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EINFRA-5-2015: Centres of Excellence for computing applications

EoCoE

Energy oriented Center of Excellence for computing applications

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D6.3 - M12
D6.3 Annual Thematic Report - Year 1

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1. Background

Task 6.1.6 of the EoCoE project consists in organisating a series of 9 thematic workshops to present research products to the other project partners. These will typically take place during regular six-monthly EoCoE project meetings. Project partners are expected to propose workshop themes based on outputs from the different work packages. These workshops can also be open to the wider end-user community.
In Year 1, two workshops were organized, which are described below.

2. First Thematic Workshop: Benchmarking and performance analysis

2.1 Aim

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, enabling the teams to make a preliminary identification of bottlenecks, and to initiate the standardisation of benchmark procedures for these codes within the EoCoE project.

As an initial step, all code developers were instructed on how to perform benchmarking within the JUBE workflow environment, which will permit measurements to be documented, shared and rigorously reproduced over the project lifetime and beyond. Developers were then able to begin analysing their applications using specific HPC tools under the guidance of HPC experts (Score-P, Scalasca, Vampir, Paraver, Extrae, among others). Based on this face-to-face collaboration and common training, small teams of code developers and HPC experts from WP 1 were established, who will follow up on the promising initial work to provide comprehensive benchmarks and performance data by the time the next workshop is held in March/April.

A very valuable outcome was the exchange of respective ideas and needs between code developers and HPC experts, as this helped clarifying the issues from either perspective and enabled both sides to interact more smoothly with a well-defined focus on the next actions to be taken. For example, the requirements for a full code 'audit' from the EoCoE and POP perspectives were clarified: here it was decided that the initial benchmarking would take place within and immediately after the workshop by EoCoE WP1 members, whereas more in-depth follow-up analyses could be passed on to POP at a later stage.

2.2 Agenda

Tuesday, Dec 8^{th} 2015

14:00 – 15:45	JUBE – Introduction	Sebastian Lührs , JSC
15:45 – 16:15	Coffee Break	
16:15 – 18:00	JUBE – Integration Hands on I	Sebastian Lührs et al.
18:30	Transfer to Hotels in Jülich	

Wednesday, Dec 9th 2015

09:00 – 10:30	Tools Intro: Score-P , Scalasca , Vampir	POP@JSC
10:30 – 11:00	Coffee Break	
11:00 – 12:30	Tools Hands-on: Score-P , Scalasca , Vampir	POP@JSC
12:30 – 13:30	Lunch	
09:00 – 10:30	JUBE – Integration Hands on II	Sebastian Lührs et al.
10:30 – 11:00	Coffee Break	
11:00 – 12:30	JUBE – Integration Hands on II	Sebastian Lührs et al.

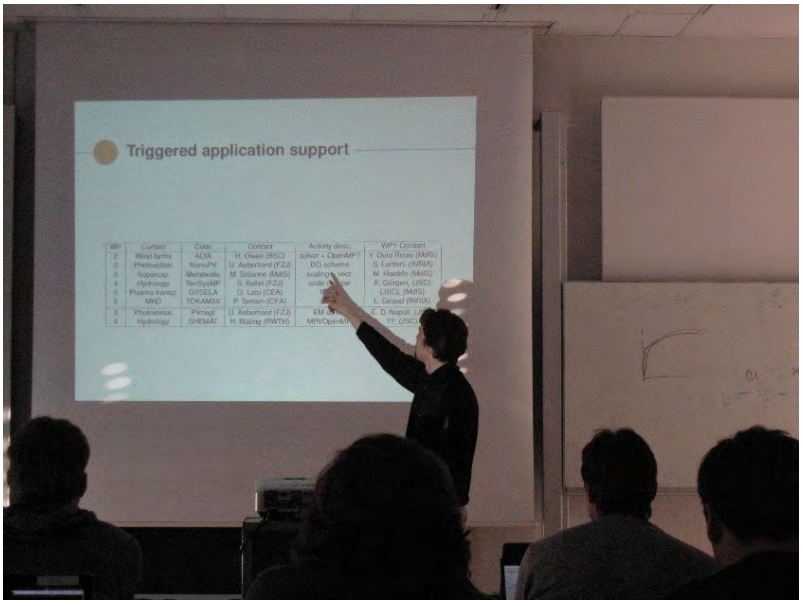
Thursday, Dec 10th 2015

13:30 – 15:00	Tools Intro: Extrae , Paraver	POP@BSC
15:00 – 15:30	Coffee Break	
15:30 – 17:30	Tools Hands-on: Extrae , Paraver	POP@BSC
12:30 – 13:30	Lunch	
13:30 – 15:00	Benchmarking Hands-on I	All
15:00 – 15:30	Coffee Break	
15:30 – 17:30	Benchmarking Hands-on I	All
	Parallel session	
13:30 – 15:00	Tools Intro: Extrae , Paraver	POP@BSC
15:00 – 15:30	Coffee Break	
15:30 – 17:30	Tools Hands-on: Extrae , Paraver	POP@BSC

