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EoCoE

Energy oriented Center of Excellence for computing applications

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D13 M24

Assessment report of course delivery

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1. Introduction

As a centre of Excellence in Computing application, EoCoE activities aim to capitalise the knowledge and expertise acquired through computational methods and application codes enhancements and disseminate it contributing to existing open libraries and providing conferences and workshops, education and trainings, consultancy and expertise to laboratories, Industries and SMEs. The expected impact of the training activities is to have more scientists and engineers trained in the use of computational methods and optimisation of applications. The main stakeholders identified by EoCoE in need of training are engineers and researchers that operate in academia, industry and SMEs.

In particular, EoCoE will disseminate the acquired knowledge and expertise through:

- 9 thematic workshops and an international conference and more generally will promote the EoCoE in main international conferences (see D6.4)
- Education and training modules to help laboratories and industry to access and use HPC methods and code modules.

In EoCoE, training involves the delivery of education to disseminate the skills, best practices and know-how of EoCoE to Doctoral/Master's/Professionals in the use of computational methods and tools and optimisation of applications. EoCoE takes advantage of the close ties it has with the PRACE Advanced Training Centres (PATCs) training infrastructure and other organisations to deliver new specific training modules.

Specific educational activities include the a) the creation of multimedia modules for academic courses and professional training, b) the delivery of short courses for professionals, c) the delivery of academic courses/modules through existing PhD/MSc programmes, d) MOOCs and e) a supplementary e-learning platform.

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2. Training Tools

As presented in D6.2-Education Course materials and platform, EoCoE uses a collaboration platform which is accessible for all members of the project at link <u>http://project.eocoe.eu</u>. The part of the platform is Document Repository that is used for storing training modules, too. All training presentations from various workshops and training activities are in the document repository in the dedicated folder. Recorded videos are available on the EoCoE public site, at <u>http://www.eocoe.eu/workshopstrainings.</u>

In addition, EoCoE committed to using a dedicated learning environment to support massive open online courses (MOOC) - online courses aimed at unlimited participation and open access via the web. Keeping its commitment, EoCoE tested the Moodle platform (the Modular Object Oriented Dynamic Learning Environment), one of the commonly used e-learning platforms. It has been around for over ten years. It is a free and open-source software learning management system written in PHP and distributed under the GNU General Public License. Developed on pedagogical principles, Moodle is used for blended learning, distance education, flipped classroom and other e-learning projects in schools, universities, workplaces and other sectors. With customizable management features, it is used to create private websites with online courses for educators and trainers to achieve learning goals. It allows for extending and tailoring learning environments using community sourced plugins.

It has to be noted however, that Moodle has not, up to this point, been adopted by EoCoE which continues to use the PRACE indico system (http://www.training.prace-ri.eu/material/index.html) to store training materials.

2.1 JUBE automation framework

The JUBE framework is highly used within the performance evaluation strategy of WP1 to allow a comparable and reproducible application instrumentation and evaluation.

JUBE offers the user an environment for configuring, compiling, and running an application on different computing systems with the accompanied tasks of result analysis and verification. Additional tools beside the application such as performance evaluation tools can be triggered and integrated into the automated run.

As part of the performance evaluation strategy three performance evaluation workshops took place were JUBE was presented to the audience to either introduce the usage of the tool as well of the evaluation strategy within EoCoE. The main new material to introduce JUBE was a presentation which is available via OpenAccess <u>http://hdl.handle.net/2128/14566</u>. This presentation extends the general JUBE documentation (<u>http://www.fz-juelich.de/jsc/jube</u>) and connects to the tutorial examples which are directly shipped with each installation of JUBE.

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Beside the course material for the performance evaluation workshops, the general JUBE documentation was extended as well by taking care of user requests and problems. For this a new FAQ section was introduced (<u>https://apps.fz-juelich.de/jsc/jube/jube2/docu/faq.html</u>), which provides additional information for the EoCoE users as well for JUBE users in general.

3. Training module development

According to the project proposal the education and training modules to be developed would have a particular focus on: HPC methods and tools - codes - optimisation of applications and they would be provided through: a)PhD/MSc courses b)MOOC Courses c)short courses for professionals and e) supplementary e-learning platform.

