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Energy Oriented Center of Excellence:
toward exascale for energy

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D7.6
Sustainability plan

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Index

Executive Summary

This document is a result of the project-spanning reflection on EoCoE's sustainability. It details the original plans that were devised during the first phase of the EoCoE project (2015-2018),

The risks are presented in the order they were mentioned on the Participant Portal in the "Critical Risks for Implementation" tag, using their full name. To help the reader, the risk mitigation measures stated in the proposal are recalled, as well as the linked work packages and the initial severity assessment. In addition, we related each risk with the impacts which it might affect.

The goal of this deliverable is to analyse the different risks and the extent to which they actually materialized, as well as the impact they had on the project.

Beyond the risks that were initially determined, the EoCoE-II project was hit by an unexpected, unforeseeable situation, as the research team has been affected by the 2020 Covid-19 pandemic and the subsequent, European-wide lockdown. We strived to precisely determine the impact of this lockdown through means that are detailed in the "Risk 7" section of this deliverable.

Drafting the EoCoE development roadmap: This includes: the refinement of services' areas of applications, the identification of the needs of the identified markets and the improvements to be made to the offered services and the business model; the barriers and how to overcome them; prepare the sustainable structure of the EoCoE-II, in close collaboration with EERA.

• Preparing the financial projections: investment needed for covering the costs, funding strategies, co-funding opportunities through different stakeholders identified through the networking activities (WP6); including internal sources, public support through EU, national programmes etc., complementary or parallel projects.

Previously considered scenarios

A. Business plan

1. *EoCoE Services.*

A sustainability model had been devised during the first phase of EoCoE; its ambition was to map a strategy based on selling HPC services.

"EoCoE offers an ever-expanding NETWORK of HPC experts in High Performance Computing and inSustainable Energies from Academia, Industry and the Public Sector. Whether you want to

- *simulate a wind power plant to optimize its production,*
- *predict the wind directions and speed over complex terrain,*
- *use our high-end numerical tools to determine the properties of new materials for photovoltaicpower panels, or for batteries and supercapacitors,*
- *monitor and improve the performance of your code using the unique methodology we havedeveloped*
- *and much more...*

EoCoE experts will support you to exploit HPC resources in all the phases of your project!"

2. *Services Evaluation.*

Code auditing and performance assessment:

- Code optimization, adaptation to new hardware architectures
- Automated performance metric extraction scripts. Seamless monitoring of code performanceduring development.
- Special-purpose algorithms: eigenstate computation for large matrices, Poisson solvers, domain decomposition[gh1] ,…
- Runtime systems
- Code refactoring
- Software package/technology integration (I/O, linear algebra,…)
- Porting codes on new HPC architectures

Tools:

- CFD air-flow modelling for wind farm assessments
- Large weather ensembles for predicting extreme events in the weather/wind/PV power forecast
- Short-term forecasting to predict power output of wind/solar plants
- Multi-scale simulation methods (molecular dynamics, kinetic Monte Carlo, quantum MonteCarlo, …) for materials modelling (solar cells, batteries, super-capacitors…)
- Geothermal and heat reservoir modelling
- Predictive hydropower capacity modelling
- State-of-the-art linear algebra methods
- Advanced programming methods for Exascale
- Visualisation

Consultancy and training:

- Training in HPC (parallel programming, new architectures, new programming paradigm,…)
- Provision of expertise to determine if simulation is relevant to improve an industrial process /business
- Assessment of the best numerical tools to tackle energy related problems (within or outsideEoCoE)
- Showcasing the state-of-the-art simulation techniques in energy related application fields.

The following table presents the prices we will apply for these services according to the time requested by every service (this estimation is a standard example. Each client request is unique and needs specifics analysis and evaluation) and the corresponding Person Month costs.

Services	PM	Time (month)	PM costs (k€)	Total cost (k€)
Code auditing and performance assessment:				
Code auditing and performance assessment thanks to an automated procedure => PM: 1; Time: 1 month; PM cost / Total cost: 5k€-10€;	1	1	5 - 10	5 - 10
Application support / performance improvement => PM: 6 to 48; Time: 6 to 24 months; PM costs: 5k€–10k€; total cost: 60k€-480k€	12 - 48	6 - 24	5 - 10	60 - 480
Tools:				
CFD air-flow modelling for wind farm assessments	Evaluation for each service by the experts. The cost of expertise will be around 1k€/day for short term mission and 5 to 10k€/month for long term mission depending on the level of expertise.			
Large weather ensembles for predicting extreme events in the weather/wind/PV power forecast				
Short-term forecasting to predict power output of wind/solar plants				
Multi-scale simulation methods (molecular dynamics, kinetic Monte Carlo, quantum Monte Carlo, …) for materials modelling (solar cells, batteries, super-capacitors,…)				
Geothermal and heat reservoir modelling				
Predictive hydropower capacity modelling				
State-of-the-art linear algebra methods				
Advanced programming methods for Exascale				
Vizualisation (Videos)				
Sofware as a service	CPU hours + software tools: 1€ / node.hour for CPU + 2€ / node.hour for software.			
Consultancy and training:				
Training in HPC (parallel programming, new architectures, new programming paradigm…): PM: 1; Time: 1 (training design) + 2x0,25 (per session) = 1,5; PM - Total cost: 15k€ per session.	1	1,5	10	15k€
Provision of expertise to determine if simulation is relevant to improve an industrial process / business and determine the numerical tools: Time: 2 days; Cost: 1k€ / day	2 days		2k€	2k€

Based on the previous services costs evaluation, it is possible to estimate the potential income in various scenarios. The lower estimate would correspond to the beginning of the service offer and the high estimate to an optimistic view of what could be achieved after a few years.

