC | Espoo, FI | 2017-09-21 | 2 |
| 2017-18 | Advanced MPI | EPCC | Cambridge, UK | 2017-09-12 | 2 |
| 2017-18 | Advanced Fortran Topics | GCS | Garching, DE | 2017-09-11 | 5 |
| 2017-18 | Hands-on Introduction to High Performance Computing for womENcourage | EPCC | Barcelona, ES | 2017-09-07 | 1 |
| 2016-17 | Modern Fortran | EPCC | Cambridge, UK | 2017-07-27 | 2 |
| 2016-17 | Message-passing Programming with MPI | EPCC | Edinburgh, UK | 2017-07-12 | 3 |

| Programme | Course title | PTC | Location | Start Date | Duration (days) |
|---|---|---|---|---|---|
| 2016-17 | Hands-on Introduction to HPC | EPCC | Edinburgh, UK | 2017-07-10 | 2 |
| 2016-17 | Efficient Parallel Programming with GASPI | GCS | Stuttgart, DE | 2017-07-03 | 2 |
| 2016-17 | Data Analytics with HPC | EPCC | Portsmouth, UK | 2017-06-29 | 2 |
| 2016-17 | Introduction to Unified Parallel C (UPC) and Co-array Fortran (CAF) | GCS | Stuttgart, DE | 2017-06-29 | 2 |
| 2016-17 | 8th Programming and Tuning Massively Parallel Systems summer school (PUMPS) | BSC | Barcelona, ES | 2017-06-26 | 5 |
| 2016-17 | Intel MIC Programming Workshop | GCS | Garching, DE | 2017-06-26 | 3 |
| 2016-17 | Workshop HPC Methods for Engineering | CINECA | Milan, IT | 2017-06-19 | 3 |
| 2016-17 | 3rd School on Scientific Data Analytics and Visualization | CINECA | Rome, IT | 2017-06-12 | 5 |
| 2016-17 | High-performance computing with Python | GCS | Juelich, DE | 2017-06-12 | 2 |
| 2016-17 | Systems Workshop: Programming ARM based prototypes | BSC | Barcelona, ES | 2017-05-12 | 1 |
| 2016-17 | Heterogeneous Programming on GPUs with MPI + OmpSs | BSC | Barcelona, ES | 2017-05-10 | 2 |
| 2016-17 | Software Carpentry | EPCC | Edinburgh, UK | 2017-05-09 | 2 |
| 2016-17 | Performance Analysis and Tools | BSC | Barcelona, ES | 2017-05-08 | 2 |
| 2016-17 | HPC code optimisation workshop | GCS | Garching, DE | 2017-05-04 | 1 |
| 2016-17 | Introduction to Scientific and Technical Computing in C | CINECA | Bologna, IT | 2017-05-03 | 3 |
| 2016-17 | Uncertainty quantification | MdS | Saclay, FR | 2017-05-02 | 3 |
| 2016-17 | Introduction to OpenACC | BSC | Barcelona, ES | 2017-04-27 | 2 |
| 2016-17 | Node-Level Performance Engineering | GCS | Stuttgart, DE | 2017-04-27 | 2 |
| 2016-17 | Advanced Optimization and Threading | CSC | Espoo, FI | 2017-04-26 | 3 |
| 2016-17 | Advanced usage on Curie supercomputer: Best practice for current and future HPC architectures | MdS | Bruyères-le-Châtel, FR | 2017-04-25 | 3 |

| Programme | Course title | PTC | Location | Start Date | Duration (days) |
|---|---|---|---|---|---|
| 2016-17 | GPU Programming with CUDA | GCS | Juelich, DE | 2017-04-24 | 3 |
| 2016-17 | Introduction to CUDA Programming | BSC | Barcelona, ES | 2017-04-18 | 4 |
| 2016-17 | C-C++ multicore application programming | MdS | Saclay, FR | 2017-04-18 | 3 |
| 2016-17 | Hands-on Porting and Optimisation Workshop: Making the most of ARCHER | EPCC | Birmingham, UK | 2017-04-04 | 1 |
| 2016-17 | Programming the Manycore Knights Landing Processor | EPCC | Leeds, UK | 2017-04-03 | 2 |
| 2016-17 | Advanced Topics in High Performance Computing | GCS | Garching, DE | 2017-04-03 | 4 |
| 2016-17 | Metagenomics Data Analysis Workshop | CSC | Espoo, FI | 2017-04-03 | 4 |
| 2016-17 | Efficient Parallel IO on ARCHER | EPCC | Durham, UK | 2017-03-29 | 2 |
| 2016-17 | Single-sided PGAS Communications Libraries | EPCC | Warwick, UK | 2017-03-27 | 2 |
| 2016-17 | 25th VI-HPS Tuning Workshop | GCS | Aachen, DE | 2017-03-27 | 5 |
| 2016-17 | Advanced Fortran Programming | CSC | Espoo, FI | 2017-03-20 | 3 |
| 2016-17 | Fortran for Scientific Computing | GCS | Stuttgart, DE | 2017-03-20 | 5 |
| 2016-17 | Spring School in Computational Chemistry 2017 | CSC | Espoo, FI | 2017-03-14 | 4 |
| 2016-17 | Simulation Environments for Life Sciences | BSC | Barcelona, ES | 2017-03-14 | 2 |
| 2016-17 | Parallel I/O and Portable Data Formats | GCS | Juelich, DE | 2017-03-13 | 3 |
| 2016-17 | OpenMP GPU Directives for Parallel Accelerated Supercomputers - an alternative to CUDA from Cray perspective | GCS | Stuttgart, DE | 2017-03-07 | 2 |
| 2016-17 | Parallel filesystems and parallel IO libraries | MdS | Saclay, FR | 2017-03-06 | 2 |
| 2016-17 | Python in High Performance Computing | CSC | Espoo, FI | 2017-03-01 | 3 |
| 2016-17 | HPC-based simulations, Engineering and Environment | BSC | Barcelona, ES | 2017-02-14 | 3 |
| 2016-17 | 13th Advanced School on Parallel Computing | CINECA | Bologna, IT | 2017-02-13 | 5 |
| 2016-17 | Advanced Parallel Programming | CSC | Espoo, FI | 2017-02-13 | 3 |
| 2016-17 | 24th VI-HPS Tuning Workshop | EPCC | Southampton, UK | 2017-02-08 | 3 |
| 2016-17 | Intel MIC Programming Workshop | GCS | Ostrava, CZ | 2017-02-07 | 2 |
| 2016-17 | Big Data Analytics | BSC | Barcelona, ES | 2017-02-07 | 4 |
| 2016-17 | Parallel Linear Algebra | MdS | Ostrava, CZ | 2017-02-02 | 2 |
| 2016-17 | Programming Distributed Computing Platforms with COMPSs | BSC | Barcelona, ES | 2017-02-02 | 1 |
| 2016-17 | Petaflop System Administration; Marenostrum III | BSC | Barcelona, ES | 2017-01-31 | 2 |
| 2016-17 | Performance portability for GPU application using high-level programming approaches | MdS | Orsay, FR | 2017-01-16 | 3 |
| 2016-17 | Introduction to hybrid programming in HPC | GCS | Garching, DE | 2017-01-12 | 1 |

**Table 5. List of PTC courses during the PRACE-5IP project.**

## 12.2 Reports from Seasonal Schools organised in PRACE-5IP

### *12.2.1 Autumn 2017 Seasonal School Report, Poland*

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

**PRACE Autumn School 2017 – Event Report**

1 Basic information about the event

1.1 Name

PRACE Seasonal School on Computational Fluid-Structure Interaction

1.2 Dates

20.11.2017 – 24.11.2017

1.3 Location

Gdańsk, Poland

1.4 Organising sites

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

1.5 Mission

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

1.6 Event URL

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

2 Organisational details

2.1 Local organising committee

- Rafał Tylman, CI TASK
- Ewa Politowska, CI TASK
- Michał Białoskórski, CI TASK
- Ondrej Jakl, VSB

2.2 Venue

Seasonal school was placed at our headquarter in Gdańsk University of Technology. It is located in city centre and close to the old city centre of Gdańsk

(approx 10 minutes by public transport). It is very easily to get there from airport (approx 20 min by train) and main train station (approx. 5 minutes). All laboratories and lecturers were held in well equipped conference room suitable for 30 persons.

3 Program & contents

3.1 Program committee

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

3.2 Designing the program

Large number of the mechanical, aerospace, civil and hydro engineering machines are operating in the complex environment. Floating offshore wind turbine or the helicopter in flight are only a reference examples of the problem. Operational loads and resulting structural response of the investigated object are coming from aerodynamic, hydrodynamic and thermal forces. Traditionally those mechanical systems are being studied w.r.t the different scientific disciplines: solid mechanics, flow mechanics, material sciences and computer methods only to name major domains. It leads to the approximate and often imprecise results of numerical simulations. Muti-physics approach is required to adequately address the complexity of the real-life operation of the mechanical systems.
Proposed Seasonal School on Computational Fluid-Structure Interaction tries to close the isolated domain analysis gap. The FSI School offers an integrated multidisciplinary training covering the comprehensive spectrum of the mathematical theorems, fluid and solid dynamics, numerical modelling techniques and all this within the framework of the HPC resources and tools able to tackle the challenging problems of the coupled multi-physics problems. Lectures will be followed with the laboratory exercises run on the CI TASK cluster. The course is addressed to wide audience ranging from PhD students to more senior researchers active in the science and industrial R&D departments.

3.3 Description of the contents

HPC – Introduction to High Performance Computing. On this seminar attendees were introduced to HPC and parallel calculation problems. On laboratories attendees were able to access to supercomputer and learn how to submit jobs to queue.
CFD – This seminar provides an introduction to the CFD methods. From basic elements to more advanced problems. On laboratories attendees conducted by trainer write their own CFD calculation programs in Fortran
FEM – Introduction to FE modelling concept. Derivation of governing equations for 1D problems (simple approach). Formulation’s generalization for 2D, ad 3D problems (weighting methods). Simplification for special cases. During laboratories attendees where working with Matlab software.

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

3.4 List of trainers

**George Barakos** – professor at School of Engineering of the University of Glasgow. George has so far delivered undergraduate and graduate-level courses on Fluid Mechanics, Aerodynamics, Aeroelasticity, Computational Fluid Dynamics and Thermodynamics, Simulation in Aerospace Engineering. He is the author of some 150 research papers and a regular contributor to national and international conferences on aerodynamics, fluid mechanics and CFD.
**Pascal Bayrasy** – Development Manager at Fraunhofer SCAI, specialised on Fluid Structure Interaction Method. Involved in R&D of MpCCI Coupling Environment software.
**Nadja Wirth** – engineer at Fraunhofer SCAI, specialised on Turbomachineru applications, and MpCCI software development.
**Maicej Kashin**, PhD – scientist and lecturer at GUT. Specialised on Finite Element Methods (FEM).
**Michał Białoskórsk**i, PhD – senior HPC specialist in CI TASK administrator involved in building first HPC clusters. During his work in CI TASK has a lot of didactic activities with students and On-demand workshops for HPC users

3.5 Computer resources

All attendees have guarantee access to CI TASK supercomputer – Tryton (https://www.top500.org/system/178552) within course accounts. There where resource reservation set for course purpose.
Laboratories were held on virtual machines with installed all software needed for course. Attendees has been connecting to the laboratory via remote desktop application.

4 Participants & feedback

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

There were 32 participants, from Poland only.

4.2 Analysis of the feedback

All participants were satisfied from the course level and contents, except one who was expecting more HPC information and less theorems.
The most attractive for attendees where CFD lab classes – 50% asks for course continuation in future.

