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Energy oriented Center of Excellence for computing applications

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Education Course materials and platform

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	Contact's e-mail:	edouard.audit@cea.fr
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	Contributors:	George Kirkos, Nicolas Jarraud (CyI)
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Abstract:

The aim of this report is to present the current state of EoCoE training materials delivered by task WP6.2.The main part of the report describe the first training modules presented during EoCoE workshop.

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1 Introduction

Deliverable D6.2 presents the current state of EoCoE training materials delivered by task WP6.2

In the EoCoE Description of Work the task 6.2 is defined as follows:
"Education will be provided through close partnerships with PRACE/PATC and other organisations and partners training facilities to disseminate the skills, best practices and know-how of EoCoE to Doctoral/Master's/Professional trainings in the use of computational methods and tools and optimisation of applications. Actions led by CyI will include: Creation of multimedia modules for academic courses and professional training, delivery of short courses for professionals, delivery of academic courses/modules through existing PhD/MSc programmes, MOOCs and a supplementary e-learning platform. PSNC, CNRS and INRIA will co-organise training sessions and participate in preparation of multimedia training materials."

Training modules should document the work achieved by EoCoE project. Therefore the tasks 6.2 should be more active in the second part of the project as results from Work Package will be ready. In the first year of the project the task 6.2 focused on two activities:

- Prepare first training session and training modules
- To find the platform for storing and delivering training modules

2 2nd Project Meeting in Rome

Face to Face EoCoE project meeting was organised in Rome, 30th November - 2nd December 2016.

This was the second of bi-annual face to face meeting of the Energy oriented Centre of Excellence in computing applications EoCoE .

The meeting consisted of three parts.

- Tutorial session held on Wednesday morning
- The public part (video recorded) is a session which presented the results of the project in a plenary session which will held on Wednesday afternoon.
- The rest of the meeting consists of different workshops and committees. These are for EoCoE members or on invitation only.

  The program of tutorial session is presented below.

Wed. November 30	EoCoE Tutorial programme
Room (seats)	**Conference Hall (100)**
8:30 AM (since)	Registration
9:00 AM	**Advanced programming methods for Exascale** Programming-model design and implementation for the Exascale, *Olivier Aumage, INRIA*
10:45 AM	Coffee break
	Energy oriented computing applications
11:00 AM	1. Computing Kernel Autotuning Using BOAST, *Brice Videau*
11:30 AM	2. Electronics structure calculations in HPC framework: Solutions for profiling, load-balancing and post-processing, *Thierry Deutsch*
12:00 PM	3. ParFlow functionalities and implementation with JUBE. *Sharples, Kollet, Naz and Görgen*
12:30 PM	4. Visualizing a grid mesh with Visir software, *Alexis Loyer, INRIA*
1:00 PM	Lunch break

Figure 1 Agenda f Rome workshop training session

The focus on the tutorial presentations is on the services provided by EoCoE project. Tutorials present what is available, and how this helps scientists in their work in energy oriented areas and how users can use the services.

All plenary sessions were recorded. The video of the tutorial session are part of training modules.

The general EoCoE recommendation for all training modules is that there should be two version of the videos: short (about 10 minutes) overview and complete recording.
From the short overview users should get the general idea about the service, what resources are available, what prerequisite are needed, where the service is available, how to start working with it and where to ask about details etc.

The complete presentation can contain more details, demos, examples etc. Some short guided exercises also can be conducted in this part if this possible and useful.

3 Training modules from Rome tutorial session

3.1 Programming-model design and implementation for the Exascale, Olivier Aumage, INRIA

The tutorial was focused on Programming models for modern architectures. In the first part the overview of Modern HPC platform was presented including runtime systems and abstraction of application workloads. The second part of the tutorial focused on practical example of using the sequential task flow programming model with the StarPU Task-Based Runtime System.

StarPU is a task-based **runtime system** for heterogeneous platforms coupling a performance modelling **scheduler** with a distributed shared-memory manager.

The tutorial based on experiences of EoCoE Partner INRIA STORM team (Statical Optimizations and Runtime Methods team). The team deals with the parallelism complexity challenge, providing a coordinated set of programming tools and techniques before (*compiler*), during (*runtime*) and after (*analysis*) program execution. Team STORM aims at combining strengths along these three directions: High level *domain specific languages*; *Runtime systems* for heterogeneous, many core platforms; *Analysis* and performance feedback tools.

The screenshot from tutorial and sample slides from tutorial presentation are presented below. The whole material is available at web page:
http://public.weconext.eu/eocoe/2016-11-30/video_id_000/index.html