Friday, Dec 11th 2015

09:00 – 10:30	Benchmarking Hands-on II	All
10:30 – 11:00	Coffee Break	
11:00 – 12:30	Audit	POP
12:30 – 13:30	Lunch	
14:00	Departure	

2.3 Pictures


Triggered application support

2.4 List of participants

Name	Surname	Affiliation	COE	Attended
Urs	Aeberhard	FZJ IEK-5	EoCoE	
Antoni	Artigues	Barcelona Supercomputing Center	EoCoE	
Jonas	Berndt	FZJ IEK-8	EoCoE	
Thomas	Breuer	FZJ JSC	EoCoE	
Dirk	Brömmel	FZJ JSC	EoCoE	
Johanna	Bruckmann	RWTH Aachen	EoCoE	
Henrik	Buesing	RWTH Aachen	EoCoE	
Metin	Cakircali	FZJ JSC	EoCoE	
Edoardo	Di Napoli	FZJ JSC	EoCoE	
Hendrik	Elbern	FZJ IEK-8	EoCoE	
Wolfgang	Frings	FZJ JSC	EoCoE	
Fabian	Gasper	FZJ JSC	EoCoE	
Paul	Gibbon	FZJ JSC	EoCoE	
Judit	Gimenez	Barcelona Supercomputing Center	POP	
Klaus	Goergen	FZJ JSC	EoCoE	
Matthieu	Haefele	Maison de la Simulation , Paris	EoCoE	
Stefan	Kollet	FZJ JSC	EoCoE	
Ketan	Kulkarni	FZJ JSC	EoCoE	
Guillaume	Latu	Maison de la Simulation , Paris	EoCoE	
Sebastian	Lührs	FZJ JSC	EoCoE	
Bernd	Mohr	FZJ JSC	POP	
Sachin	Nanavati	FZJ JSC	EoCoE	
Yacine	Ould-Rouis	Maison de la Simulation , Paris	EoCoE	
Herbert	Owen	Barcelona Supercomputing Center	EoCoE	
Wei	Qu	RWTH Aachen , E.ON Energy Research Center	EoCoE	
Daniel	Rohe	FZJ JSC	EoCoE	
Dirk	Schmidl	RWTH Aachen	POP	
Harald	Servat	Barcelona Supercomputing Center	POP	
Bo	Wang	RWTH Aachen	POP	
Brian	Wylie	FZJ JSC	POP	
Ilya	Zhukov	FZJ JSC	POP	
Lukas	Poodhuis	FZJ JSC	EoCoE	
Marc-André	Hermanns	FZJ JSC	POP	

2.5 Core metrics of the workshop

Date	Dec 8^{th} to Dec 11^{th} 2015
Location	Jülich Supercomputing Centre at Forschungszentrum Jülich
Hours of training	16,5h , 4,5h of these theory and 12h hands-on
Number of instructors	19 (not all present all days, specific attendance instead)
Number of trainees	14
Number of evaluation tools	6
Codes evaluated	see separate table
Platforms used	JURECA , JUQUEEN , partially other “home” systems
Range of cores used	1 – 3.072

3. Second Thematic Workshop: Benchmarking and performance analysis

3.1 Aim

The second EoCoE-POP workshop at Maison de la Simulation on benchmarking and performance analysis brought together, in a similar way as the first workshop, code 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 the same as the first workshop and we refer the reader to the report of the first workshop for more informations.

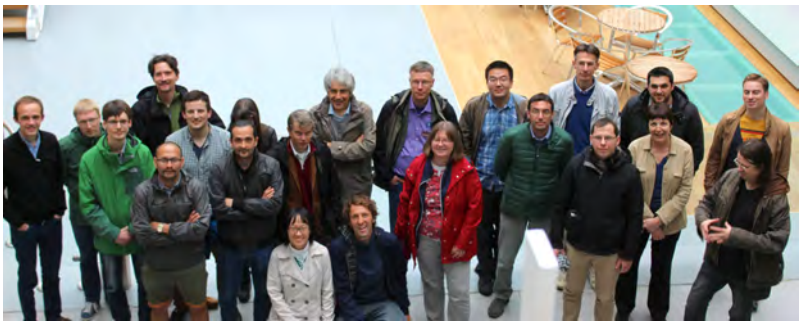
The format and the means were also very similar to the first workshop. The only difference for code developers is that they could start their JUBE integration from a first template this time rather than from scratch as it was the case during the first workshop. As a consequence, code developers could progress much faster and all code teams could reach objectives that were not met during the first workshop. This showed us that our methodology is improving and we plan to improve it further for the next workshop that will likely take place in January 2017.