4.3 Awareness activities, outreach

Information was published on PRACE event portal and disseminated in HPC centres in Poland as well as researchers working with fluid dynamics.
The maximal number of registrants was reached.

5 Conclusions & lessons learned
Organisation of Seasonal School was very valuable experience and it was not as difficult as we thought it would be.

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

### *12.2.2 Winter 2018 Seasonal School Report, Slovakia*

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

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

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

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

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

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

   3.2. Final program (table (appendix))
   See appendix
   3.3. List of trainers (full list of trainers as an appendix with contact information and description of expertises)
   - Prof. Erik Bongcam Rudloff: biologist and computer scientist. He is Professor of Bioinformatics and the head of SLU-Global Bioinformatics Centre at the Swedish University of Agricultural Sciences. His main research deals with development of bioinformatics solutions for the Life Sciences community; erikbong@mac.com

- Dr. Seija Sirkiä: Data scientist at CSC - Scientific computing Ltd., Finland.; seija.sirkia@csc.fi
- Mr. Apurva Nandan: Software specialist at CSC - Scientific computing Ltd., Finland. Works in the Data Analytics group building big data and cloud-based applications; apurva.nandan@csc.fi
- Dr. Kimmo Mattila: Bioinformatics specialist at CSC - Scientific computing Ltd., Finland; kimmo.mattila@csc.fi

3.4. Designing the program

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

3.5. Description of the contents

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

eases the learning for practicing bioinformaticians. Spark is constantly growing with new libraries for bioinformatics analysis, although widespread usage will take some time because the traditional methods need some rewriting in Spark. But, with the community constantly evolving, it is good chance to learn Spark and implement your own methods in it, for doing large scale data analysis.

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

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

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

4. Participants & feedback

4.1. Number of participants by country

| Country | Count |
|---|---|
| Slovakia | 32 |
| Czech Republic | 1 |
| Germany | 1 |

4.2. Process for selecting the participants (if applicable)

No selection applied

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

4.4. Analysis of the feedback

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

Positive:

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

Negative:

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

5. Conclusions & lessons learned

We are aware that this school may have been too advanced for non-negligible fraction of participants due to a lack of programming skills. However, if we would explicitly state, that the event is suitable for skilled programmers, we would hardly attract this many

participants (especially among biologists). We nevertheless strongly believe that the school was inspiring for many of them and by enlarging the community of researched using bioinformatics tools in HPC environment, even more researchers will be attracted to this area. Despite rather small participation of foreign researchers we were positively surprise that we could attract local researcher from various institutions across the country. Most of the attendees are not HPC users (yet) that we could effectively disseminate the information not only about our local computing resources and opportunities but also about PRACE to a brand new community.

*12.2.3 Autumn 2018 Seasonal School Report, Slovenia*

**1. Basic information about the event**

**Name**

PRACE Autumn School 2018 - HPC for Engineering and Chemistry

**Dates**

24.-26. 9. 2018

**Location**

Ljubljana, Slovenia

**Organizing sites**

University of Ljubljana, Faculty of mechanical engineering (ULFME), University of Ljubljana, Faculty of Chemistry and Chemical Technology (FKKT), National institute of Chemistry (NIC), University of Ljubljana, Faculty of medicine (UL FM)

**2. Organizational details**

**Local organizing committee (table)**

| Name | Organization |
|---|---|
| Prof. dr. Leon Kos | UL FME |
| Prof. dr. Janez Povh | UL FME |
| Mateja Maffi | UL FME |
| dr. Jernej Stare | National Institute of Chemistry |

**Venue**

Event was organised at University of Ljubljana, Faculty of mechanical Engineering, Aškerčeva cesta 6, 1000 Ljubljana in 2 classrooms, suitable for parallel groups up to 40 people.

**Realized workload**

| **Name** | **PMs** |
|---|---|
| Prof. dr. Leon Kos | 1 |
| Prof. dr. Janez Povh | 1 |
| Mateja Maffi | 1 |

**Synergetic events**

None

**3. Program & content**

**Program committee:**

| **Name** | **Organization** |
|---|---|
| Leon Kos, ULFME (programme chair) | UL FME |
| Prof. dr. Janez Povh | UL FME |
| Dr. Matej Praprotnik, | National Institute of Chemistry |
| Brane Leskošek | UL FM |

**Final program**

See Appendix 1.

**List of trainers:**

5.1.1. Aleksander Grm, University of Ljubljana, speaker at Hands-on tutorial on solving engineering problems with OpenFoam

5.1.2. Milan Hodošček, National Institute of Chemistry, Speaker at Hands-on tutorial on Molecular dynamics and at QM/MM

5.1.3. Alain Kassab University of Florida, speaker at

- Multiscale CFD modeling for congential heart disease
- Multiscale CFD modeling for left ventricular assist device
- An introduction to Finite Element, Boundary Element, and Meshless Methods - with applications in heat transfer and fluid flow
- Conjugate heat transfer and proper orthogonal decomposition

5.1.4. Franci Merzel, NIC; speaker at Classical and ab-initio molecular dynamics

5.1.5. Matej Praprotnik, speaker at Multiscale modeling & simulation

5.1.6. Jurij Sablić, NIC, speaker at Hands-on tutorial on Espresso++

5.1.7. Jernej Stare, NIC, Speaker at

- Hands-on tutorial on Quatum methods (Gaussian, cpmd...)
- Quantum methods

6. Caspar van Leeuwen SURFsara; Speaker at

- MPI
- Parallel Computing
- OpenMP

7. Jens H. Walther, Technical University of Denmark, Denmarks; speaker at

- Hands-on tutorial on Molecular dynamics and Computational fluid dynamics for nanofluidics
- Nanofludics

**4. Designing the program**

The program was designed to attract more researchers from the field of mechanical engineering and chemistry. In today's competitive product development, high performance computing (HPC) delivers outstanding value in these two areas. Parallel computing increases understanding, productivity and accuracy of the simulation - a faster turnaround, reduced costs, systematic design variations and more complex models. The PRACE Autumn School communicated and discussed issues and perspectives of HPC targeting engineering applications arising from evaluation performance and/or design of products, e.g. equipment and processes, with a particular emphasis on the automotive, aerospace, and energy fields. The PRACE Autumn School placed priority on algorithms, simulation strategies, and programming techniques for complex fluid flow simulations, structural mechanics and computational chemistry with intensive use of HPC

resources. PRACE was presented as the main organization for HPC in Europe. Autumn school targeted industry users to get acquainted with advanced technology and the possibilities of HPC. In designing the Autumn School program, we wanted to have a broad awareness of the school spread by attendees and by additional awareness activities. Having this in mind we specially tailored program to be understandable and at the same time have insight into real world challenging problems that can be solved on supercomputer only by following simulations with commercial suite of programs, custom solvers and plugins that helps with the simulations.

## 5. Description of the contents

The training event targeted to:

8. Esperienced researchers from academia fro several slovenian research institues and universities;
9. young researchers from academia and engineers from industry looking for competencies in advanced CFD, FEM, Lattice Boltzmann, Monte Carlo numerical simulations, using state-of-the-art software and hardware tools. Representatives of several existing industrial partners (Pipistrel - aircrafts), Akrapovič (motorcycle exhausts), Domel (pumps, stirrers, vacuum cleaners) that engineers from SMEs will find this course of particular interes.
10. master students from mechanical and chemical engineering that wanted to get competent for the most demanding numerical simulations in engineering;

We started with presenting of the EU and Slovenian HPC space. Then we made shot introduction to parallel programming with C and MPI.
Benefits of HPC for industry were presented with special speaker from the domain of mechanical engineering and with tutorials on OpenFoam.
Chemical engineering people were given several extensive hand-on trainings about the most important HP methods and HP software used chemistry: classical and ab-initio molecular dynamics, multiscale modeling & simulation, Espresso++https://events.prace-ri.eu/event/729/contributions/582/, Quatum methods (Gaussian, cpmd...).

We provided access to the following computer resources

11. Supercomputer HPCFS-U at ULFME with accounts for the event is being prepared that will give attendees KDE GUI environment with all required tools and icons required for tutorials. ULFME owns a license for 25 seats and 256 core parallel ANSYS research associate. Nearby computing classrooms were prepared for NX client remote terminal access. Time limited WiFi hot spot access with the same credentials as for HPC were given to all attendees so that they could access internet from their (not required) laptops and smart phones.

## 6. Participants & feedback

### 6.1. Number of expected participants

39 people registered for the school:

| Country | Count |
|---|---|
| Iran, Islamic Republic of | 2 |
| Italy | 2 |
| Romania | 2 |
| Slovenia | 33 |

| | |
|---|---|
| Spain | 1 |
| **Total** | **39** |

Out of them, only 30 showed up:

| **Country** | **Count** |
|---|---|
| Iran, Islamic Republic of | 1 |
| Italy | 0 |
| Romania | 2 |
| Slovenia | 27 |
| Spain | 1 |
| **Total** | **30** |

### 6.2. Process for selecting the participants

No selection applied

### 6.3. Statistics of the feedback survey

An extensive survey was sent to all participants. We collected 11 answers. The summary of these answers is presented as Appendix 2.

### 6.4. Analysis of the feedback

Here we only recall the most important facts collected by the respondents.
Overall, we can conclude that the participants were satisfied or very satisfied with almost all elements of the school. They liked most the hands-on exercises, while the lowest satisfaction was with speakers who only gave fast, high level lectures in some specific area. This was also the main observation of the organising committee team.
We also got several ideas for the next autumns school, like cuda programming, linear algebra solvers etc.

### 6.5. Conclusions & lessons learned

We are aware that this school may have been too advanced for small fraction of participants due to a lack of programming skills, while for few of those that are already using some specific HPC software some topics were too easy. But we would target more specifically to the people with appropriate background, we would hardly attract these many participants. We are nevertheless strongly confident that the school was inspiring for many of them and we have nicely mixed people from mechanical and chemical engineering domains and therefore initiated new multidisciplinary collaborations.

*12.2.4 Winter 2018 Seasonal School Report, Bulgaria*

1. Basic information about the event

1.1. Name

- PRACE Winter School on Computational Chemistry, Biochemistry and Medicinal Chemistry – Methods and Tools

1.2. Dates

- 26-29 November 2018

1.3. Location

- Institute of Information and Communication Technologies, Bulgarian Academy of Sciences (IICT-BAS), Hall #2, Acad. Georgi Bonchev str., Bl.25A 1113 Sofia, Bulgaria

1.4. Organizing sites:

Association National Centre for Supercomputing Applications (NCSA), Bulgaria

2. Organizational details

2.1. Local organizing committee (table)

| Name | Organisation |
|---|---|
| Prof. Nevena Ilieva-Litova nevena.ilieva@parallel.bas.bg | NCSA |
| Dr. Iva Nikolova inni@tu-sofia.bg | NCSA |
| Nedu Karaivanov nkaraivanov@parallel.bas.bg | NCSA |

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

Institute of Information and Communication Technologies, Bulgarian Academy of Sciences, Sofia, Bulgaria, Training Hall #2: IICT-BAS provided all the necessary conditions for conducting the school, including a hall with the needed capacity and the most up-to-date technical equipment for lectures and practical classes on the topic of the school. This includes a beamer and screen with multiple connection options for presentation computers, a tele-conference system, 3D presentation system (smart lab) and lecture hall with 50 seats in a classroom setting as well as a stable wireless internet connection. The Hall provides excellent facilities especially designed to accommodate training courses, lectures, labs, etc in the field of Computer Science. It also provided enough space for registration and coffee breaks. In addition IICT's location is close enough to Sofia airport (5km) and there is a number of 3 and 4 star hotels within 1km of the training location, so that once accommodated, all foreign participants could reach the venue by foot

2.3. Budgeting (fluid text: reasoning behind the budget; table: the budget together with realized expenses (appendix)):

The major other direct costs incurred for the event covered the usual activities necessary for running a training event: Covering the cost of two-way air-plane tickets to Sofia and back and transport to/from their hotel for the four invited speakers from abroad; cost of speakers' accommodation covering the period of the School (accommodation in a four-star hotel for 60 euro per day per person). The costs for food and catering refer to organized lunch for all the participants for all four days of the training event, coffee breaks organized at the premises of the training twice every day during the School, as well as an organized dinner. In addition, extra materials were designed especially for the event and distributed to participants (badges, event programs, certificates). NCSA has observed the principles of best value for money and all costs for the listed services are at or below average prices on the local market. The total incurred other direct costs amount to 3,763.65 Eur.