Figure 2 Title slide from the training module

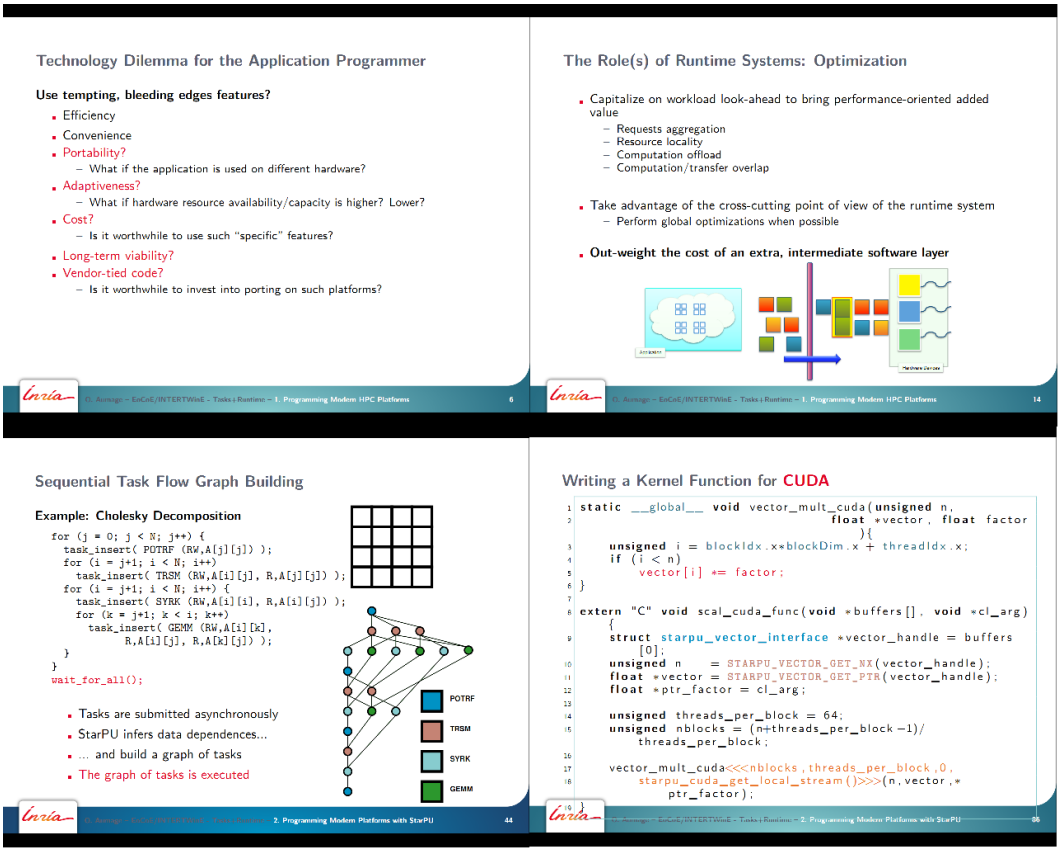

Figure 3 Sample slides from tutorial presentation

3.2 Computing Kernel Autotuning Using BOAST

The tutorial presents BOAST metaprogramming framework in order to do some autotuning on scientific applications kernels.

BOAST is aiming at generating parametrized source code. The aim is for the programmer to be able to orthogonally express optimizations on a computing kernel, enabling a thorough search of the optimization space. This also allows a lot of code factorization and thus code base reduction.
BOAST allows the description of a computing kernel and its possible optimization using and embedded domain specific language (EDSL). The kernel and a combination of optimization can then be generated in a target programming language of choice (FORTRAN, C, CUDA or OpenCL). BOAST can then benchmark (using a selected compiler and compiler options) and test the generated kernel for regressions.

The tutorial presents the idea of BOAST and practical example of using BOAST with Gysela.

The screenshot from tutorial and sample slides from tutorial presentation are presented below. The whole material is available at web page:
http://public.weconext.eu/eocoe/2016-11-30/video_id_001/index.html