Through the implementation of the project new training material was developed, including new modules based on the technical breakthrough and methodological advances generated by the project that complements the more general training material offered through the PATC network. A number of these modules have been delivered in partnership with the PATCs training infrastructure (see Section 4) and are available through a dedicated page on the EoCoE website.

The development of MOOC courses have not yet been implemented but they are under consideration, especially by the CyI.

4. Training Activities

EoCoE carried out both internal and external training activities and it sought to carry out its training activities in collaboration with other relevant structures such as the PRACE Advanced Training Centres (PATCs) and other Pan-European structures dedicated to industrial/academic consortia funding. This practice allowed for reduce training costs, larger audience, more effective dissemination and greater impact. In this section, the training activities carried out in the second reporting period of EoCoE are presented. The following table presents the Training activities carried out by EoCoE:

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Event	Date	Location	Notes
1st Joint EoCoE-POP application benchmarking workshop	December 2015	JSC, Germany	Reported In Deliverable D6.3
2nd Joint EoCoE-POP application benchmarking workshop	30th May to 2nd June 2016	MdlS, France	Reported In Deliverable D6.3
Training session at EoCoE Face to Face Bi-annual project meeting	30th November - 02nd December 2016	ENEA, Italy	Reported In Deliverable D6.2
Evaluation Workshop EoCoE / PoP: 3rd joint workshop on benchmarking and performance analysis	24-27 April 2017	BSC, Spain	Reported In Deliverable D6.4
International HPSC TerrSys Fall School 2017	25-29 September 2017	Bonn University, Germany	WP1 related

Table 1: EoCoE Training activities

4.1.First Thematic Workshop: Benchmarking and performance analysis

The first EoCoE-POP workshop on benchmarking and performance analysis brought together code developers of community codes associated with WP2-5 with HPC experts associated with WP1 and HPC experts from the CoE \POP". The goal was to familiarise the developers from WP2-5 with state-of-the-art HPC performance analysis tools.

Code developers were instructed on how to perform benchmarking within the JUBE workflow environment. Developers were then able to begin analysing their applications using specific HPC tools under the guidance of HPC experts (Score-P, Scalasca, Vampir, Paraver, and Extrae, among others). The training was 16,5h hours long (12h hands-on) and was attended by 14 participants.

Detailed presentation of the First Thematic Workshop can be found in Deliverable 6.3.

4.2. Second Thematic Workshop: Benchmarking and performance analysis

The second EoCoE-POP workshop at Maison de la Simulation on benchmarking and performance analysis brought together developers of community codes associated with WP 2-5 with HPC experts associated with WP 1 and HPC experts from the CoE \POP". In addition, this time two external partners (EDF and BRGM) joined the event and brought codes and code developers. The goal was to improve codes developed by the participants. In this workshop code developers could start their JUBE integration from a provided template so they could progress much faster.

The training was 17h hours long (12h hands-on) and was attended by 12 participants. Detailed presentation of the Second Thematic Workshop can be found in Deliverable 6.3.

4.3. 3rd Training Workshop: Evaluation (EoCoE, PoP, with support from PRACE)

In a joint effort, the two centres of excellence EoCoE and PoP collaborated once again to hold a workshop on HPC benchmarking and performance analysis. This was the third event of its kind and was held at BSC in Barcelona and it was supported by the <u>French PATC</u> and the <u>Spanish PATC</u>.

Improving again an already proven concept, it has brought together 17 experts from topical fields in energy research and tools and 11 experts from HPC science in order to tackle the transition of current R&D codes and applications towards exascale.

The EoCoE performance analysis methodology has once again passed a new level of maturity. Experts from topical fields could really learn how to use advanced performance evaluation tools, get insight of the performance bottlenecks of their applications and bring back home JUBE based benchmarking tool to repeat, in a reproducible manner, this analysis on future optimised versions of their code. The following courses were presented in the workshop:

- JUBE Introduction, Sebastian Lührs, JSC
- JUBE Integration Hands on I, Sebastian Lührs et al.
- Tools Intro: Score-P, Scalasca, Vampir, POP@JSC
- Tools Hands-on: Score-P, Scalasca, Vampir, POP@JSC
- Tools Intro: Extrae, Paraver, POP@BSC
- Tools Hands-on: Extrae, Paraver, POP@BSC
- JUBE Integration Hands on II, Sebastian Lührs et al.
- JUBE Integration Hands on II, Sebastian Lührs et al.
- Benchmarking Hands-on I, All
- Benchmarking Hands-on II, All
- Audit, POP

4.4. International HPSC TerrSys Fall School 2017

The Centre for High-Performance Scientific Computing in Terrestrial Systems (HPSC TerrSys), with support from the Energy Orientated Centre of Excellence for Computing (EoCoE WP4), offered a Fall School for Master and PhD students as well as Postdocs interested in *Terrestrial Modelling and High-Performance Scientific Computing*.