2.4. Realized workload (table: person and total working hours spent for the event):
A total of 15 persons who committed 452 person-hours were engaged in the event

2.5. Synergetic events (listing: was there any other PRACE activity during the event which would have utilized the venue or other effort):

3. Program& content

3.1. Program committee

Prof. Tony Spassov - Head of Department Applied Inorganic Chemistry, Faculty of Chemistry and Pharmacy, University of Sofia "St. Kl. Ohridski", TSpassov@chem.uni-sofia.bg
Dr. Ilian Todorov - Head of Computational Chemistry Group, Scientific Computing Department –Science and Technology Facilities Counci, UK, ilian.todorov@stfc.ac.uk
Prof. Irini Doychinova –Tzekova – Head of Department of General and Inorganic Chemistry , Faculty of Pharmacy – Medical University of Sofia, idoytchinova@pharmfac.net

3.2. **Final program (table (appendix))**

| DAY 1 | |
|---|---|
| 9:00-9:30 | **Registration** |
| 9:30 | **Opening Address**<br>**Prof. Tony Spassov**- *Head of Department Applied Inorganic Chemistry Faculty of Chemistry and Pharmacy, University of Sofia "St. Kl. Ohridski"* |

| | |
|---|---|
| 9:40 | **The Hartree Centre Experience**<br>**Dr. Ilian Todorov -** *Scientific Computing Department –Science and Technology Facilities Council* |
| 10:00-11:00 | **UK Industrial Innovation via Hartree Centre's Computational Soft Matter R&D**<br>**Dr. Michael Seaton -** *Scientific Computing Department - Science and Technology Facilities Council* |
| **11:00 – 11:30 Coffee Break** | |
| 11:30-13:00 | **Factors governing the metal ion selectivity in ion channels: Insights from DFT/CDM calculations**<br>**Determinants of the host–guest interactions between α-, β- and γ-cyclodextrins and group IA, IIA and IIIA metal cations: a DFT/PCM study**<br>**Prof. Todor Dudev** - *Faculty of Chemistry and Pharmacy, University of Sofia "St. Kl. Ohridski*" |
| **13:00 – 14:00 Lunch Break** | |
| 14:00 – 15:00 | **Biomolecular simulations for more efficient drug delivery**<br>**Prof. Anela Ivanova -** *Faculty of Chemistry and Pharmacy, University of Sofia "St. Kl. Ohridski*" |
| **15:00 – 15:30 Coffee Break** | |
| 15:30 – 17:00 | **In-silico methods in Drug design**<br>**Prof. Ilza Pajeva -** *Institute of Biophysics and Biomedical Engineering- IBBE-BAS* |

| | |
|---|---|
| **DAY 2** | |
| 9:00-10:00 | **Prof. Sonia Ilieva- Reaction mechanism in organic chemistry**<br>*Faculty of Chemistry and Pharmacy, University of Sofia "St. Kl. Ohridski*" |
| **10:00 – 10:30 Coffee Break** | |
| 10:30-12:00 | **Prof. Irini Doychniova - Tzekova Case studies in drug design** |

| | |
|---|---|
| | *Faculty of Pharmacy – Medical University of Sofia* |
| 12:00-13:00 | **Prof. Boris Galabov – Computer modeling of π-hydrogen bonding in organic systems and Grapheme**<br>*Faculty of Chemistry and Pharmacy, University of Sofia "St. Kl. Ohridski"* |
| **13:00 – 14:00 Lunch Break** | |
| 14:00 – 15:00 | **Assoc. Prof. Hristiyan A. Aleksandrov- Modeling of metal and metal oxides systems relevant for catalytic applications**<br>*Faculty of Chemistry and Pharmacy, University of Sofia "St. Kl. Ohridski"* |
| **15:00 – 15:30 Coffee Break** | |
| 15:30 – 18:00 | **Dr. Peicho Petkov,**<br>*National Centre for Supercomputing Applications (NCSA), Bulgaria*<br>**Prof. Anela Ivanova**<br>*Faculty of Chemistry and Pharmacy, University of Sofia "St. Kl. Ohridski"*<br>**MD Simulations Training** |
| **DAY 3** | |
| 9:00-11:00 | **Dr. Ilian Todorov - Introduction to DL_POLY Part 1**<br>*Scientific Computing Department - Science and Technology Facilities Council, UK* |
| **11:00 – 11:30 Coffee Break** | |
| 11:30-13:00 | **Dr. Ilian Todorov - Introduction to DL_POLY Part 2**<br>*Scientific Computing Department - Science and Technology Facilities Council, UK* |
| **13:00 – 14:00 Lunch Break** | |
| 14:00 – 15:00 | **Dr. Ivelina Georgieva - Simulations of metal-organic complexes**<br>*Institute of General and Inorganic Chemistry – Bulgarian Academy of Sciences* |
| **15:00 – 15:30 Coffee Break** | |

| | |
|---|---|
| 15:30 – 16:45 | **Dr. Ivelina Georgieva - Simulations of metal-organic complexes - demo and training**<br>*Institute of General and Inorganic Chemistry – Bulgarian Academy of Sciences* |
| **18:00 – 22:00 Dinner** | |
| **DAY 4** | |
| 9:00- 11:00 | **Dr. Chin Yong - Introduction to DL_FIELD**<br>*Scientific Computing Department - Science and Technology Facilities Council, UK* |
| **11:00 – 11:30 Coffee Break** | |
| 11:30- 13:00 | **Dr Michael Seaton - Introduction to DL_MESO**<br>*Scientific Computing Department - Science and Technology Facilities Council, UK* |
| **13:00 – 14:30 Lunch Break** | |
| 14:30 – 17:00 | **Dr. Ilian Todorov, Dr. Chin Yong, Dr. Michael Seaton, Dr. Alin Elena**<br>**Training:** Practicals with DL_POLY_4.09 |
| **Closing Words** | |

3.3. List of trainers (full list of trainers as an appendix with contact information and description of expertises)

- Dr. Ilian Todorov (ilian.todorov@stfc.ac.uk), Scientific Computing Department, STFC, UK: Lead of the Computational Chemistry Groups at STFC. The group provides support to a number of CoSeC consortia on behalf of the Scientific Computing Department as well as to the industrial and emerging technology ambitions of the Hartree Centre. Dr. Todorov's work focus has been in the area of application development in molecular simulations. He has carried out extensive HPC software engineering research in the area of molecular dynamics algorithms and methodology by driving the development of the DL_POLY flagship code. Has scientific interests in the calculation of properties and thermodynamics of solid state materials as well as soft matter using classical molecular simulations such as Molecular Dynamics, Dissipative Particle Dynamics, Monte Carlo and Lattice Dynamics. Dr. Todorov has organized and carried out a large number of training events promoting molecular simulation methodologies via the CCP5 software suite supporting a number UK consortia such as CCP5, HEC-MCC and

UKCOMES. And has been involved in a number of PRACE training events promoting software engineering skills and methodology relevant to emerging technologies.

- Dr. Chin Yong ( chin.yong@stfc.ac.uk) – Scientific Computing Department, STFC, UK is a Senior Research Scientist of the Computational Chemistry Group at Daresbury Laboratory since October 2000. He has extensive research experience in a wide-range of molecular modelling fields including polymers, particle bombardment, nano-surface contacts, mineral surface interactions and biological simulations, using a variety of techniques such as the molecular dynamics, Monte Carlo and ab-initio electronic calculations. Since November 2008 he has been an active support scientist for the CCP5 community, in particular, in areas of potential model development and also the lead developer of DL_FIELD, a powerful force field model development and editing software tool for DL_POLY molecular dynamics package as a result of culmination of many years experiences in molecular modelling research.

- Dr. Alin Marin Elena ( alin-marin.elena@stfc.ac.uk ) is currently a Computational Scientist at Daresbury Laboratory, STFC, UK. His main activity relates to methods and software development, DL_POLY4. Dr Elena has a strong interest in new technologies and High Performance Computing and their application to statistical physics and is also involved in the Xeon Phi and many-core versions of DL_POLY.

- Dr. Michael Seaton – Hartree Centre, STFC ( michael.seaton@stfc.ac.uk )
- Prof. Tony Spassov ( TSpassov@chem.uni-sofia.bg ) – Head of Department Applied Inorganic Chemistry, Faculty of Chemistry and Pharmacy, University of Sofia “St. Kl. Ohridski". Research experience:
  Structural Analysis Techniques: Optical Microscopy, Electron Microscopy (TEM, SEM), Electron and X-ray Diffraction;
  Thermal Analysis Techniques: Differential Thermal Analysis, Differential Scanning Calorimetry, Rapid Heating Techniques, Thermogravimetry. Electrical Properties Measurements. Magnetic properties measurements;
  Electrochemical and gas-phase techniques for hydriding/dehydriding of metallic alloys;
  Rapid Quenching Techniques: Splat-quenching, Melt-spinning. Mechanical Alloying.

- Prof. Boris Galabov ( bgalabov@chem.uni-sofia.bg )– Faculty of Chemistry and Pharmacy, University of Sofia “St. Kl. Ohridski": Boris Galabov has published 132 scientific papers, most of which in prestigious international journals. He has delivered 35 plenary and invited lectures at international scientific conferences as well as many lectures in foreign universities. He is member of the Editorial

Boards of the Journal of Molecular Structure, Asian Journal of Spectroscopy and Open Spectroscopy Journal. The principal scientific interests of B. Galabov are in the fields of physical organic chemistry and vibrational spectroscopy.

- Prof. Todor Dudev (t.dudev@chem.uni-sofia.bg) - Faculty of Chemistry and Pharmacy, University of Sofia “St. Kl. Ohridski”. Todor Dudev is a full professor at Sofia University. He leads research in computational methods in Chemistry/Biochemistry. Previously he was a Senior Research Associate at Academia Sinica (Taiwan) and a Postdoctoral Researcher at Tokyo Institute of Technology (Japan).
  Areas of Expertise:
  Computational Chemistry/Biochemistry/Biophysics; Metals in Biology and Medicine; Molecular Modeling; Coordination Chemistry; Chemoinformatics; Infrared and Raman Spectroscopy; Teaching / Course Design;

- Prof. Anela Ivanova (aivanova@chem.uni-sofia.bg); Faculty of Chemistry and Pharmacy, University of Sofia “St. Kl. Ohridski". Prof. Ivanova teaches or has taught the following university courses:
  Quantum chemistry and chemical bonding – core course for B.Sc. level (lectures)
  Structure of matter – core course for B.Sc. level (lectures)
  Molecular design, Quantum chemistry – elective coursec for B.Sc. level (seminars)
  Molecular modelling of functional materials – elective course for B.Sc. level (seminars)
  Molecular dynamics and Monte Carlo simulations – core course for M.Sc. level (lectures)
  Quantum chemistry for molecular systems – core course for M.Sc. level (seminars)
  Physical and Colloid Chemistry 1 – mandatory course for M.Sc. level, Pharmacy major (seminars)

- Prof. Ilza Pajeva (pajeva@biomed.bas.bg ) – Institute of Biophysics and Biomedical Engineering – Bulgarian Academy of Sciences (IBBE-BAS) has deep expertise in: Pharmacology, Theoretical Chemistry and Medicinal Chemistry.