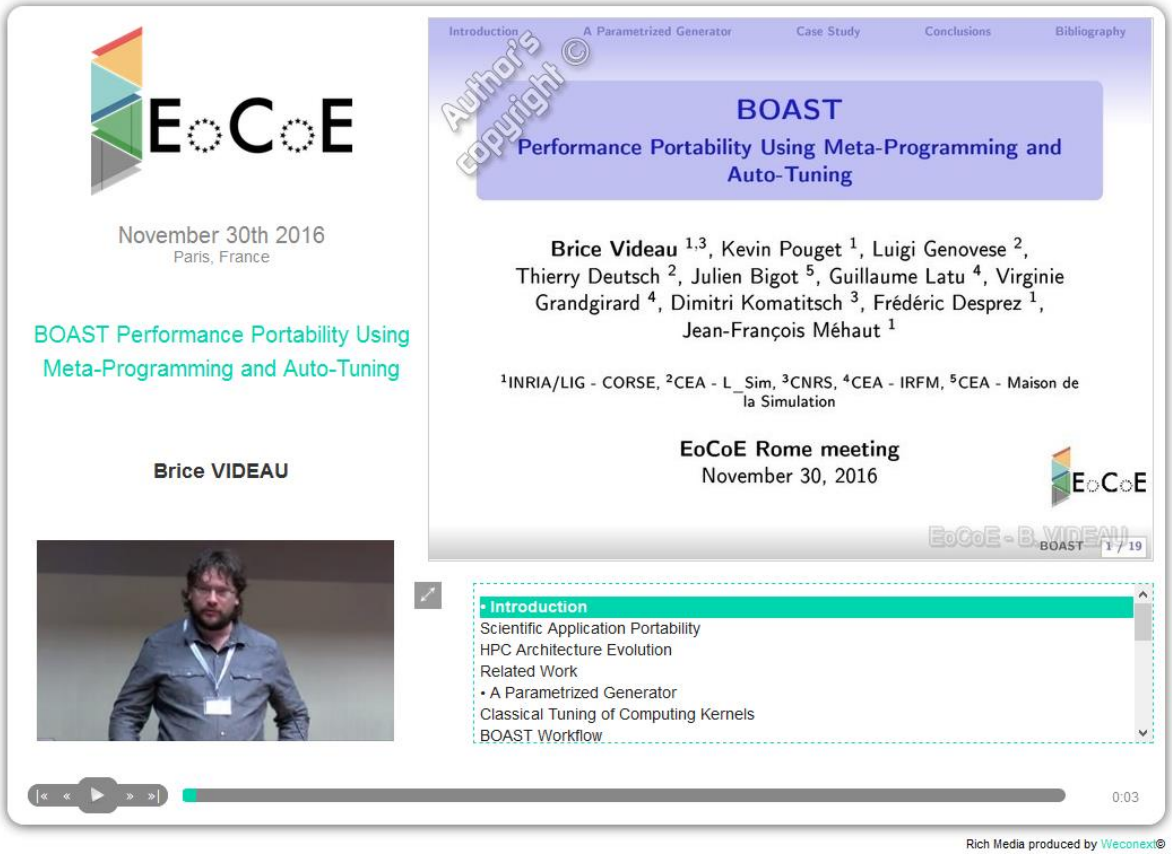

Figure 4 Title slide from the module

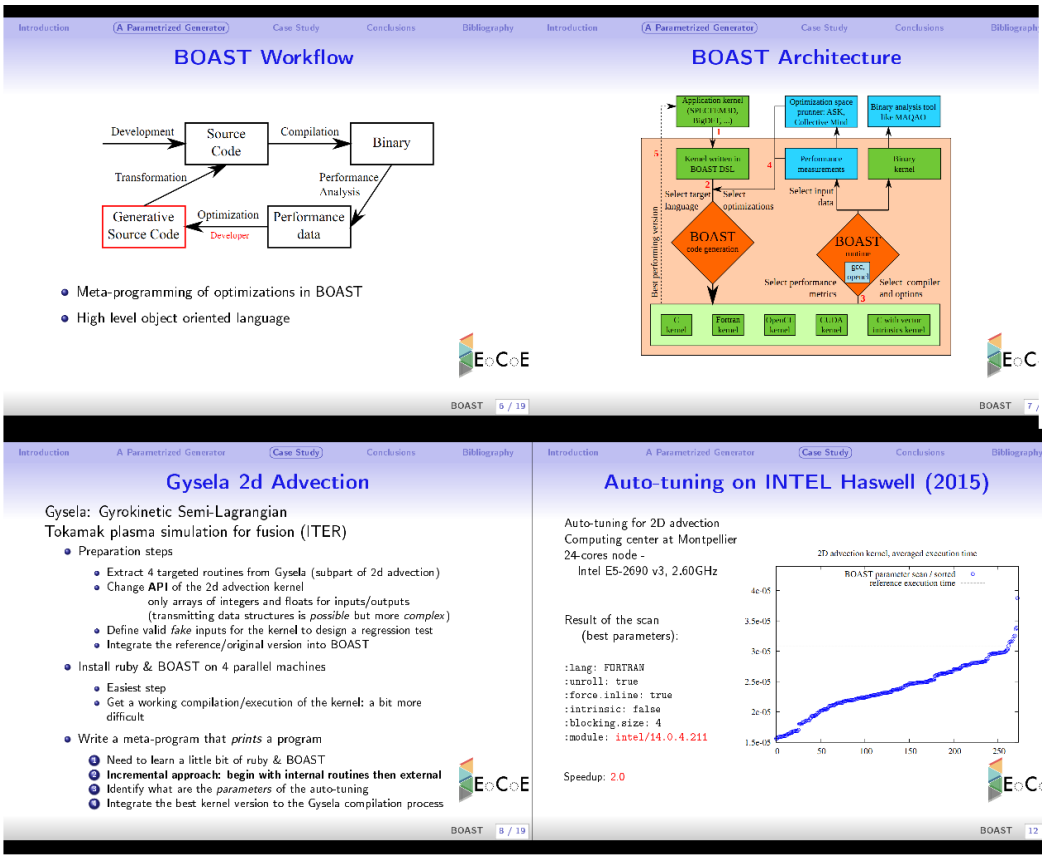

Figure 5 Sample slides from tutorial presentation

3.3 Electronics structure calculations in HPC framework: Solutions for profiling, load-balancing and post-processing

The tutorial focused on how to investigate and interpret performance issues and performance opportunities in view of exascale applications in the context of electronic structure calculations. BigDFT tool is used which help computational physicist to focus on the preparing algorithms and computation input rather than dealing with specific hardware optimisations. The presentation included example input description in YAML based language.

BigDFT is a DFT massively parallel electronic structure code (GPL license) using a wavelet basis set. Wavelets form a real space basis set distributed on an adaptive mesh (two levels of resolution in our implementation). GTH or HGH pseudopotentials are used to remove the core electrons. Thanks to our Poisson solver based on a Green function formalism, periodic systems, surfaces and isolated systems can be simulated with the proper boundary conditions.

More information about the tool can be found at www.bigdft.org/

The screenshot from tutorial and sample slides from tutorial presentation are presented below. The whole material is available at web page:
http://public.weconext.eu/eocoe/2016-11-30/video_id_003/index.html