The objective of this applied course was to provide the theoretical and technical context of terrestrial modelling in high-performance scientific computing (HPSC) environments utilizing stand-alone and coupled hydrologic, land surface and atmospheric models. Utilizing the Terrestrial Systems Modelling Platform (TerrSysMP), the course took a complete tour of terrestrial modelling and HPSC in connection with real-world observations and data assimilation including:

- setting up a terrestrial model and performing simulations in massively parallel supercomputer environments at the Jülich Supercomputing Centre
- parallel performance analysis and profiling
- parallel data assimilation using TerrSysMP-PDAF (Parallel Data Assimilation Framework)
- post-processing and visualization in the age of big data

The learning Outcomes of the School were to provide the participants with the generic capabilities of terrestrial modelling and data assimilation in supercomputing environments with a focus on TerrSysMP(-PDAF) including parallel performance analysis and profiling utilizing freely available software tools, and handling of very large data sets in the analyses and visualization process.

Attendance to the School required Basic knowledge of LINUX/UNIX and programming languages such as R, Python, C/C++, or FORTRAN as well as data formats such as NetCDF is an advantage.

The following courses were presented at the workshop:

- Introduction to MPI short course
- Introduction to fundamentals of environmental (climate, hydrology, georesources, terrestrial systems) modelling
- Characteristics and handling of HPC resources
- Setup of regional terrestrial models and performing simulations
- The OASIS coupler
- Continue morning projects and inspection of results with real data
- Visualization and big data strategies
- Parallel performance and profiling
- Performance and profiling analysis
- Ensemble data assimilation
- Ensemble data assimilation with TerrSysMP
- Ensemble data assimilation with TerrSysMP

International HPSC TerrSys Fall School 2017 Poster:



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4.5. Other Trainings

Listed below are training events on disciplinary and HPC-related topics where EoCoE members participated as tutors or guest speakers, presenting courses developed by EoCoE.

Date	Event	Торіс	Venue	Web	EoCoE WP
June 2017	EAWAG Summer School 2017 - Principles of catchment-scale hydrological modelling	Hydrology	Lecce (Italy)		WP4
May 2016	Spring school Maths-CS-HPC	Math, Computer Science	St Germain au mont d'or (Lyon)	https://mathsinfohpc.sciencesconf.org/	WP1
July 2016	E-CAM workshop	Soft matter	MdIS, France	https://www.cecam.org/workshop- 1512.html	WP1
6-7 March 2017	PRACE-PATC- EoCoE training on Parallel filesystems and parallel IO libraries		Mdls, France	https://events.prace-ri.eu/event/569/	WP1
13-15 March 2017	Parallel I/O and Portable Data Formats (PATC course)		JSC, Germany	https://events.prace-ri.eu/event/565/	WP1

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High performance computing (HPC) is based on advanced fundamental research in both applied mathematics and computer science. Motivated by both performance and power objectives, today's computing infrastructures evolve toward architectures with an increasing complexity, including sophisticated memory organizations. This has exposed the need for parallel programming and related code optimizations to a larger public. Research communities in computer science (architecture, compilation) and applied mathematics (numerical simulation) are not always aware of this need; at least their work do not always spread enough across the other discipline to lead to mutual influence. Automatic code optimizations and tools also require a better evaluation of their applicability. The goal of the research school was to make the link between some of the most recent advances in computer science (program optimizations, in particular polyhedral techniques and tools) and applied mathematics (schemes for numerical simulation), in relation with application needs.

