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

# EoCoE

# Energy oriented Center of Excellence

for computing applications Grant Agreement Number: EINFRA-676629

> D6.1 EoCoE web platform

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EoCoE	Project Title:	Energy oriented Centre of Excellence	
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Project and Deliverable Information Sheet

\* - The dissemination level are indicated as follows: PU – Public, CO – Confidential, only for members of the consortium (including the Commission Services) CL – Classified, as referred to in Commission Decision 2991/844/EC.

Document Control Sheet

Document	Title :	EoCoE web platform
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#### Document Keywords:

Web platform; Internet web site

Executive Summary:

This deliverable gives the address and main structure of the Energy oriented Centre of Excellence in computing applications web site

Note:

This deliverable is realised using a structured and modular writing method for technical documents: Information Mapping <sup>R</sup>. It benefits from the specific limap package of  $L^{A}T_{E}X$  language.

# EoCoE web platform deliverable overview

Abstract	This deliverable gives the address, main structure of the Energy oriented Centre of Excellence in computing applications web site and editorial infras- tructure		
Table of content	This deliverable contains the following topics		
	FoCoF web platform		
		, 	
	Annex I : Contribution to: DELIVERABLE 6.1 7 Suggestions for Services Web Page		

# EoCoE web platform

the Energy oriented Centre of broject is to:
rnance of the project
al public audience
and eventually more tech- ars and transversal basis "work
emic and industrial
nities of the project
computing applications web
ject coordinator assisted by the Work package 6 (Knowledge ne editorial team is com-posed of ho have the rights to update the
pal project: www.drupal.org
t who won a public procure-
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Continuing...

### EoCoE web platform, Continued

Web site updates The web platform is updated by the PEC members as necessary. The hidden address accessible by login and password: www.eocoe.eu/user gives access to an "Edition" tag which allows to change the web platform content.



### Annex 1

### **Contribution to: DELIVERABLE 6.1**

### **Suggestions for Services Web Page**

### Background

The EoCoE website (http://www.eocoe.eu/) was set up early on in the project (Deliverable 6.1 of the project). However, in the recent EU review of the project, recommendation 1.1 stated:

Recommendation 1.1. Resubmit D6.1 "EoCoE web platform". The document is not discussing the concept and approach to address the different EoCoE target groups, the approach to make the potential users aware about the offered services or trainings and is a very short overview on the procedures and approaches taken. While the web page is following a nice design the lack of concept how to address the users and gain awareness about the offered services is confirmed with the implemented web page that is given too much attention on the project structure and members and not enough on the services offered. Update the web page to be targeted around the services and document the concept and approach for the different target groups in an updated version of D6.1

In an effort to improve on this situation, the partners agreed at the Poznan meeting that CyI would conduct a survey of Work Package Leaders, as well as potential end-users, in order to better define which services EoCoE can provide, and what demand exists for those services. These results are presented in a separate report.

### Location of the Services Page

Currently, a visitor to the EoCoE site can only find out about the services through clicking on the "Transversal Basis" icon and from there scrolling to the bottom of the page, where they can see a static bullet list:

## **Tools and services for HPC**

The cooperative actions within the transversal basis focus on performance evaluation, continuous code integration, benchmarking, post-processing, visualisation, and handling of big data. An overview of the resulting actions is given in the list below:



- Performance analysis;
- Systematic benchmarking of coupled Multiphysics codes;
- Development of automatic integration and benchmarking tools;
- Visualization of:
  - large ensembles of simulations, and derived products;
  - parallelisation degree of concentrated solar power model;
  - solar nowcasting results;
  - o large data sets containing atomic configurations;
  - the electronic and solvent 3D densities for large molecular systems;
  - o time series of subsurface geothermal reservoir behaviour.
- Development of high order finite element reader in HDF5-Pixie format for Visit and Paraview;
- Data mining tool;
- Development of novel approaches regarding diagnostics for extreme weather events;
- Concept for solutions to handle the BigData output for high resolution, time dependent 3D geothermal reservoir behaviour.