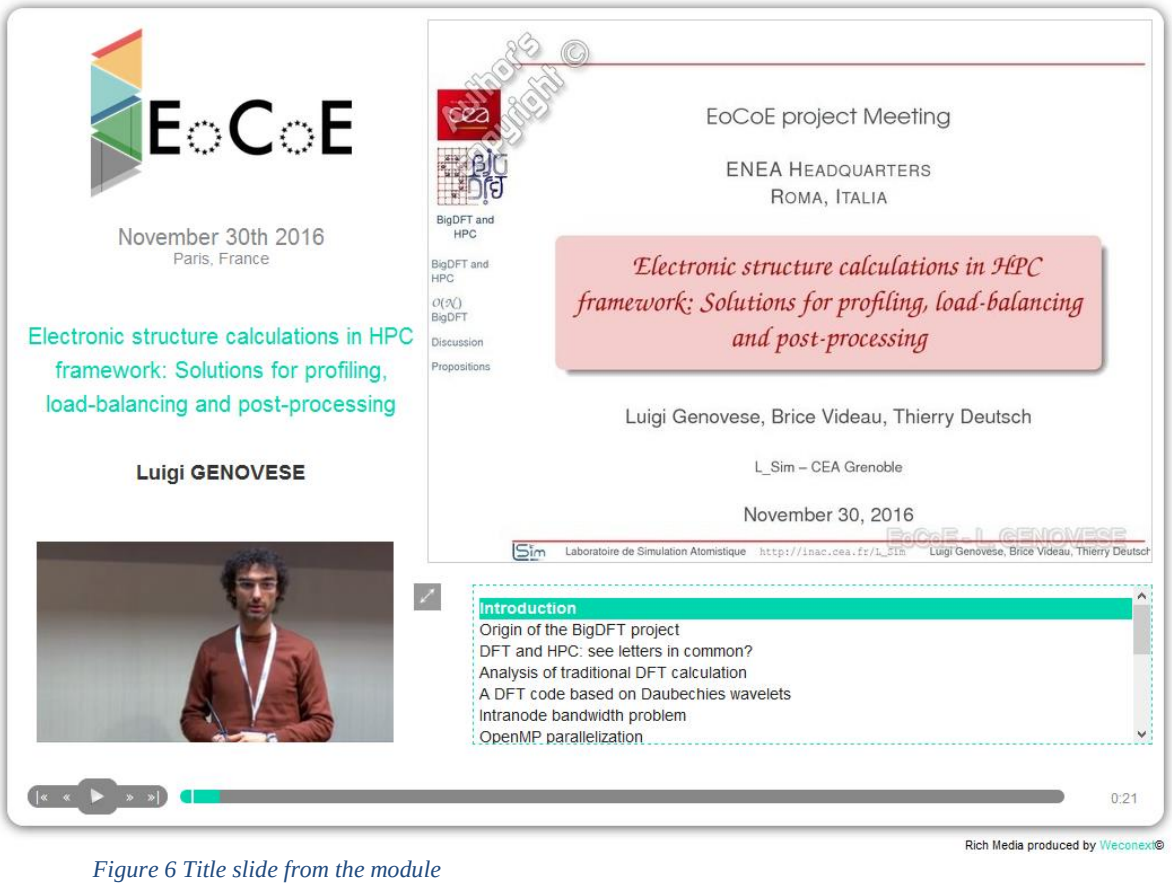

Figure 6 Title slide from the module

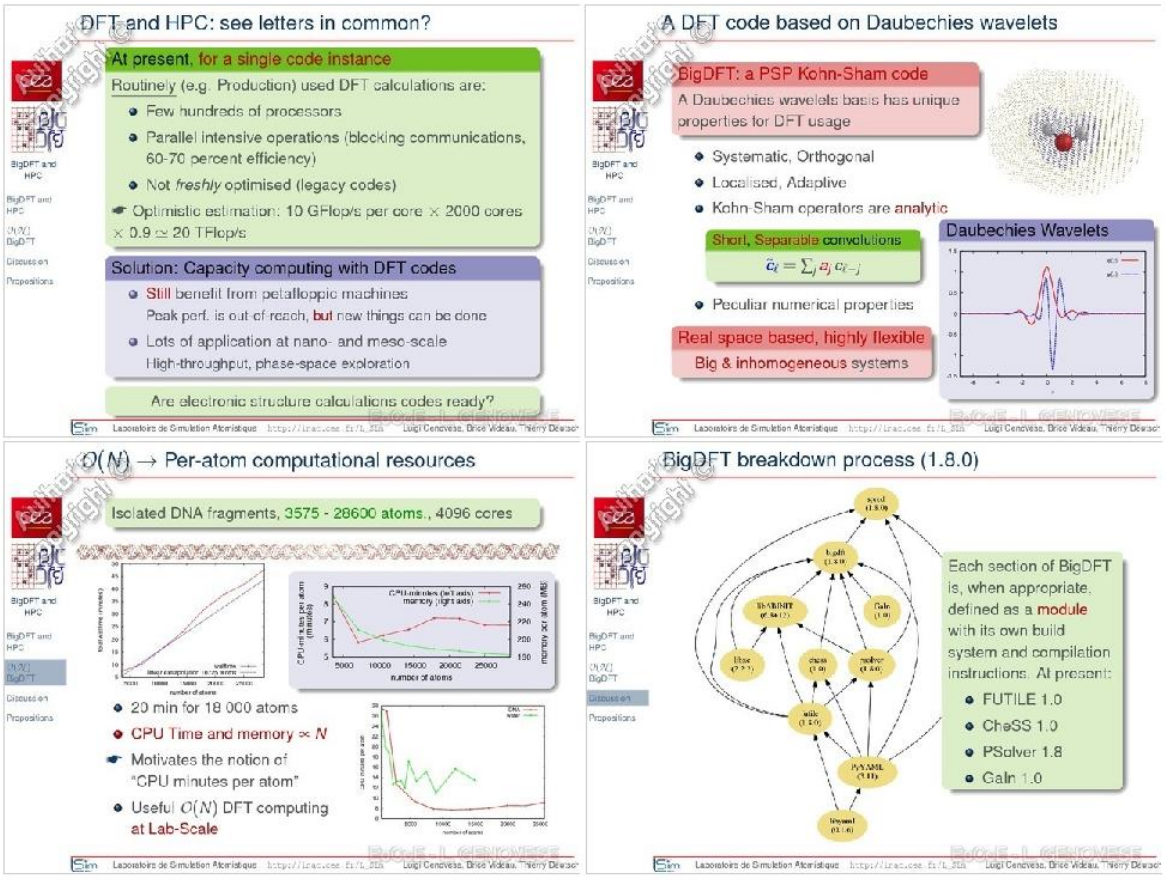

Figure 7 Sample slides from tutorial presentation

3.4 ParFlow functionalities and implementation with JUBE.

JUBE is one of the main tool used in our workshop and it was enhanced thanks to EoCoE. Some team were formed during the workshops, with this tutorial EoCoE member at large are aware the possibility offered by the performance analysis tools and methodology developed within EoCoE