Services	Total cost (k€)	Number of projects / revenue in k€ Low estimate	medium estimate	high estimate
Code auditing and performance assessment:				
Code auditing and performance assessment thanks to an automated procedure => PM: 1; Time: 1 month; PM cost / Total cost: 5k€-10€;	5 - 10	1 / 7k€	5 / 35k€	10 / 70k€
Application support / performance improvement => PM: 6 to 48; Time: 6 to 24 months; PM costs: 5k€–10k€; total cost: 60k€-480k€	60 - 480	0 / 0k€	1 / 100k€	3 / 300k€
Tools:				
CFD air-flow modelling for wind farm assessments	1k€ / days 5k€-10k€ / month	3 days / 3k€	10 days / 10k€	2 month / 15k€
Large weather ensembles for predicting extreme events in the weather/wind/PV power forecast				
Short-term forecasting to predict power output of wind/solar plants				
Multi-scale simulation methods (molecular dynamics, kinetic Monte Carlo, quantum Monte Carlo, …) for materials modelling (solar cells, batteries, super-capacitors,…)				
Geothermal and heat reservoir modelling				
Predictive hydropower capacity modelling				
State-of-the-art linear algebra methods				
Advanced programming methods for Exascale				
Vizualisation (Videos)				
Sofware as a service	3€ / hour	50 hours / 0k€	1000 / 3k€	10 000 / 30k€
Consultancy and training:				
Training in HPC (parallel programming, new architectures, new programming paradigm…): PM: 1; Time: 1 (training design) + 2x0,25 (per session) = 1,5; PM - Total cost: 15k€ per session.	15k€	1 / 15k€	3 / 45k€	6 / 90k€
Provision of expertise to determine if simulation is relevant to improve an industrial process / business and determine the numerical tools: Time: 2 days; Cost: 1k€ / day	2k€	1 / 2k€	5 / 10k€	10 / 20k€
Total income		27k€	203k€	525 k€

In the above table, the actual *cost* of the service has not been deducted from the income, which means that the amount left for actually running and developing the CoE will be significantly smaller. In any case we believe that relying on such estimates is rather hazardous and as detailed in the next section, analysis of already running projects shows that developing such a service offer is rather difficult

A. EoCoE I / CoE original vision and perspectives.

The services offer presented above is a classical approach to transfer directly the research carried out by the EoCoE teams to the industry. It relies on the fact that many industries/SMEs have activities in area very closely related to the research done in EoCoE and should therefore be interested in the expertise that EoCoE can provide.

However, doing benchmarking on similar actions carried out at national or European levels, we have realized that this approach is in fact rather difficult and sometime not as efficient as one might expect. First of all, the dissemination of HPC to industries/SMEs is an objective shared by many projects bothat the European and national levels. Many of these projects offer full support,

scientific expertise and CPU time on large systems, for a much reduced cost (if any at all). The "free" offer in the field of HPC for industries/SMEs is therefore numerous and diverse, from small to very ambitious projects, training, consultancy. The most visible projects proposing this offer are: Fortissimo (1 and 2), PRACE/SHAPE, PRACE/PATC, POP, Simseo (France), Fraunhofer Alliance for Numerical Simulation (Germany), andequivalent programmes in several other EU states. Even for these projects/programs which are "free" and sometimes fully dedicated to SMEs/Industry, engaging with industry has proven to be a rather difficult and lengthy process. For example, there are only about 10% of industrial participants at the PRACE/PATC trainings even though some PATCs have designed training session specifically dedicated for SMEs. The PRACE/SHAPE project was also designed to "*help European SMEs overcome barriers to using HPC, such as cost of operation, lack of knowledge and lack of resources".* This project has been running for 9 years, has a significant budget (~75PM/year in the current PRACE project), benefits from the dedicated and experienced PRACE dissemination team and from the support from allmajor European computing centers. Nevertheless, over these 9 years, a very limited number of SMEs/industries have been participating.

Promoting the usage of simulation tools within the industry, and particularly for SMEs, is certainly an objective of primary importance. From the feedback of the above mentioned projects, and of many others, the following points can be noted:

- Engaging with SMEs on a simulation/HPC project is a very difficult task, with which evenspecially dedicated projects have had only modest success rates so far.
- The services offer in this domain is rather large and mostly free, but it does however not seemto easily attract SMEs/Industries.
- Achieving a significant amount of self-sustainability for the CoEs in the actual context basedon this classical service offer does not seem to be a realistic objective.