This provides no advice as to how to get in touch with service providers nor what these services entail.

It is recommended to add a "Services" tag at the top of the front page, not only in the navigation links at the bottom.



# **Transversal Basis**

Instead of simple text as in the picture above, we could have a "button" looking something like this:





## **Content of the Services Page**

### 1. List of Services

When the visitor clicks on the Service tag, they should be able to address a page which is a one-stop shop

for accessing services or requesting new services.

As such, one should start by having a list of potential services:

#### There should be an introductory text, such as:

EoCoE offers an ever-expanding range of HPC services to end-users involved in Sustainable Energies from Academia, Industry and the Public Sector. Whether you want to simulate a wind farm to optimize its production, predict the wind behaviour over complex terrain, use our high-end numerical tools to determine the properties of new materials for PV, batteries or super capacitors, monitor and improve the performance of your code using the unique methodology we have developed or much more... EoCoE experts will support you through all the phases of your project.

Examples of our services are described below, but you can always complete the form at the end of this page should you not find the exact service you are looking for, remembering to enter the reference number of the service closest to your need from the table below, so we can put you in touch with the relevant EoCoE expert.



SERVICE CATEGORY	DESCRIPTION	SECTOR	Service delivery approach
Optimisation of codes/applications : code refactoring for performance	Multi scale modelling of organic solar cells, perovskite solar cells and batteries	Materials for Energy	<ul> <li>Virtual support (e.g. sending codes and receiving the performance analysis) electronically</li> <li>Live virtual support (work simultaneously with the service provider in a virtual workspace)</li> <li>Face-to-face workshops/trainings</li> <li>Online tutorials/MOOCS/on-demand courses, On-demand courses or resources which end-users can download in their own time</li> </ul>
Optimisation of codes/applications : software package/technolog y integration	<ol> <li>Support to develop new numerical models to design new and improved materials for energy applications.</li> <li>Support in using optimized software package to manage grand challenge simulations.</li> <li>Support to compute physical and chemical quantities of interest in the energy field.</li> </ol>	Materials for Energy	<ul> <li>Face-to-face workshops/training</li> <li>Mentoring/consultancy: despatch support staff to end user for a short time</li> <li>Secondment: end-user embed their staff in one of the service providers for hands- on learning</li> </ul>
Access to computational modules and application codes from open libraries	Open libraries for electronic structure software such as:         - Low-level       libraries         (input/output, memory allocations, scheduler, signal,)         - Computing       the eigenstates and values for large matrices Poisson solvers	Materials for Energy	Access to open libraries
Optimisation of codes/applications : code refactoring for performance	Optimising molecular dynamics and kinetic Monte Carlo codes	Materials for Energy	<ul> <li>Virtual support (e.g. sending codes and receiving the performance analysis) electronically</li> <li>On-demand courses or resources which end-users can download in their owr time</li> </ul>