The JUBE benchmarking environment provides a script based framework to easily create benchmark sets, run those sets on different computer systems and evaluate the results

Benchmarking a computer system usually involves numerous tasks, involving several runs of different applications. Configuring, compiling, and running a benchmark suite on several platforms with the accompanied tasks of result verification and analysis needs a lot of administrative work and produces a lot of data, which has to be analysed and collected in a central database. JUBE provides a benchmarking environment and all these steps can be automated..

For each benchmark application the benchmark data is written out in a certain format that enables the benchmarker to deduct the desired information. This data can be parsed by automatic pre- and post-processing scripts that draw information, and store it more densely for manual interpretation.

More information about JUBE can be found at
http://www.fz-juelich.de/ias/jsc/EN/Expertise/Support/Software/JUBE/_node.html

The screenshot from tutorial and sample slides from tutorial presentation are presented below. The whole material is available at web page:
http://public.weconext.eu/eocoe/2016-11-30/video_id_002/index.html

Figure 8 Title slide from the module

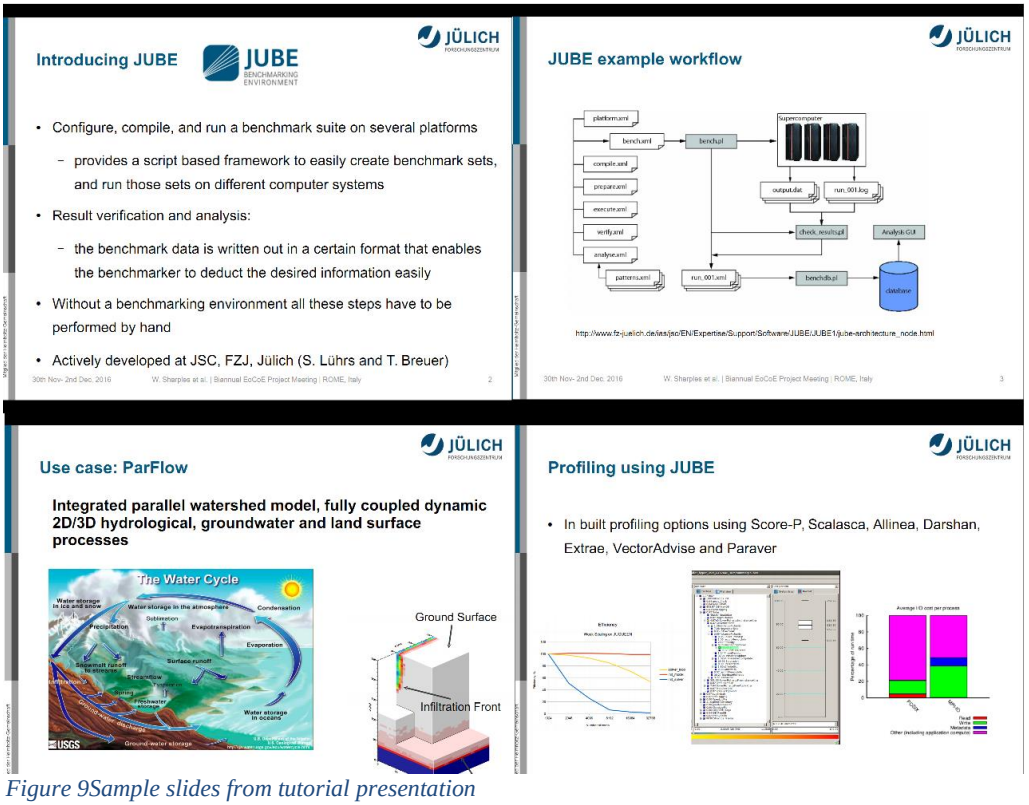

Figure 9Sample slides from tutorial presentation

3.5 Visualizing a grid mesh with Visir software

The tutorial presented the example usage of Visir software for generation, optimisation and visualisation of mesh.

Vizir is an interactive mesh visualization and modification software, which aims at gathering INRIA dynamic libraries (3D mesh generator, 3D adaptative remeshers, solvers...). The primary intent is to facilitate the computation process, from the geometry recuperation to the solving step, through the mesh generation.