- Prof. Sonia Ilieva ( ohtsi@chem.uni-sofia.bg )- Faculty of Chemistry and Pharmacy, University of Sofia “St. Kl. Ohridski", Research Interests:
  Application of quantum-chemical calculations for interpretation of intensities in vibrational spectra; IR spectroscopy; Molecular modeling and quantitative structure-activity relationship (QSAR) of biologically active compounds
  Lectures: Instrumental methods in chemistry, Methods for analysis and control of medicines, Molecular modeling and QSAR, Ab initio MO calculations.

- Prof. Irini Doychinova- Tzekova ( idoytchinova@pharmfac.net) – Head of Department of General and Inorganic Chemistry , Faculty of Pharmacy – Medical University of Sofia,

- Assoc. Prof. Hristiyan Aleksandrov (haa@chem.uni-sofia.bg )- Faculty of Chemistry and Pharmacy, University of Sofia “St. Kl. Ohridski", Research interests: Quantum chemical modelling of: materials and catalysts with focus on microporous materials, oxide surfaces and nanoparticles; transition metal surfaces, nanoparticles and small clusters; complexes of transition metal ions ; reaction occurring on catalytic systems; drug delivery systems

- Dr. Peicho Petkov (peicho.petkov@gmail.com) - National Centre for Supercomputing Applications (NCSA), Bulgaria has been working in the field of Molecular dynamics simulations since 2006. He joined the CMS collaboration at CERN in 2001 and since 2010 he has been involved in the PRACE initiative. His main interests encompass high energy physics, molecular simulations, parallel computing and numerical algorithms. Within the PRACE project, his main activities have been running molecular dynamics simulations with GROMACS, NAMD and LAMMPS on BlueGene/P and BlueGene/Q as well as machines with hybrid Intel Xeon – Intel Xeon Phi architecture.

- Assoc. Prof. Ivelina Georgieva ( ivelina@svr.igic.bas.bg )– Institute of General and Inorganic Chemistry;

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

The program aimed at demonstrating and exposing the use of Computational (incl. HPC) methods and tools in the fields of Chemistry, Biochemistry and Medicinal Chemistry, areas in which the academics in Bulgaria have shown visible progress recognized globally. The experience of the UK’s Hartree Centre and the STFC Scientific Computing Department were also used to show that knowledge exchange between scientists with different academic experience and between academia and industry is the facilitation process for setting collaborative projects in which academic and industrial interests, experiments, HPC modeling and application development meet to provide drive for one another.
The program also discussed the methodologies, numerical methods and their implementation used by the state-of-the-art codes in the HPC environment.
A number of examples where the use of HPC modeling has been essential in solving scientific problems at atomic and molecular level were also presented.
Discussions and interaction with the lecturers was an integral part of the training process.

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

Dr. Ilian Todorov
The Hartree Centre Challenge-led applied research & innovation presented by Dr Ilian Todorov

The presentation outlined the historical set up and current ambitions of the Hartree Centre at UKRI STFC, UK. The Hartree Centre together with IBM-UK provides a collaborative environment for commercial partners to set up and explore R&D project ideas in the computational area, including HPC Software Engineering, ML and AI. Its main function is to help advance and stimulate industrial innovation in the UK by applying academic methodologies and computational methods to industrially relevant problems.
Dr Michael Seaton, - Hartee Centre of Science and Technology Facilities Council:
UK Industrial Innovation via Hartree Centre's Computational Soft Matter R&D presented
The talk included a number of Hartree Centre research lines with commercial partners such as IBM and Unilever in the area of Soft Matter Computational Chemistry.

Prof. Todor Dudev - Faculty of Chemistry and Pharmacy, University of Sofia "St. Kl. Ohridski":
(a) Factors governing the metal ion selectivity in ion channels: Insights from DFT/CDM calculations.
The thermodynamic aspects of metal ion competition in various ion channels (sodium, potassium, calcium and magnesium) have been systematically studied by a combination of density functional theory (DFT) calculations and continuum dielectric method (CDM) computations. The effect of different factors, such as the metal type, composition and architecture of the ion channel selectivity filter, solvent exposure of the pore and its rigidity, and the degree of the permeant ion hydration is assessed and major factors governing the metal ion selectivity in these systems determined.

(b) Determinants of the host–guest interactions between α-, β- and γ-cyclodextrins and group IA, IIA and IIIA metal cations: a DFT/PCM study
By employing density functional theory (DFT) calculations combined with polarizable continuum model (PCM) computations, we assess how the interaction between cyclodextrins of different size and a number of metal cations depends on (1) the size, valence state and preferred coordination number of the guest metal cations, (2) the size and flexibility of the host molecule, and (3) the dielectric properties of the environment. The major determinants of the process of cyclodextrin-metal recognition are established.

Prof. Anela Ivanova (FCP-SU) - Faculty of Chemistry and Pharmacy, University of Sofia "St. Kl. Ohridski"
Biomolecular simulations for more efficient drug delivery
The workflow of a typical molecular dynamics (MD) simulation of bioactive components in the liquid phase is presented with focus on some specifics of biosimulations. An overview of the relevant MD algorithms is made, introducing their basics. Software packages are summarized, where these algorithms are implemented. The concepts are illustrated with sample results from recent atomistic MD simulations of different (supra)molecular building blocks of systems for efficient drug delivery of a model chemotherapeutic agent

Prof. Ilza Pajeva (IBBE-BAS) - Institute of Biophysics and Biomedical Engineering-IBBE-BAS
In-silico methods in Drug design
The basics of *in silico* drug design was presented focusing on: concepts and principles of complementarity in the drug-receptor interactions, main types of ligand-receptor

interactions, classifications of the methods in computer-aided drug design, examples and limitations.

Prof. Irini Doichinova (FP-MU Sofia)
Case studies in drug design
Drug design is a rational computer-aided approach for drug discovery and development applying a wide variety of in silico methods. Some of the main methods like quantitative structure-activity relationships (QSARs), proteochemometrics, and molecular docking and their applications in drug design was considered in the lecture by real case studies.

Prof. Boris Galabov
Computer modeling of π-hydrogen bonding in organic systems and grapheme
π-Hydrogen bonding is an important phenomena in chemistry, biology, physics, and material science. Computational modeling combined with FTIR spectroscopy reveals details of the interactions leading to the formation of π-hydrogen bonded complexes. Density functional theory and MP2 ab initio computations predict with a remarkable accuracy the shifts of O-H stretching vibration frequencies upon π-hydrogen bonding with benzene derivatives and graphene. It is shown that the O-H frequency shifts may be employed as an experimental measure of chemical reactivity for aromatic compounds.

Dr. Peicho Petkov, Prof. Anela Ivanova
Hands-on Training on Molecular Dynamics using GROMACS

Dr. Ilian Todorov
Introduction to DL_POLY
DL_Software is the collective term that refers to the computational chemistry software suites developed at Daresbury Laboratory. DL_POLY is a general purpose molecular dynamics simulation package developed at Daresbury Laboratory by I.T. Todorov and W. Smith under the auspices of EPSRC and in support of CCP5. It can be used to simulate a wide variety of molecular systems including simple liquids, ionic liquids and solids, small polar and non-polar molecular systems, bio- and synthetic polymers, ionic polymers and glasses, solutions, simple metals and alloys.

Ivelina Georgieva, Natasha Trendafilova (IGIC-BAS)
Training – Simulations of metal-organic complexes

Dr. Chin Yong
Introduction to DL_FIELD
DL_FIELD is a computer program package written in C that primarily serves as a support application software tool for DL_POLY molecular dynamics simulation package. DL_FIELD is developed at Daresbury Laboratory by C.W. Yong under the auspices of EPSRC and in support of CCP5. The primary function of the Program is to convert users' atom models, in particular those of large complex bio molecular systems for a wide range of force fields (CHARMM, AMBER, OPLS, DREIDING, PCFF, CVFF, INORGANIC), into file formats that are recognisable by, and ready to run using, DL_POLY with minimum intervention by the user. The DL_FIELD operates with a minimum set of directive and, without having to learn any scripting languages, users can also easily fine tune force field models and set up their own force field library.

Dr. Michael Seaton
Introduction to DL_MESO
DL_MESO is a general purpose mesoscale simulation package developed at Daresbury Laboratory by M.A. Seaton under the auspices of EPSRC and in support of CCP5. It is written in Fortran90 and C++ and supports both Lattice Boltzmann Equation (LBE) and Dissipative Particle Dynamics (DPD) methods. It is supplied with its own Java-based Graphical User Interface (GUI) and is capable of both serial and parallel execution.

Dr. Alin Elena
Further Training with GROMACS 4.09

3.6. Computer resources: (fluid text: comment if they were sufficient for the event)

Remote access to Avitohol Supercomputing System via dedicated student accounts and local secure wi-fi connection. The multifunctional high-performance computer Avitohol has 300 CPU Intel Xeon E5-2650v2, 300 co-processors Intel Xeon Phi 7120P, 9.6 TB memory and performance of 420 TFLOPS;local. The resources proved to be sufficient for the purposes of the School: The network ‘s data traffic capacity was sufficient and there were enough dedicated accounts for all the participants to access the supercomputing system and learn about the different modeling capabilities of the applied software. (listing: supercomputer accesses as well as local IT infra available for the attendees;

4. Participants

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

| Participants | Country |
|---|---|
| 26 | Bulgaria |
| 2 | Italy |
| 1 | Czech Republic |
| 1 | Spain |

*12.2.5 Winter 2019 Seasonal School Report, Belgium*

1. **Basic information about the event**

**1.1. Name**

**PRACE Winter School – Introduction to Machine Learning for Scientist**

**1.2. Dates**

04.03.2019 – 08.03.2019

**1.3. Location**

Leuven, Belgium

**1.4. Organizing sites**

KU Leuven
U Hasselt
Flemish Supercomputing Center (VSC)
With the collaboration of HPE

**2. Organizational details**

2.1. **Local organizing committee (table)**

| Name | Institution |
|---|---|
| Geert Jan Bex | Hasselt University |
| Jan Ooghe | KU Leuven |
| Ewald Pauwels | Ghent University |
| Stefan Becuwe | University of Antwerpen |
| Ingrid Barcena | KU Leuven |

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

The event took place in one of the computer rooms of the KU Leuven ICTS building in de Arenberg Campus of the University of Leuven. The room was selected based on the possibility to accommodate comfortably all participants (40 people), the availability of computers (in case some participants have problems with their own laptop), the projection facilities and the good internet connectivity to the HPC KU Leuven cluster that needed to be used for the hand-on sessions. In the building was also available a room for having lunches and coffee breaks to promote networking among the participants. The venue was well connected and easy to reach from the city center. The venue is part of the KU Leuven facilities and therefore could be used without no cost.