3.2 Agenda

From Monday May 30^{th} at lunchtime to Thursday June 2^{nd} lunchtime 2016
It was the same format than the fist workshop, but about different codes to evaluate. refer to firtst workshop agenda for more details. Following is a short summary of what happened and when.

Mon 14:00 – 18:00	JUBE – Introduction + hands-on	Sebastian Lührs , JSC
Tue 09:00 – 18:00	Performance tools introduction + hands-on (POP)	Brian Wylie, Judit Gimenez
Wed 09:00 – 18:00	Hands-on JUBE code integration	All
Thu 09:00 – 12:00	Hands-on JUBE code integration	All

3.3 Pictures



3.4 Codes Evaluated and progresses made so far

EoCoE code benchmarking and analysis progress sheet - checkpoint July 2016

Code	WP	JSC Account	Data server account	Gitlab account	JUBE integration	Benchmarks defined in JUBE	Tools integrated in JUBE	Allinea report	Score-P profile	Score-P trace	Scalasca analysis	Vampir analysis	Extrae measurement	Paraver analysis	Darshan results	VTune analysis	Advisor analysis	Performance report	Total Progress (%)
ALYA	WP 2	2	2	2	2	2	2	2	2	2	2	2	2	2	2	2	2	2	100
ESIAS	WP 2	2	2	2	2	1	1	0	2	1	1	0	0	0	1	0	0	2	100
Metalwalls	WP 3	2	2	2	2	2	2	2	2	2	2	0	2	2	2	0	2	2	100
PVnegf	WP 3	2	2	2	1	0	0	0	0	0	0	0	0	0	0	0	0	0	32
SHEMAT	WP 4	2	2	2	2	2	1	2	1	1	1	0	2	2	2	0	0	0	90
ParFlow	WP 4	2	2	2	2	0	1	1	1	1	1	1	1	1	1	1	0	0	82
GYSELA	WP 5	2	2	2	2	2	2	1	1	1	1	0	2	2	2	0	0	0	90
nowcast system	WP 2	1	2	2	2	2	1	2	2	2	2	0	0	0	2	0	0	0	90
CP2K	WP 3	2	2	2	2	2	0	0	1	0	0	0	1	0	2	0	0	0	64
MDFT	WP 3	2	2	2	2	2	2	2	2	2	2	0	2	2	0	0	0	2	100
TELEMAC	ext	1	2	2	2	2	1	2	2	2	2	2	2	2	0	0	0	0	90
COMPASS	ext	2	2	2	2	2	1	2	2	2	2	2	2	2	0	0	0	0	90
EIRENE	WP 5	2	2	2	2	2	1	2	2	1	1	0	1	0	2	0	0	0	90

Legend

0	not started
1	in progress
2	established

3.5 Core metrics of the workshop

Date	May 30^{th} to June 2^{nd} 2016
Location	Maison de la Simulation Saclay, France
Hours of training	17h , 5h of these theory and 12h hands-on
Number of instructors	10
Number of trainees	12
Number of evaluation tools	6
Codes evaluated	6
Platforms used	JURECA , JUQUEEN , Mare Nostrum
Range of cores used	1 – 2.048

4. Next workshops for Year 2

For the coming year, three workshops are already planned :

1) A third and last *Benchmarking and performance analysis workshop* will be organised in BSC (Barcelona, Spain). This workshop will focus on the remaining EoCoE core applications that have not yet been through the evaluation process. Several external teams, including from industry, have also shown interest to participate to this workshop.

2) A workshop on *HPC for renewable energies: new programming models and strategies for the emerging exascale architectures*, has been proposed for the European HPC Summit Week in May 2017. This workshop will review the state of the art in the available programming models that have been proposed for upcoming exascale architectures, focusing on those that enable attaining good performance on a range of different architectures, and have a significant user base. Talks will be given both by the developpers of the systems, as well as by advanced user sharing their experience with renewable energy applications from, for example, the areas of wind-, solar-, hydro and geothermal power, nuclear fusion and high-capacity batteries. .

3) A EoCoE workshop will be organized at the Large-Scale Scientific Computations (LSSC 2017) Conference in Sozopol (Bulgaria) in June 2017. The topic of the workshop will be : *Large-Scale Numerical Computations for Sustainable Energy Production and Storage*. It will bring together application scientists, applied mathematicians and computer scientists, to focus on numerical issues for high-performance simulations concerning low-carbon energy production and storage. Topics of interest include (but are not limited to) numerical algorithms and scientic software libraries for high-performance computations in the areas of meteorology for energy, geothermal and hydropower systems, fusion for energy, materials for energy generation and storage.