Vizir is based on various technologies:

- Qt and OpenGL for graphic interfaces.
- libmesh6

More information about Visir can be found at
https://www.rocq.inria.fr/gamma/gamma/vizir/

The screenshot from tutorial and sample slides from tutorial presentation are presented below. The whole material is available at web page:
http://public.weconext.eu/eocoe/2016-11-30/video_id_004/index.html

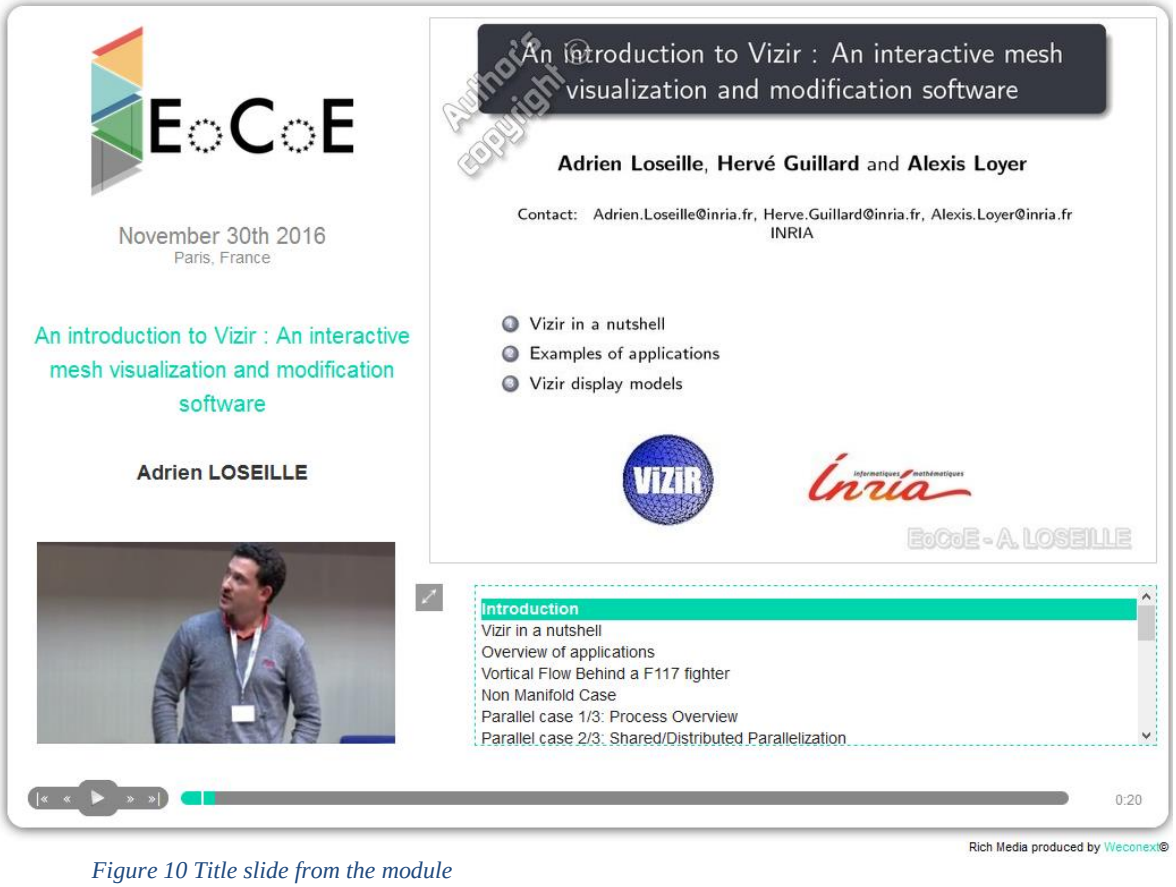

Figure 10 Title slide from the module

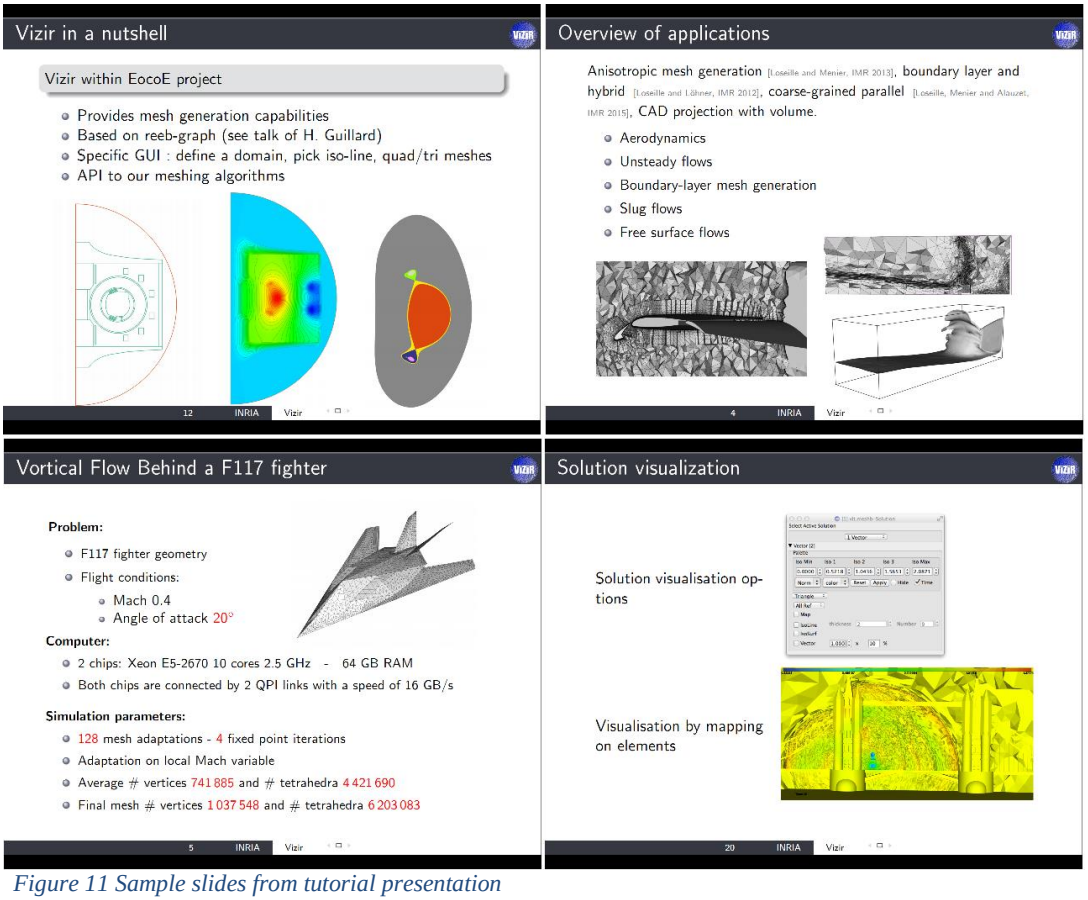

Figure 11 Sample slides from tutorial presentation

4 Partnerships with PRACE/PATC

EoCoE participates in PRACE Training. The following sessions have beneficiated from EoCoE expertise:

- Parallel filesystems and parallel IO libraries @MdlS https://events.prace-ri.eu/event/569/ 6-7 Mars, organized by M. Haefele
- Scientific workflows, "on demand" event, organized by PATC France, EoCoE and ECAM Organizers: M. Kern, M. Mancip, M. Plociennik, date TBA (Apr / May 17)
- Parallel I/O and Portable Data Formats organised by JSC, EoCoE Participant Sebeastian Lührs, 13 - 15 March

5 Training modules repository

5.1 EoCoE document repository