Matthieu Haefele represented EoCoE in this School delivering a course on 'Architectures & Code Optimizations'. The course material of the school which had 70 participants can be found here: <u>https://mathsinfohpc.sciencesconf.org/resource/page/id/5</u>



4.5.1. E-CAM Extreme-Scale State-of-the-Art Workshop

The central goal of the 1st E-CAM Extreme-Scale State-of-the-art Workshop was to provide a forum for fellow E-CAM application end users and developers to:

- 1. Identify emerging extreme-scale computing requirements across the centre, including from both academia and industry partners
- 2. Increase the centre's awareness of current and emerging HPC hardware and software technologies on the road to exascale computing
- 3. Increase the centre's awareness of PRACE services (Advanced Training, software enablement, and industry interactions)
- 4. Interface with other members of the European HPC community
- 5. Identify themes of future interest for the centre on the road to exascale computing

Matthieu Haefele represented EoCoE in this workshop delivering a course on 'Exascale Challenges: The view from EoCoE' where he presented the methodological aspects on application performance monitoring and how this has triggered the first performance improvement achieved in the framework of support activities. More details on the course which had 31 participants can be found here: https://www.cecam.org/workshop-0-1512.html

4.5.2. PRACE-PATC-EoCoE training on Parallel file systems and parallel IO libraries

The increase in computational power goes hand in hand with an increase in the size of the data to be managed, both on the input and on the output sides. IO can easily become a bottleneck for large scale architectures. The understanding of parallel file system mechanisms and parallel IO concepts enables users to efficiently use existing high level libraries like Netcdf or HDF5. In addition this course provided an introduction to the well-established IO technology in the climate community: XIOS.

The specific topics of the training included:

- HDF5 High level IO libraries (3h)
- Parallel HDF5 and focus on MPI-IO hints (3h)
- Parallel file systems: Lustre (1h30)
- XIOS: IO server and online post-processing (4h30)

After this course, participants are expected to understand the trade-offs implied by using a parallel file-system, and know how to efficiently use parallel IO libraries.

Matthieu Haefele organised the course for EoCoE. The course material of the course which had 62 participants can be found here: <u>https://events.prace-ri.eu/event/569/</u>.

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4.5.3. PRACE-PATC-Parallel I/O and Portable Data Formats

Numerical simulations conducted on current high-performance computing (HPC) systems face an ever growing need for scalability. Larger HPC platforms provide opportunities to push the limitations on size and properties of what can be accurately simulated. Therefore, it is needed to process larger data sets, be it reading input data or writing results. Serial approaches on handling I/O in a parallel application will dominate the performance on massively parallel systems, leaving a lot of computing resources idle during those serial application phases.

In addition to the need for parallel I/O, input and output data is often processed on different platforms. Heterogeneity of platforms can impose a high level of maintenance, when different data representations are needed. Portable, self-describing data formats such as HDF5 and netCDF are examples of already widely used data formats within certain communities.

This course introduced the basics of I/O, including basic I/O-relevant terms, an overview over parallel file systems with a focus on GPFS, and the HPC hardware available at JSC. Different I/O strategies were presented. The course also introduced the use of the HDF5, the netCDF and the SIONlib library interfaces as well as MPI-I/O. Optimization potential and best practices were discussed.

The course was organised by JRC and EoCoE who was represented by Sebastian Lührs. The course material of the course which had 8 participants can be found here: <u>https://events.prace-ri.eu/event/565/</u>.



Parallel I/O and Portable Data Formats HDF5

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Jülich, March 14th, 2017



Parallel I/O and Portable Data Formats PnetCDF and NetCDF 4

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Jülich, March 13th, 2017



Parallel I/O and Portable Data Formats I/O strategies

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Jülich, March 13th, 2017

5. Success indicators

Targets	Indicator Description	Indicator target value	Current Indicator Value
	Number of conferences where EoCoE HPC simulation message is delivered specifically to SMEs and industry	> 10	0
	Number of HPC courses modules created or updated with new EoCoE expertise (ex: FTI, I/Os)	5	4
	Number of PATCs' sessions using EoCoE training materials	20	5
Academia, industry and SMEs engineers and researchers	Number of attendees to training sessions with EoCoE training materials	150 persons	186
	Number of course session dedicated to SMEs	2	0
	Number of hired personnel mentored by EoCoE experts	>20	17

N/A-Not available

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