**2.3. Budgeting (fluid text: reasoning behind the budget; table: the budget together with realized expenses (appendix))**

The costs presented in the table has been made as follows:

- **Facilities:** the Seasonal School took place at KU Leuven owned facilities so it was no cost associated with the use of this facilities.
- **Trainers travel expenses**: HPE did cover the travel expenses of 3 HPE trainers (Sorin Cheran, Al Amin and Vlad Stoican). The trainers from VSC had no travel expenses associated. Therefore no travel expenses were needed.
- **Trainers accommodation expenses**: Accomodation for the the 3 HPE trainers

was provided : 4 nights for Sorin Cheran and Vlad Stoican and 3 nights for Al Amin VSC trainers had no accommodation extensions associated.

- **Catering coffee breaks**: We offered 2 coffee breaks (morning and afternoon) during the 3 central days and 1 (afternoon) for the first day and 1 (morning) the last day.
- **Catering lunch:** In order to facilitate logistics and facilitate networking between the attendees, we offered lunch catering. during the 3 central days.
- **Social event:** Tuesday evening was organized a guided walk in the city center and a dinner.

For realized expenses see appendix 1.

2.4. **Realized workload (table: person and total working hours spent for the event)**

The total realized workload was 1.9 PM distributed as follows:

| Person | Task | Effort (hours) |
|---|---|---|
| Geert Jan Bex | Program | 100 |
| Jan Ooghe | Program | 100 |
| Kristel Hoydonckx | Logistic arrangements:<br>• Facilities<br>• Accommodation<br>• Catering<br>• Course materials<br>• Hosting and Registration | 40 |
| Ehsan Moravveji | Support during hands-on | 15 |
| Martijn Oldenhof | Support during hands-on | 15 |

**2.5. Synergetic events (listing: was there any other PRACE activity during the event which would have utilized the venue or other effort)**

No additional PRACE activity were organized during the event.

**3. Program & content**

3.1. **Program committee (table)**

| Name | Institution |
|---|---|
| Prof. dr. Bart Goethals | Universiteit Antwerpen |
| Prof. dr. Ann Nowé | Vrije Universiteit Brussel |
| Prof. dr. Dirk Valkenborg | Universiteit Hasselt |
| Prof. dr. Luc De Raedt | KU Leuven |

3.2. **Final program (table (appendix))**

See appendix 2.

3.3. **List of trainers (full list of trainers as an appendix with contact information and description of expertises):**

- Sorin Cheran (HPE): HPC and AI Strategist, Distinguished Technologist at Hewlett Packard Enterprise. He obtained his PhD in Computer Science (Artificial Intelligence) from Universita degli Studi di Torino in Italy. Sorin has been

driving emerging technologies adoption in the industry and is currently leading the part of the AI initiative within HPE.

- Geert Jan Bex (U Hasselt): He works as HPC analyst and consultant at KU Leuven and UHasselt. He has a M.Sc. in Physics (UAntwerpen) and a Ph.D. (UHasselt) in physics studying the properties of neural networks using statistical physics. He has worked as a knowledge engineer developing decision support systems for businesses where he mainly focused on applications of computational linguistics and machine learning. Returning to academia, he switched research topics to computer science working on inference of grammars for semi-structured data, leading to a PhD. in computer science. and also did research on bioinformatics applications.
- Al Amin (HPE): HPE AI expert giving support during the hands-on.
- Vlad Stoican (HPE): HPE AI expert giving support during the hands-on.
- Martijn Oldenholf (KU leuven): After his Master degree in Engineering he specialized himself in Distributed and Parallel systems. Now more than 10 years professional experience in the field of High Performance Computing and currently pursuing an advanced Master degree in Artificial Intelligence at KU leuven.
- Ehsan Moravveji (KU Leuven)

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

Machine learning is increasingly being used as a tool to explore, understand, and explore the data that is generated in a wide variety of scientific domains. Classic approaches to data processing start to break down under the avalanche of data produced by modern measurement and diagnostic techniques.
This seasonal school was designed to provide researchers with an overview and a solid understanding of machine learning algorithms, and how they can be used to solve various research questions. The theory was complemented with a large amount of hand-on sessions to allow the attendees to put the learned concepts into practice.

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

- Introduction to AI and applicability: this introduction covers motivation for using AI techniques, illustrated with examples from industry. An overview of the history of the field is provided, as well as a discussion the state of the art and future directions.
- Linear regression: although useful in itself, this method mostly serves as a "warm up" exercise and a motivation why more sophisticated algorithms are required. Most interesting data is not linearly separable.
- Multilayer networks: this type of neural network was introduced three decades ago, but the backpropagation algorithm introduced in this session to train them is still used in the context of deep learning today.
- Frameworks and software ecosystem: modern machine learning frameworks such as Keras and Tensorflow make it much easier to apply machine learning

techniques. A decade ago, coding a neural network would take days, while it can now be done in minutes using these frameworks. An overview of the strong and weak points of a wide variety of frameworks is provided.

- Supervised learning , CNN and RNN: convolutional neural networks (CNNs) are widely applied in tasks related to images. These deep neural network discover the low-level features of the images in the lower layers, learning more abstract properties in the higher layers. CNNs have been successfully applied to object recognition tasks among others. Recurrent neural networks (RNNs) can be used to handle data that is represented as sequences of varying length. The key feature is that information should be retained over a long range of items in the sequence. RNNs are used extensively in natural language applications such as sentiment classification and machine translation.
- Unsupervised learning: while neural networks as well as many other machine learning techniques required labeled data, unsupervised learning algorithms try to infer structure in unlabeled data by separating it into categories. A number of these clustering algorithms are discussed. Dimensionality reduction can be used to detect the most salient features in the data, to reduce the number of dimensions for visualization purposes, or to reduce the number of features for machine learning tasks.
- Reinforcement learning: these techniques are intended to infer the optimal behavior of an agent in an environment, e.g., a computer playing a game (Alpha-go zero) or in robotics. The relevant mathematical background, current algorithms and applications are discussed.
- Scikit-learn pipelines: a proper methodology is paramount to the success of machine learning and AI projects. Data needs to be preprocessed or curated consistently during the training, testing and production phases. The Scikit-learn software package implements a lot of relevant algorithms and allows to build streamlined pipelines for reliable and consistent data processing.
- AI Ethics: it is clear that wide scale application of AI in services and industry will lead to ethical and societal issues. Researchers in the field of AI or in domain that apply it should be aware of these issues.
- AI at scale: using multiple GPUs: large data sets and complex algorithms require massive compute power, often more than is (realistically) available from a single GPU. Approaches to parallelize training over multiple GPUs and multiple compute nodes are discussed. Examples and scaling experiments are shown.

3.6. **Computer resources (listing: supercomputer accesses as well as local IT infra available for the attendees; fluid text: comment if they were sufficient for the event)**
Participants could use their own laptop or one of the 40 computers available on the computer room. For running the hand-on sessions both an HPE training cluster and the KU Leuven GPU infrastructure were used.

**4. Participants & feedback**

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

| Contry | Count |
|---|---|
| Belgium | 27 |
| Germany | 7 |
| Portugal | 2 |
| United Kingdom | 1 |
| Cyprus | 1 |
| Netherlands | 1 |
| Iceland | 1 |

4.2. **Process for selecting the participants (if applicable, fluid text)**
No selection applied

4.3. **Statistics of the feedback survey (tables (appendix))**
See appendix 3.

4.4. **Analysis of the feedback (fluid text: analyze the feedback in general and all specific very good or bad comments)**
We received 25 replies to the evaluations. The general evaluation of the school was very positive. Almost half of the participants were from outside Belgium and very diverse science field background (Bioinformatics, Engineering, Astrophysics, Material Science, Computer Science. Medicine, Climate, Physics, …) were represented. Most participants were from the academia but there was also 3 attendees from industrial companies.
The participants were very enthusiast and participative which contributed to make the sessions very interactive. In addition, during breaks and lunches participants engaged in very interesting conversations both with the teachers and other attendees.
As part of outreach activities we have made a video about the seasonal school that includes interviews to some participants:
https://dms.licdn.com/playback/C4D05AQE7LBg8vQBI-A/9cc7ff5a818c4bd5af2031dc9f2a7ccd/feedshare-mp4_3300-captions-thumbnails/1507940147251-drlcss?e=1553796000&v=beta&t=sJVGQk4GultPGNKSwjm2qNiwiaGEORgZjQ2XIuWLGwo
From the evaluation survey we can conclude:
Positive:

- The majority of the respondents found the venue, the catering, the overall organization and the registration excellent or good.
- Most respondents (> 90%) agree that the topic was relevant for their research and / or inspiring.
- Most respondents (>90%) agree that the teaching materials were well prepared and the hands-on valuable.
- A majority of respondents (80%) agree that the pace of teaching was right.
- 88% of respondents rated the school with grade 8 to 10 (10 is the best).

Negative:

- 12% of the respondents didn't agree that lectures were "clearly presented and comprehensible"

## 5. Conclusions & lessons learned (fluid text)

The overall conclusion of the seasonal school was very positive. After announcing the school we reached the maximum number of participants in very short time and we had a waiting list of more than 10 people. This clearly shows that there is a big interest among researchers of many disciplines in learning and apply to their fields machine learning techniques. Therefore it would be a good idea to organize more editions of this seasonal school.
In addition, the organization of the seasonal school gave us the opportunity to reach out to some potential users of both our HPC infrastructure and PRACE services.

## Appendix 1: realized expenses

| **Concept** | **Cost (EUR)** |
|---|---|
| Facilities | No cost |
| Trainers travel | No cost |
| Trainers accommodation | 1,996.66 |
| Catering (8 coffee breaks and 3 lunches for 48 people) | 4,223.20 |
| Social event (guided walk) | 144.00 |
| Social event (dinner for 28 people) | 840.00 |
| KU Leuven goodies | 70.18 |
| **Total** | **7,274.04** |

## Appendix 2: final timetable

**Monday 4/03**
**The Flemish Supercomputing Center (VSC)**
13:00 – 13:30
**Introduction to AI and applicability**
13:30 - 14:00
**How does deep learning work: From linear regression to neural networks**
14:00 - 15:00
**Coffe break**
**Hands-on: Linear regression**
15:20 - 17:30

**Tuesday 5/03**
**Hands-on: multilayer networks**
9:00 – 10:30
**Coffee break**
**Supervised learning: classification: Frameworks and Software ecosystem**
10:50 - 12:00
**Lunch**
12:00 - 13:00
**Supervised learning: classification: Frameworks and Software ecosystem: Hands-on: Frameworks**
13:00 - 14:00
**Supervised learning: classification: Convolutional Neural Networks**
14:00 – 14:30
**Supervised learning: classification: Hands-on: CNN**
14:30 – 15:00
**Coffe break**

**Supervised learning: classification: Hands-on: CNN**
15:20 – 17:30
**Social event: Guided walking tour in Leuven and dinner**
**18.00-21.00**

**Wednesday 6/03**
**Supervised learning: classification. Recurrent Neural Networks**
9:00 – 10:00
**Supervised learning: classification. Recurrent Neural Networks: Hands-on: RNN**
10:00 –10:30
**Coffe break**
**Supervised learning: classification. Recurrent Neural Networks: Hands-on: RNN**
10:50 –12:00
**Lunch**
12:00 - 13:00
**From Training to inference. The life of a model: Looking at Inference. Loading Models**
13:00 – 13:45
**Coffe break**
**Unsupervised learning: clustering: Methods and algorithms**
14:10 – 15:00
**Coffe break**
**Unsupervised learning: clustering: Hands-on**
15:20 - 16:30
**Unsupervised learning: dimensionality reduction: Methods and algorithms**
16:30 - 17:30