EoCoE uses a collaboration platform which is accessible for all members of the project at link project.eocoe.eu. The part of the platform is Document Repository. It was decided that in the first project phase it will be used for storing training modules, too. All training presentation from Rome workshop are available in the document repository in the dedicated folder. Recorded videos are available at WeWonext site and linked to the main project page. This solution is adequate for first project phase, while the number of training modules isI not yet big. After review of the results and feedback from Rome session and after taking into account the types of training materials produced by EoCoE we conclude that it is advantageous to use specialised training service.

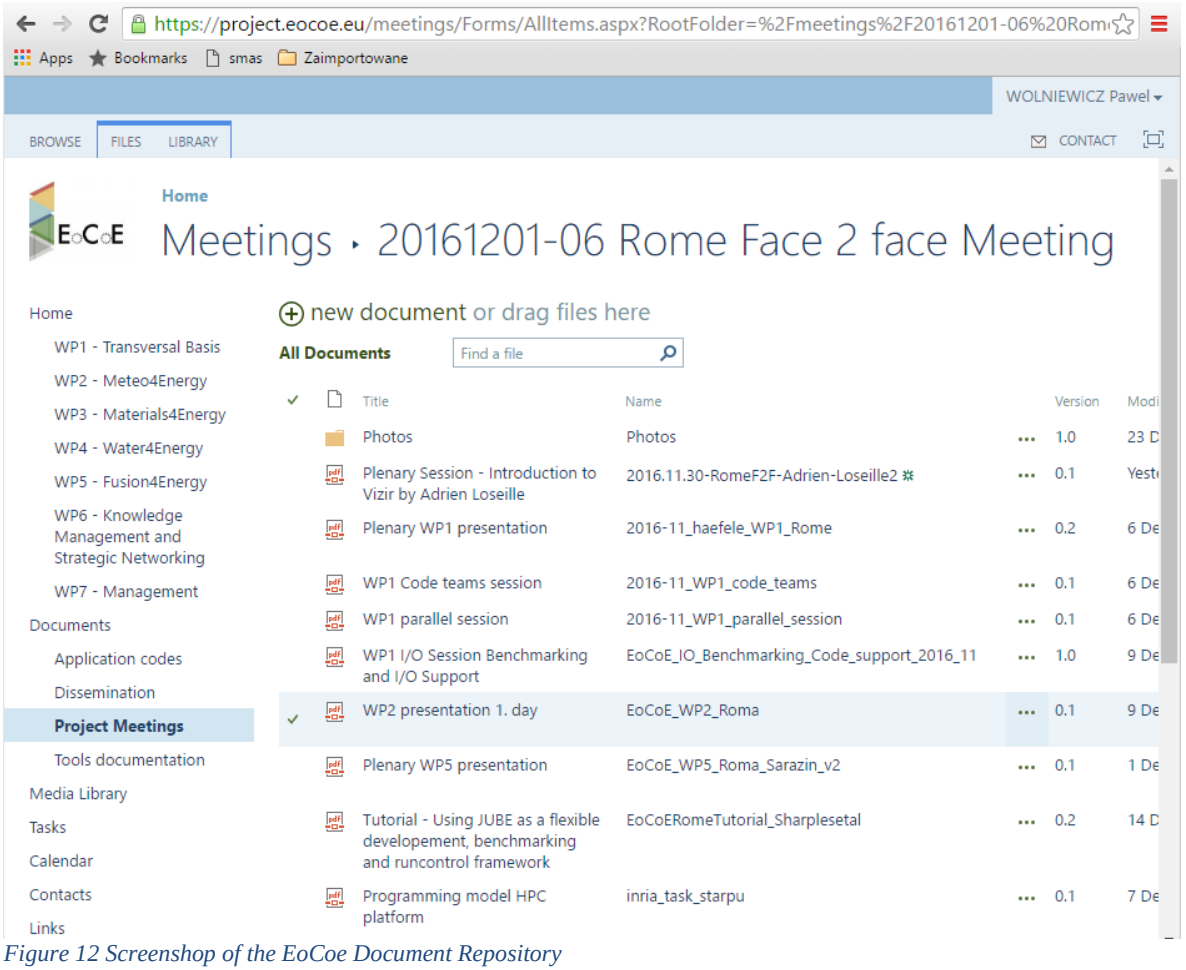

Figure 12 Screenshop of the EoCoe Document Repository

5.2 WeConext video repository

Videos from Rome tutorials were recorded by WeConext and stored and their repository avaible at http://public.weconext.eu/eocoe/2016-11-30/index.html

All modules are prepared in the same style and contain:

- Video of the presenter
- Current slide
- Index of slides

The view of the page with Rome training materials is shown below.