Access to computational modules and application codes from open libraries	CFD Wind flow modelling for wind farm assessment	Meteorology for Energy	Secondment: end-user embed their staff in one of the service providers for hands-on learning
Finished products	Large weather ensembles for predicting large-error events in the weather/ wind/PV power forecast.	Meteorology for Energy	Not an HPC service <i>per se</i> but the results are of interest to grid operators.
Performance Analysis of codes/applications	A range of performance analysis services provided for the Meteorology for Energy Community	Meteorology for Energy	<ul> <li>Virtual support (e.g. sending codes and receiving the performance analysis) electronically</li> <li>Live virtual support (work simultaneously with the service provider in a virtual workspace)</li> <li>Face-to-face workshops/trainings</li> <li>Online tutorials/MOOCS/on-demand courses</li> <li>Mentoring/consultancy: despatch support staff to end user for a short time</li> </ul>
Performance Analysis of Codes/Application s	Code audit - initial performance profiling	Water for Energy	<ul> <li>Virtual support (e.g. sending codes and receiving the performance analysis) electronically</li> <li>Live virtual support (work simultaneously with the service provider in a virtual workspace)</li> <li>Face-to-face workshops/trainings</li> </ul>
Optimisation of codes/applications : code refactoring for performance	Incorporation of solver libraries which run on heterogeneous architecture to improve run times	Water <u>f</u> or Energy	<ul> <li>Virtual support (e.g. sending codes and receiving the performance analysis) electronically</li> <li>Live virtual support (work simultaneously with the service provider in a virtual workspace)</li> <li>Face-to-face workshops/trainings</li> </ul>
Performance Analysis of Codes/Application s	Automated performance metrics extraction scripts	Water for Energy	<ul> <li>Virtual support (e.g. sending codes and receiving the performance analysis) electronically</li> <li>Live virtual support (work simultaneously with the service provider in a virtual workspace)</li> <li>Face-to-face workshops/trainings</li> </ul>

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Access to computational modules and application codes from open libraries	Software that provides flux-surface aligned mesh-grids in the poloidal plane. Input data: magnetic equilibrium + code requirements. Output = mesh that fills the needs of different simulation codes (on the basis of the codes which are members of the EoCoE project)	Fusion	Secondment: end-user embed their staff in one of the service providers for hands- on learning
Optimisation of codes/applications : software package/technolog y integration	Optimized techniques to couple fluid-like and kinetic/particle codes/descriptions - Metric for multi-code complexity (analysis) Metric for measuring convergence in hybrid FD/stochastic algorithms	Fusion for Energy	<ul> <li>On-demand courses or resources which end-users can download in their own time (upcoming)</li> </ul>
Performance Analysis of Codes/Application s	Provide a report with a list of standard and dedicated performance metrics with their interpretations. An optimisation roadmap is given when possible.	Transversal Basis	<ul> <li>Live virtual support (work simultaneously with the service provider in a virtual workspace)</li> <li>Face-to-face workshops/trainings</li> </ul>
Optimisation of codes/applications : code refactoring for performance	Activity that starts with a version of a scientific application and delivers a more performant version of the application. This work is performed in collaboration with the application developers	Transversal basis	<ul> <li>Live virtual support (work simultaneously with the service provider in a virtual workspace)</li> <li>Face-to-face workshops/trainings</li> <li>Principally remote work with periodic meetings</li> </ul>
Optimisation of codes/applications : software package/technolog y integration	Integration of IO or linear algebra software package in a scientific application	Transversal basis	<ul> <li>Virtual support (e.g. sending codes and receiving the performance analysis) electronically</li> </ul>



### 2. Service request form

The page should also contain a service request form, where visitors, having read the table of services above can complete the following fields (\* = compulsory fields):

- 1. Name of the requestor\*
- 2. E-Mail address\*
- 3. Institution\*
- 4. Energy sector\*
- 5. Type of institution\* [drop-down of government, SME, industry, academic, or "other"]
- 6. I would like to request more information on the following type of service [drop down menu based on the services described in the table above?]
- 7. I would like to request a service not listed in the table [Here, the user must be given a field to describe the type of service they are looking for]

This short form must be sent to a centralised e-mail account (i.e. a new mailing list which for the moment goes to the inbox of George Kirkos and Nathalie Girard) – so that the information can be centralised. The recipient of the e-mail will then judge which work package to approach, and will filter irrelevant requests. We should also have at the backend a database that stores the data from these request, for statistical purposes.

#### 3. Information on upcoming courses/events/workshops

Here, we just need a hyperlink and short text driving them to the events page.

#### 4. Access to open Libraries

On this page, we should also list and provide hyperlinks to all existing EoCoE open libraries.

#### 5. Virtual classroom

Probably the educational materials deserve a separate page of their own. Here we can simply have a hyperlink to that page.

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