**Thursday 7/03**
**Reinforcement learning: How does it work and when to use it**
09:00 - 10:30
**Coffee break**
**Reinforcement learning: Hands-on**
10:50 - 12:00
**Lunch**
12:00 - 13:00
**Using scikit-learn pipelines to streamline**
13:00 - 14:00
**Coffe break**
**AI Ethics and possible future scenarios**
14:20 – 16:30

**Friday 8/03**
**Deep learning using multiple nodes with GPUs: Emphasis on efficiency and scaling**
09:00 - 10:00
**HPE deep learning cookbook (AI)**
10:00 – 11:00
**Coffe break**
**Hands-on: wrap-up**
11:20 – 12:00

## 12.3 PRACE-5IP Y2 On-demand Events Reports

**On-demand Events Application Form Template**

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

### *12.3.1 E-CAM Workshop on Particle-Based Models and HPC*

1. Basic information about the event
1.1. PRACE E-CAM Workshop on Particle-Based Models and HPC
1.2. 7-9.6.2017
1.3. CSC - IT-center for science
1.4. CSC, Aalto university
2. Organizational details
2.1. Local organizing committee
Jan Åström, CSC
Mikko Alava, Aalto
Antti Puisto, Aalto
2.2. A workshop on particle based models and HPC, was arranged because such methods have emerged more and more as important tools for science research. In comparison to more standard methods based on numerical solution for differential equations, particle methods more directly deal with the underlying physics of a problem. In contrast, these methods are much more demanding in terms of compute power requirements.
2.3. Workload, person ~hours
Jan Åström ~ 150h

2.4. Synergetic events: The workshop fit as a natural part of CSC and Aalto courses on HPC methods in science.
3. Program & content
3.1. Program committee
Jan Åström
Mikko Alava
Antti Puisto
3.2. Final program: attached appendix
3.3. List of trainers (appendix)
3.4. Designing the program: The idea behind the program was to find a suitable mix of experts on particle models and HPC experts. The HPC part was focused on implementing particle models on GPUs, and the particle model part focused on models for fracture and fragmentation as well as the Lattice Boltzmann method for fluid dynamics.
3.5. Description of the contents (brief commentary of each lecture and lab/exercise)
3.6. Computer resources: table top work stations with GPUs in the CSC lecture room.
4. Participants & feedback
4.1. Number of participants by country:
Finland: 17
Estonia: 1
Holland: 1
Hungary: 1
Germany: 1
4.2. Process for selecting the participants (all who expressed interested could attend )
4.3. Statistics of the feedback survey (only one person feedback received. Maximum positive feedback 5/5 on all points.)
4.4. Analysis of the feedback (only one person feedback – not statistically representative. On-site personal feedback at the closing overwhelmingly positive - “very useful” was the general comment.)
5. Conclusions & lessons learned (A very positive experience in general.)

### *12.3.2 Energy-aware application development for heterogeneous computing*

1. Basic information about the event
1.1. Name Energy-aware application development for heterogeneous computing
1.2. Dates: November 21st, 2017
1.3. Location: Barcelona
1.4. Organizing sites: Barcelona Supercomputing Center (BSC)
2. Organizational details
2.1. Local organizing committee: Rosa M. Badia, Jorge Ejarque, TANGO Project, Computer Science Dept, BSC Education and Training Team of BSC under the management of Maria-Ribera Sancho.
2.2. Venue: The course was hosted by BSC on the Nord Campus Premises of UPC. We used the standard set-up applied for the PATC courses we run.
2.3. Realized workload (table: person and total working hours spent for the event)
2.4. Synergetic events (listing: was there any other PRACE activity during the event which would have utilized the venue or other effort)
No

3. Program & content

3.1. Program committee

The role of convener was assigned to Jorge Ejarque, a researcher working at the Computer Science department of BSC

3.2. Final program (see table in Appendix))

3.3. List of trainers (see Appendix)

3.4. Designing the program

With this course, we aimed to present the TANGO toolbox which provides a set of tools to simplify and optimize the usage of distributed heterogeneous computing environments. We mainly targeted to attract students, HPC application developers and System administrators which can benefit from the tools we developed at the TANGO project.

3.5. Description of the contents

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

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

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

3.6. Computer resources

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

4. Participants & feedback

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

Spain 13

Brazil 1

Iran 1

4.2. Process for selecting the participants

All students registered were accepted.

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

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

5. Conclusions & lessons learned

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

APPENDIX

PROGRAM

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

- Overview of Heterogeneous distributing computing
- Why TANGO?

Coffee Break 10:30

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

- Introduction to the TANGO Toolbox Components
- Demos

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

- Programming Model Syntax

Lunch Break 13:00 to 14:00

Session 4 / 14:00 pm- 17:30 pm: Programming Model Hands-on
- Environment Setup
- Sample application overview
- Exercise with an incomplete sample code
- Compilation and execution
- Monitoring and Debugging
- Final notes

Coffee Break 16:00
END of COURSE
LIST OF TRAINERS
Name Institution Contact Details
Jorge Ejarque, Workflows and Distributed computing group, Computer Sciences Dept BSC
jorge.ejarque@bsc.es
Karim Djemame University of Leeds
David Garcia Atos Research and Innovation

### *12.3.3 Programming and optimizing the Knights Landing*

1. Basic information about the event
1.1. PRACE Workshop on “Programming and Optimizing the Intel Knights Landing Manycore Processor”
1.2. Dates: 24-25.04.2018
1.3. Location: HPC2N, Umeå University, Sweden
1.4. Organizing sites: HPC2N, Umeå University
2. Organizational details
2.1. Local organizing committee
Jerry Eriksson, HPC2N
Pedro Ojeda-May, HPC2N
Birgitte Brydsö, HPC2N
2.2. A two day workshop with instructors from Intel. The course focused on programming and optimizing the Intel ® Xeon Phi™ Manycore Processor, codenamed "Knights Landing (KNL)" and how to best use it efficiently. Code examples were profiled on KNL processors. Participants were encouraged to bring their own code, which Intel instructors helped them optimize.
2.3. Workload, person ~hours
Jerry Eriksson ~ 100h
Pedro Ojeda-May ~ 100h
2.4. Synergetic events: The workshop was a natural fit for HPC2N and the NLAFET group with a focus on HPC programming and optimization.
3. Program & content
3.1. Program committee
Jerry Eriksson
Mikko Byckling
Asma Farjallah
3.2. Final program: https://www.hpc2n.umu.se/events/courses/knl-spring-2018
3.3. List of trainers: Mikko Byckling and Asma Farjallah, Intel Corporation
3.4. Designing the program: The idea was to offer training on KNL programming, on vectorization, and on optimization from experts in the field.

3.5. Description of the contents: (brief commentary of each lecture and lab/exercise)
3.6. Computer resources: Kebnekaise KNL partition at HPC2N.
4. Participants & feedback
4.1. Number of participants by country:
Finland: 1
Germany: 1
Mexico: 1
Sweden: 10
Denmark: 2
Jordan: 1
Canada: 1
Vietnam: 1
4.2. Process for selecting the participants (all who expressed interested could attend )
4.3. Statistics of the feedback survey (evaluation results to be added.)
4.4. Analysis of the feedback (evaluation results to be added.)
5. Conclusions & lessons learned (A very positive experience in general. More comments to follow.)

### *12.3.4 Advanced CFD and Turbulence Modelling Targeting HPC*

1. Basic information about the event
1.1. Name: Advanced CFD and Turbulence Modelling Targeting HPC
1.2. Dates: 3-5 October, 2018
1.3. Location: BSC, Barcelona
1.4. Organizing sites: BSC and STFC Daresbury Laboratory
2. Organizational details
2.1. Local organizing committee (table)
Charles Moulinec, STFC Daresbury Laboratory
Education and Training Team of BSC under the management of Maria-Ribera Sancho.
2.2. Venue : The course was hosted by BSC on the Nord Campus Premises of UPC. We chose a computer lab this time because of the technical requirements of the course, preparing all the simulations on the local simulations before sending over the relevant files to MareNostrum, for overnight simulations mainly.
2.3. Budgeting: €1,040 from PRACE. €6,000 from CECAM (Daresbury node) for meals, instructors trips and half of the room rental.
2.4. Realized workload
Charles Moulinec, STFC, 40-60 hours
Carolina Olmo, 15 hours

1.1. Synergetic events (listing: was there any other PRACE activity during the event which would have utilized the venue or other effort) No
2. Program & content
2.1. Program committee (table) ?
2.2. Final program : Please see Appendix 1
2.3. List of trainers :
Charles Moulinec, STFC Daresbury Laboratory
Stefano Rolfo, STFC Daresbury Laboratory

Antonio Toti, EFD Energy
Juan Uribe, EFD Energy
2.4. Designing the program The programme is about advanced CFD and turbulence modelling targeting HPC.
2.5. Description of the contents (see Appendix 1, in italic)
2.6. Computer resources: As it happened that the local PCs provided by UPC were Windows machines only, a Virtual Machine (Linux - ubuntu 16.4) was created and installed there on the 20 available local PCs, knowing that we were expecting 18 attendees, which all turned up. Accounts to MareNostrum were created for each student from our support department.
3. Participants & feedback
3.1. Number of participants by country:
UK: 3
Spain: 10
Italy: 3
France: 1
Mexico: 1
3.2. Process for selecting the participants: There was no filter applied. All students who applied were accepted.
3.3. Statistics of the feedback survey (tables (appendix))
3.4. Analysis of the feedback
Good feedback was received from all the students. The most impressive achievement was to be able to attract a lady from Mexico (Diana Perez) who travelled especially for the course, and is now keen in working with Code_Saturne. There is even a plan to organise a course with UNAM in Mexico City in the feature.
4. Conclusions & lessons learned: In the future we are planning to make this course a regular PTC event. We are considering doing it in a regular room (instead of a computer lab) next time, as the concept of Virtual Machine worked fine this year (Note this was the first year the teachers were using this concept, as they were always used to have access to identical local Linux PCs before). It should be more affordable and there would be more places available.
APPENDIX 1/Programme
CECAM/PRACE Training Course - 2018
Advanced CFD and Turbulence Modelling Targeting HPC
Wednesday 3th of October 2018:
-09:30-10:00 Registration
-10:00-10:30 Introduction and welcome
-10:30-11:00 Introduction to Code_Saturne (Lecture by Juan Uribe)
-11:00-11:20 Coffee break (at the nearby cafetaria)
-11:20-13:00 Hands-on tutorial: Laminar tube bundles using the GUI (Setting up a small case for local PC and first touch of Code_Saturne)
-13:00-14:00 Lunch (at the nearby cafetaria)
-14:00-15:00 HPC presentation and introduction to Marenostrum (Lecture by Charles Moulinec - Simulations + tests carried out with Code_Saturne are presented to illustrate the issues of running on Tier-0 machines)
-15:00-17:00 Hands-on tutorial: LES tube bundles + GUI (Setting up the case (GUI) on the local PC, preprocessing the mesh, copying the settings to MareNostrum, and submitting a simulation to be run overnight)
Dinner at 19:30 - Pati Blau
Thursday 4th of October 2018:

-09:00-10:00 Presentation: Turbulence modelling and LES (Lecture by Juan Uribe)
-10:00-10:30 Postprocessing of LES results (Getting the results from MareNostrum on the local PC and visualising them using ParaView and xmgrace)
-10:30-11:00 Coffee break (at the nearby cafetaria)
-11:00-11:30 Use of subroutines in Code_Saturne (Lecture by Juan Uribe)
-11:30-13:00 Hands-on tutorial: LES with user subroutines (Setting up the previous case using user subroutines, and follow-up simulation on MareNostrum)
-13:00-14:00 Lunch (at the nearby cafetaria)
-14:00-14:30 Introduction to turbomachinery including some code-code coupling (Lecture by Stefano Rolfo)
-14:30-17:00 Hands-on tutorial: pump – joining vs coupling algorithms (Setting up 2 simulations, using 2 main features of the code, for the flow in a pump - This is done on the local PC, studies are copied to MareNostrum, and both simulations are running overnight).
Dinner at 19:30 - La Montiel
Friday 5th of October 2018:
-09:00-10:30 Postprocessing pump results (Copying files back. Using ParaView for visualisation)
-10:30-11:00 Coffee break (at the nearby cafeteria)
-11:00-12:00 Hands-on tutorial: Effect of partitioning + (MPI vs MPI+OpenMP) and scalability of the code (MareNostrum is used for this purpose).
-12:00-13:00 Lunch - End of the workshop

### *12.3.5 ANTAREX: Monitoring, Compilation and Autotuning Approach for Energy-Efficient HPC Systems*

1. Basic information about the event
1.1. Name
ANTAREX: Monitoring, Compilation and Autotuning Approach for Energy-Efficient HPC Systems
1.2. Dates
October 22-23, 2018
1.3. Location
I IT4Innovations, VSB – Technical University of Ostrava, Ostrava, Czech Republic
1.4. Organizing sites
IT4Innovations and ANTAREX Project consortium, http://www.antarex-project.eu/
2. Organizational details
2.1. Local organizing committee (table)

| *Name* | *Affiliation* |
|---|---|
| Nina Špániková | IT4Innovations |
| Ondřej Jakl | IT4Innovations |

2.2. Venue (name, its description and why it was selected; fluid text: analysis how good the selection was for the event)
The school was hosted by IT4Innovations in its large modern building, located in the campus of VSB-TUO in Ostrava-Poruba. In this building, we have a room dedicated to training, which can accommodate up to 40 participants. Besides common components of a modern tutorial room (wireless network, data projectors, whiteboards, etc.) it features an adjacent kitchen. Moreover, it

is located near the supercomputer hall, so the participants could enjoy almost direct contact with their target machine.

2.3. Budgeting (fluid text: reasoning behind the budget; table: the budget together with realized expenses (appendix))

The budget of the event had two sources: ANTAREX and PRACE. PRACE co-funding was used in two ways:

- Catering: The cost of two lunches, three coffee breaks and two social events (dinners) was 21 327 Kč (cca 820 EUR)
- Accommodation: The cost of accommodation for three selected young non ANTAREX project participants (master degree or doctoral students) at the university Garni hotel was 4 900 Kč (cca 190 EUR)

2.4. Realized workload (table: person and total working hours spent for the event)

| Name | Working hours |
|---|---|
| Nina Špániková | 100 |
| Ondřej Jakl | 20 |
| Kateřina Slaninová | 70 |
| Jan Martinovič | 70 |

2.5. Synergetic events (listing: was there any other PRACE activity during the event which would have utilized the venue or other effort)

No synergetic events

3. Program & content

3.1. Program committee (table)

| *Name* | *Affiliation* |
|---|---|
| Kateřina Slaninová | IT4Innovations |
| Jan Martinovič | IT4Innovations |
| Cristina Silvano | Politecnico di Milano |
| João MP Cardoso | Universidade do Porto |

3.2. Final program (table (appendix))

See List 1 in the Appendix

3.3. List of trainers (full list of trainers as an appendix with contact information and description of expertises)

See List 2 in the Appendix

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

The programme was designed with the effort that the participants should understand the main challenges of the ANTAREX project and learn about the result of its research. In particular they were motivated to learn how to express application self-adaptivity at design-time and how to runtime manage and autotune applications for green and heterogeneous High Performance Computing (HPC) systems. Programme blocks were focused on hands-on-approaches based on representative benchmarks, and on the tools provided by the ANTAREX project.

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

- Opening session and the role of PRACE Welcome and info about PRACE and its training activities
- Introduction to Supercomputing Centers and HPC Infrastructures, Visit to IT4Innovations Supercomputing Center About IT4Innovations Supercomputing Center and its Infrastuctures; excursion

- Introduction to Parallel and Distributed Computing at the IT4I Supercomputing Center Parallelism, TOP500, Anselm, Salomon
- Introduction to Monitoring, Runtime Autotuning, DSL + Source to Source Compilation About Domain-Specific Languages (DSLs), examples, about Source to Source (S2S) Compilers, ANTAREX motivation and approach
- Overview of the ANTAREX Approach About the ANTAREX project
- DSL and Source to Source Compilation: hands-on-approach and the Clava+LARA approach Clava, LARA, hands-on session
- Runtime Autotuning: hands-on-approach and the mArgot approach mARGOt autotuning framework
- Energy-Efficiency Run-time: hands-on-approach and the COUNTDOWN approach Overview, infrastructure monitoring, ExaMon and COUNTDOWN tools
- Use of the ANTAREX toolflow and experiments with representative benchmarks and ANTAREX Use Cases Autotune Matrix Multiplication with mARGOt, HDF5 interface generation with CMake plugin

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

- The main computing resource for the event was the Salomon supercomputer at IT4Innovations, which is an SGI cluster deployed in 2015. This platform could meet very well the requirements of the event, because of dedicated allocation of nodes and a high throughput queue.
- To approach these resources and the Internet from their own laptops, the participants made use of local wireless network.

4. Participants & feedback

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

| *Country* | *Number of participants* |
|---|---|
| Czech Republic | 10 |
| Italy | 2 |
| Portugal | 1 |

4.2. Process for selecting the participants (if applicable, fluid text)

The participants were selected on the first come – first served basis.

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

There were two surveys available to the participants.

1. A short paper survey 1 for immediate impressions was distributed at the end of the event. Its results are summarized in Appendix in Table 1.
2. Later, an electronic survey 2 was attached to the web page of the event. Its results are summarized in Appendix in Table 2.

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

Both surveys show high evaluation of the event by the participants. In particular, the results of survey 1 with 14 participants witness in our conditions and compared with other trainings at IT4Innvoation a great satisfaction. Survey 2 and its question about overall satisfaction, compatible with standard PRACE surveys, also shows high average score of 8,75.

There were no special comments from the participants.

5. Conclusions & lessons learned (fluid text)

This on-demand event organized with ANTAREX proved to be a very useful complement of the traditional PRACE training. It had great knowledge dissemination effect and helped shaping the local/national HPC training infrastructure through collaboration with another institutions.

Appendix

List 1: Final program

See also https://events.it4i.cz/event/14/timetable/

Monday 22 October 2018 – 1st day

- Registration - (12:00-12:30)
- Opening session and the role of PRACE - (14:00-14:30)
- Introduction to Supercomputing Centers and HPC Infrastructures, Visit to IT4Innovations Supercomputing Center - (14:30-15:30)
- Introduction to Parallel and Distributed Computing at the IT4I Supercomputing Center - (16:00-17:00)
- Introduction to Monitoring, Runtime Autotuning, DSL + Source to Source Compilation - (17:00-18:00)

Tuesday 23 October 2018 – 2nd day

- Opening session - (09:15-09:30)
- Overview of the ANTAREX Approach - (09:30-10:00)
- DSL and Source to Source Compilation: hands-on-approach and the Clava+LARA approach - (10:00-11:00)
- Runtime Autotuning: hands-on-approach and the mArgot approach - (11:30-12:30)
- Energy-Efficiency Run-time: hands-on-approach and the COUNTDOWN approach - (14:00-15:00)
- Use of the ANTAREX toolflow and experiments with representative benchmarks and ANTAREX Use Cases - (15:00-16:15)
- Panel about Open Challenges, Exascale opportunities and challenges, Heterogeneity and the use of Hardware Accelerators, Machine Learning, etc. - (16:45-17:45)
- Closing session - (17:45-18:00)

Table 1: Survey 1 (paper)

Questions

Q1. Would you recommend this training to your colleagues? [YES-NO]

Q2. How valuable was the training for your work? [5 = very much ... 1 = not at all]

Q3. How well did the training meet your expectations? [5 = very much ... 1 = not at all]

| Questions | Results | Average |
|---|---|---|
| Q1 | 14x YES, 0x NO | -- |
| Q2 | 1x 1, 0x 2, 3x 3, 1x 4, 9x 5 | 4,21 |
| Q3 | 0x 1, 0x 2, 1x 3, 3x 4, 10x 5 | 4,64 |

Table 2: Survey 2 (electronic)

Questions

1. Subject was clearly presented
2. Slides were well prepared
3. Teaching pace was appropriate
4. Demonstrations and examples were useful and illustrative

5. The event was well organized
6. Overall benefit of the training for you

Possible answers
☐For questions 1-5 the participants could make use of the following values:

0 - don't know
1 - excellent
2 - good
3 - not good nor bad
4 - bad
5 - very bad
☐For question 6 the possible values were from 0 (waste of time) to 10 (full satisfaction).

Results (4 responses)

| Name and Surname [optional] | Are you user of IT4I computing resources? | 1. Subject was clearly presented | 2. Slides were well prepared | 3. Teaching pace was appropriate | 4. Demos and examples were useful and illustrative | 5. The event was well organized | 6. Overall benefit of the training for you |
|---|---|---|---|---|---|---|---|
| Named | no | 1 | 1 | 1 | 1 | 1 | 10 |
| Named | yes | 2 | 1 | 1 | 2 | 1 | 7 |
| Named | yes | 1 | 1 | 1 | 1 | 1 | 9 |
| <anonymous> | No | 1 | 1 | 1 | 1 | 1 | 9 |

Notes and comments of the participants on the quality of the event:
There wasn't much time for experimenting with the tasks for the software.

### *12.3.6 Workshop on Deep Learning*

1. Basic information about the event
   1.1. Name - PRACE Deep Learning workshop @PDC/KTH
   1.2. Dates - 20-21 March, 2019
   1.3. Location – PDC, KTH, Lindstedtsvägen 24, 100 44 Stockholm Sweden
   1.4. Organizing sites – SNIC-KTH
2. Organizational details
   2.1. Local organizing committee (table) – Lilit Axner, Henric Zazzi
   2.2. Venue (name, its description and why it was selected; fluid text: analysis how good the selection was for the event) - room Fantum, at KTH, Lindstedtsvägen 24, 100 44 Stockholm, Sweden

2.3. Budgeting (fluid text: reasoning behind the budget; table: the budget together with realized expenses (appendix)) – about 1400€ for lunches and coffee breaks, about 910€ for travel and accommodation of lecturers from CSC, Finland, about 420€ for the lection room.

2.4. Realized workload (table: person and total working hours spent for the event) Lilit Axner – 1Pm, Henric Zazzi – 1PM

2.5. Synergetic events (listing: was there any other PRACE activity during the event which would have utilized the venue or other effort) - No

3. Program & content

3.1. Program committee (table) – Henric Zazzi, Lilit Axner

3.2. Final program (table (appendix)) – see below

3.3. List of trainers (full list of trainers as an appendix with contact information and description of expertises)

Kjartan Thor Wikfeldt kthw@kth.se

Henric Zazzi hzazzi@kth.se

Markus Koskela markus.koskela@csc.fi

Mats Sjöberg mats.sjoberg@csc.fi

3.4. Designing the program (fluid text: reasoning and goals-setting behind the program) – We have had previously a similar PRACE workshop in November and noticed the high demand in Deep learning knowledge. Thus we have decided to organize this workshop based on that.