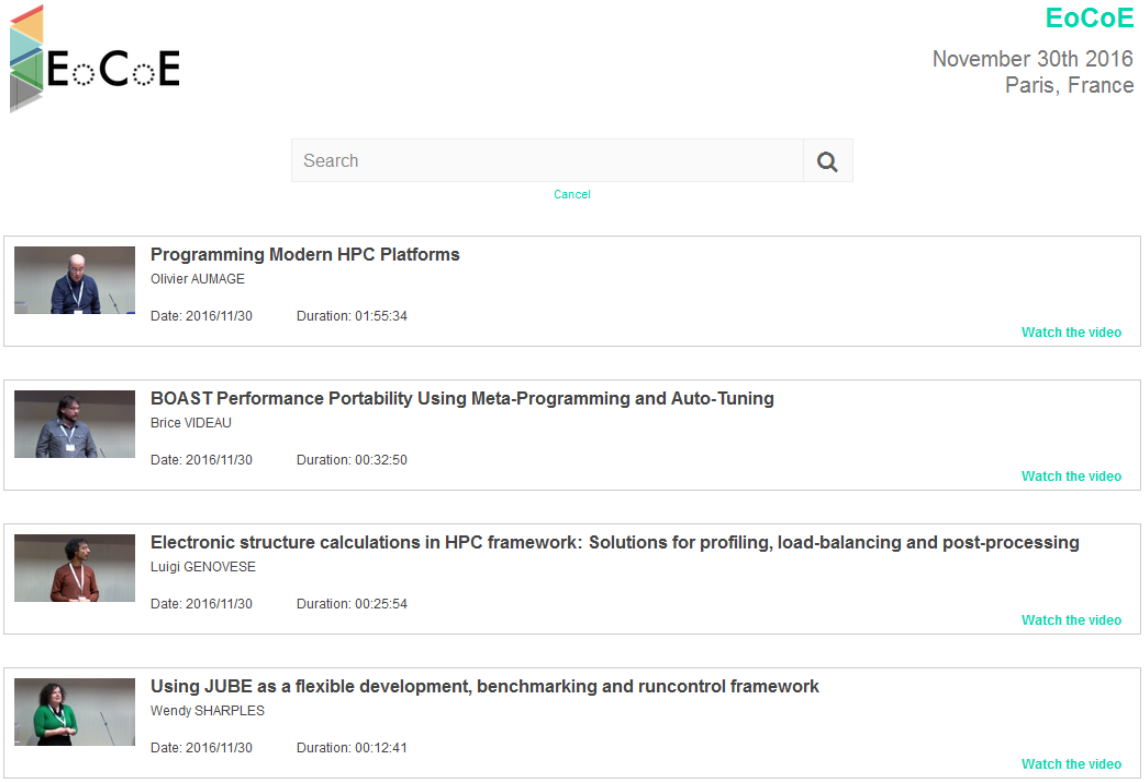

Figure 13 Training materials available at WeConext site

5.3 MOOC platform

Document server is focused on storing project files. Weconext site is perfect for publicise EoCoE recorded events. But modern training platform could be more than just repository of videos or files. To deliver a high quality training it is recommended to provide a specialised services on top of a training modules repository. Advanced training repository should support **massive open online courses** (**MOOC**) - online courses aimed at unlimited participation and open access via the web. In addition to traditional course materials such as filmed lectures, readings, and code examples, many MOOCs provide interactive user forums to support community interactions among students, professors, and teaching assistants (TAs). MOOCs are a recent and widely researched development in distance education which were first introduced in 2008 and emerged as a popular mode of learning in 2012

There are different possibilities to evolve from simple storage repository into an advanced learning platform .

- Adapt project repository to training requirements. EoCoE collaborative platform consist of a set of tools that can be useful for learning platform: document repository, media library, calendar, wiki etc. However there are same problems to solve while using it as learning platform. The most important issues include access permissions to all materials and the structure of repository.
- To use WeConext platform. With the Weconext platform it is easy to maintain an online space of reference to efficiently federate a network of experts. It supports working at distance while keeping control on data and share knowledge with a reinforced safety. The platform have a range of tools including storage of all types

of data, shared calendars, forums, surveys and reporting tools.
- To use a dedicated learning environment. Some tests and analysis of different MOOCs learning environments were conducted in the first year of the project and as a result we recommend Moodle as a training service. Moodle (the Modular Object Oriented Dynamic Learning Environment) 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. allows for extending and tailoring learning environments using community sourced plugins.

With the feedback from users of the first training modules we will be able to assess user's experiences and requirements and to recommend the possible evolution of EoCoE learning platform.

6 Summary and plans for the next period

First EoCoE training session was conducted during Rome workshop. Based on this experience the project can continue with delivering more training and preparation of training modules.

The tutorials from Rome workshop are only the first EoCoE training modules and more modules will be prepared when the results from workpackages will be ready. The experience from the firsts training sessions show that the training modules can consist of presentations, short videos, complete videos, code example, documentation etc. Taking it into account we can conclude that simple repository in the form of document server is suitable for handling limited number of training materials, but should be enhanced towards MOOC in the next part of the project.