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

3.6. -

4. This workshop gave a practical introduction to deep learning, convolutional and recurrent neural networks, GPU computing, and tools to train and apply deep neural networks for natural language processing, images, and other applications. It consisted of lectures and hands-on exercises. Keras (https://keras.io/) and PyTorch (https://pytorch.org/) were used in the exercise sessions.

After the workshop the participants had the skills and knowledge needed to begin applying deep learning for different tasks and utilizing the GPU resources available at PDC for training and deploying their own neural networks.

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

Participants got access to the PDCs GPU system Tegnér during the workshop

5. Participants & feedback

5.1. Number of participants by country (table, full list of participants as an appendix) 33 from Sweden 2 from Finland. See below the list.

5.2. Process for selecting the participants (if applicable, fluid text) first come first in.

5.3. Statistics of the feedback survey (tables (appendix)) – Overall very positive feedback both for the workshop lectures and organization.

5.4. Analysis of the feedback (fluid text: analyze the feedback in general and all specific very good or bad comments) – In the future we would be happy to organize similar workshops as the demand is quite high.

6. Conclusions & lessons learned (fluid text)
   It was a very successful workshop with exactly 35 participants of which 5 organisers and lecturers. The only point is that the participants were requesting a certificate that they have participated at the workshop. However, PRACE do not provide such and thus KTH provided a document confirming their participation.

Time Day 1 / March 20, 2019

09:00-10:30 Lecture: Introduction to deep learning

10:30-11:00 Exercises: Introduction to Notebooks, Keras fundamentals

11:00-12:00 Lecture: Image data, multi-layer percepton networks, convolutional neural networks

12:00-13:00 Lunch

13:00-14:00 Exercises: Image classification with MLPs, CNNs

14:00-15:00 Lecture: Text data, embeddings, neural NLP, recurrent neural network

15:00 - 16:00 Exercises: Text sentiment classification with CNNs, RNNs

Time Day 2 / March 21, 2019

09:00-10:00 Lecture: GPUs, batch jobs, using PDC-GPU

10:00-12:00 Exercises: Image classification

12:00-13:00 Lunch

13:00-14:00 Exercises: Text categorization and labelling

14:00-15:00 Lecture: Cloud, GPU utilization, multiple GPUs

15:00-16:00 Exercises: Using multiple GPUs

## 12.4 Feedback from the International HPC Summer School 2017 and 2018

| Question | Strongly disagree | | Disagree | | Neutral | | Agree | | Strongly agree | | Total |
|---|---|---|---|---|---|---|---|---|---|---|---|
| My goals for attending the international HPC Summer School were achieved | 0% | 0 | 2% | 1 | 12% | 8 | 55% | 36 | 32% | 21 | 66 |
| The summer school was well organized | 0% | 0 | 0% | 0 | 5% | 3 | 36% | 24 | 59% | 39 | 66 |
| I am satisfied with the delivery format of the summer school | 0% | 0 | 5% | 3 | 6% | 4 | 53% | 35 | 36% | 24 | 66 |
| I am satisfied with my interaction with my mentor during the mentoring/work sessions | 0% | 0 | 3% | 2 | 14% | 9 | 24% | 16 | 59% | 39 | 66 |
| I meaningfully engaged with a mentor during the summer school | 2% | 1 | 3% | 2 | 14% | 9 | 29% | 19 | 53% | 35 | 66 |
| I plan on keeping in contact with my mentor after the summer school | 2% | 1 | 6% | 4 | 18% | 12 | 35% | 23 | 39% | 26 | 66 |
| I plan on keeping in contact with a staff member after the summer school | 2% | 1 | 6% | 4 | 23% | 15 | 41% | 27 | 29% | 19 | 66 |
| I am satisfied with the student/mentor matching process | 2% | 1 | 3% | 2 | 23% | 15 | 33% | 22 | 39% | 26 | 66 |
| I meaningfully engaged with other students at the summer school | 0% | 0 | 3% | 2 | 2% | 1 | 32% | 21 | 64% | 42 | 66 |
| The fact that students from other countries participated in the summer school contributed to my learning | 0% | 0 | 2% | 1 | 6% | 4 | 30% | 20 | 62% | 41 | 66 |
| The knowledge/skills I gained during this summer school will significantly contribute to my work/research | 2% | 1 | 0% | 0 | 11% | 7 | 41% | 27 | 47% | 31 | 66 |
| I know the next step for me to build on what I learned at this summer school | 0% | 0 | 2% | 1 | 20% | 13 | 36% | 24 | 42% | 28 | 66 |

| | | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|
| I am interested in learning more about the resources/opportunitie s available through Compute/Calcul Canada, PRACE, RIKEN, or XSEDE as a result of this experience | 0% | 0 | 2% | 1 | 6% | 4 | 36% | 24 | 56% | 37 | 66 |
| I plan on obtaining (or currently have) access to Compute/Calcul Canada, PRACE, RIKEN, or XSEDE resources | 0% | 0 | 2% | 1 | 9% | 6 | 32% | 21 | 57% | 37 | 65 |
| The lodging was adequate | 2% | 1 | 5% | 3 | 6% | 4 | 49% | 32 | 38% | 25 | 65 |
| Overall I would rate my experience as successful | 0% | 0 | 0% | 0 | 8% | 5 | 24% | 16 | 68% | 45 | 66 |

**Table 6. Feedback from 66 responses from the International HPC Summer School 2017 in Boulder, Colorado.**

# 2018 IHPCSS Student Post Survey Response

Response Rate: 96% (75/78)

Q2 - To what extent do you agree with the following statements regarding your experience in the International HPC Summer School?

| # | Field | Strongly disagree | Disagree | Neutral | Agree | Strongly agree | Total |
|---|---|---|---|---|---|---|---|
| 1 | My goals for attending the international HPC Summer School were achieved | 1.39% 1 | 1.39% 1 | 15.28% 11 | 47.22% 34 | 34.72% 25 | 72 |
| 2 | The summer school was well organized | 0.00% 0 | 5.56% 4 | 11.11% 8 | 31.94% 23 | 51.39% 37 | 72 |
| 3 | I am satisfied with the delivery format of the summer school | 1.41% 1 | 4.23% 3 | 12.68% 9 | 50.70% 36 | 30.99% 22 | 71 |
| 4 | I am satisfied with the amount of hands-on activities | 2.78% 2 | 16.67% 12 | 18.06% 13 | 40.28% 29 | 22.22% 16 | 72 |
| 5 | I am satisfied with my interaction with my mentor during the mentoring/work sessions | 1.39% 1 | 9.72% 7 | 13.89% 10 | 34.72% 25 | 40.28% 29 | 72 |
| 6 | I am satisfied with the technical assistance available during the summer school (i.e. mentors, session facilitators, extra help sessions, etc) | 4.17% 3 | 5.56% 4 | 13.89% 10 | 36.11% 26 | 40.28% 29 | 72 |
| 7 | I meaningfully engaged with a mentor during the summer school | 0.00% 0 | 9.86% 7 | 12.68% 9 | 30.99% 22 | 46.48% 33 | 71 |
| 8 | I plan on keeping in contact with my mentor after the summer school | 1.41% 1 | 9.86% 7 | 33.80% 24 | 33.80% 24 | 21.13% 15 | 71 |
| 9 | I plan on keeping in contact with a staff member after the summer school | 1.41% 1 | 5.63% 4 | 32.39% 23 | 35.21% 25 | 25.35% 18 | 71 |
| 10 | I am satisfied with the student/mentor matching process | 6.94% 5 | 5.56% 4 | 22.22% 16 | 38.89% 28 | 26.39% 19 | 72 |
| 11 | I meaningfully engaged with other students at the summer school | 0.00% 0 | 0.00% 0 | 6.94% 5 | 41.67% 30 | 51.39% 37 | 72 |
| 12 | The fact that students from other countries participated in the summer school contributed to my learning | 0.00% 0 | 5.56% 4 | 5.56% 4 | 26.39% 19 | 62.50% 45 | 72 |
| 13 | The knowledge/skills I gained during this summer school will significantly contribute to my work/research | 0.00% 0 | 5.56% 4 | 13.89% 10 | 41.67% 30 | 38.89% 28 | 72 |
| 14 | I know the next step for me to build on what I learned at this summer school | 0.00% 0 | 1.39% 1 | 15.28% 11 | 43.06% 31 | 40.28% 29 | 72 |

| | | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|
| 15 | I am interested in learning more about the resources/opportunities available through Compute/Calcul Canada, PRACE, RIKEN, or XSEDE as a result of this experience | 0.00% | 0 | 1.39% | 1 | 12.50% | 9 | 27.78% | 20 | 58.33% | 42 | 72 |
| 16 | I plan on obtaining (or currently have) access to Compute/Calcul Canada, PRACE, RIKEN, or XSEDE resources | 0.00% | 0 | 4.29% | 3 | 21.43% | 15 | 22.86% | 16 | 51.43% | 36 | 70 |
| 17 | The lodging was adequate | 2.82% | 2 | 2.82% | 2 | 14.08% | 10 | 32.39% | 23 | 47.89% | 34 | 71 |
| 18 | Overall I would rate my experience as successful | 1.39% | 1 | 0.00% | 0 | 5.56% | 4 | 34.72% | 25 | 58.33% | 42 | 72 |

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| # | Field | Mean | Std Deviation | Count |
|---|---|---|---|---|
| 1 | My goals for attending the international HPC Summer School were achieved | 4.13 | 0.82 | 72 |
| 2 | The summer school was well organized | 4.29 | 0.87 | 72 |
| 3 | I am satisfied with the delivery format of the summer school | 4.06 | 0.85 | 71 |
| 4 | I am satisfied with the amount of hands-on activities | 3.63 | 1.09 | 72 |
| 5 | I am satisfied with my interaction with my mentor during the mentoring/work sessions | 4.03 | 1.03 | 72 |
| 6 | I am satisfied with the technical assistance available during the summer school (i.e. mentors, session facilitators, extra help sessions, etc) | 4.03 | 1.07 | 72 |
| 7 | I meaningfully engaged with a mentor during the summer school | 4.14 | 0.98 | 71 |
| 8 | I plan on keeping in contact with my mentor after the summer school | 3.63 | 0.97 | 71 |
| 9 | I plan on keeping in contact with a staff member after the summer school | 3.77 | 0.94 | 71 |
| 10 | I am satisfied with the student/mentor matching process | 3.72 | 1.12 | 72 |
| 11 | I meaningfully engaged with other students at the summer school | 4.44 | 0.62 | 72 |
| 12 | The fact that students from other countries participated in the summer school contributed to my learning | 4.46 | 0.83 | 72 |
| 13 | The knowledge/skills I gained during this summer school will significantly contribute to my work/research | 4.14 | 0.85 | 72 |
| 14 | I know the next step for me to build on what I learned at this summer school | 4.22 | 0.75 | 72 |
| 15 | I am interested in learning more about the resources/opportunities available through Compute/Calcul Canada, PRACE, RIKEN, or XSEDE as a result of this experience | 4.43 | 0.76 | 72 |

| | | | | |
|---|---|---|---|---|
| 16 | I plan on obtaining (or currently have) access to Compute/Calcul Canada, PRACE, RIKEN, or XSEDE resources | 4.21 | 0.92 | 70 |
| 17 | The lodging was adequate | 4.20 | 0.97 | 71 |
| 18 | Overall I would rate my experience as successful | 4.49 | 0.73 | 72 |

**Table 7. Feedback from 72 responses from the International HPC Summer School 2017 in Ostrava, Czech.**