Based on these experiences, we will try to propose new means to develop relationships with SMEs/industries. Services should probably be more focused and take advantage of the potential high added value of the research activities carried out in the network. A proper balance will have to be established between very specific research activities where EoCoE would provide unique added valueand a more generic approach in order to keep a reasonably large potential customer basis. In order to be more attractive and show concrete example of simulation tools, the EoCoE consortium decided to develop a Software as a Service (SaaS) platform (see below for more details).

EoCoE II sustainability strategy

B. Training HPC researchers and experts to maximize results exploitation.

To enforce the plan above, the EoCoE II consortium planned actions aimed at enlarging the network of experts in EoCoE-II with users and future collaborators from academia, industry and SMEs, building on existing collaborations links.

What the EoCoE consortium learned during EoCoE-I project is that the advertisement of EoCoE's services to stakeholders is not only a matter of what the services of EoCoE really are but also how they are offered and how they are presented to stakeholders. Without any doubt, EoCoE's services are recognized by the scientific and technological communities as services of very high quality and matching state-of-the-art in know-how and applications. Moreover, the services of EoCoE are able to provide unique support to implement exascale strategies in the energy field and address successfully the open technological problems that are holding back the quick energy transition to low-carbon economy. The lesson learned in EoCoE-I was that a different language and attitude is needed to bring EoCoE participants to offer their scientific and technological services. Thus, it was agreed in the consortium that a professional external support is needed to present EoCoE services to stakeholders.

To this end, a company, META Group, was selected, and a contract with META Group was concluded. META Group's role was to help the consortium, with a two-fold approach:

- Raise the average level of knowledge of the EoCoE participants regarding exploitation strategies,

- Select three key exploitable results, and target them for professional actions.

META Group has provided presentations to the EoCoE community about exploitable results and helped EoCoE with the selection of the aforementioned three exploitable results. The activity spanned both half of the project, with dissemination and communication activities designed accordingly. It also impacted WP7 activities in what regards to services' design and planning and associated exploitation plans.

The support provided by META through ENEA was an opportunity for all the partners of EoCoE II to discuss the use of project results and their exploitation routes, therefore contributing to maximize the impact of EoCoE II. The selected outcomes of the research work were considered to be Key

Exploitable Results (KERs). KERs were results identified by the partners as the ones with a commercial and/or societal significance. They were discussed from an exploitation point of view, the approach being to determine what will be used after the end of EoCoE II to generate and maximize impact.

Being involved in exploiting EoCoE II results is not only commercializing the novel solutions/services but it is also, in some cases, making sure that they are used and increase their TRL by addressing additional competitive funding programmes in an effective way.

The approach used was the market/customer demand or societal needs/user point of view.

The Exploitation support provided the relevant EoCoE teams with the opportunity to work on:

 The most important elements for exploitation and dissemination;

 The unique value proposition and the use model;

 An implementation roadmap for the activities to be performed after the project end (steps, timing, responsibilities, milestones, financial needs and sources);

 A targeted communication strategy centered on a short presentation of the KER and its exploitation (pitch).

The following KERs have been identified by the partnership in order to represent the some of the main categories of results envisaged by EoCoE II:

No.	Name of the KER
1	Software Library for solving linear equations
2	High Fidelity Simulator for wind energy applications (farms and turbines)
3	EoCoE Software as a Service Portal

A detailed description of what this collaboration with META Group entailed can be found in D6.3, “Assessment report on dissemination, communication and networking”.

The objectives initially considered when this collaboration was set up were indeed reached, as the EoCoE consortium received a specialized training, through which they were exposed to novel concepts and ideas on how to maximize the exploitation of their scientific outputs. The pitch sessions were oriented towards presenting the EoCoE results to industrial stakeholders, and we can

safely assess that the EoCoE partners came out of these exchanges better prepared to disseminate their results outside of the scientific community.

C. The EoCoE Software as a Service Portal

Amongst the conclusion to the initial EoCoE sustainability plan was the need for a tool that would allow the consortium to promote the flagship codes of the project, demonstrating their capabilities and potential, and ultimately attracting new users. To this end, the EoCoE team set up a Software as a Service (SaaS) platform, available at https://eocoe.psnc.pl/.

This platform offers access to software developed by EoCoE partners and from its third parties, in a very targeted and simple way. The portal focuses on simple and clear use cases, with a limited number of parameters, so that the potential users of EoCoE can run example jobs with limited resources. This web portal has been largely advertised, especially through the project's partnerships with EERA and other large networks.

There were several aims for the platform:

 Show the potential of EoCoE simulation tools via concrete examples

 Attract engineers from SMEs/industries to easily test EoCoE services and check its potential

 Create an efficient dissemination channel targeted to the interested end-users

 Present the EoCoE service portfolio with use cases that can eventually provide the opportunity to develop more ambitious collaborations between interested users and scientific teams of EoCoE.

Portal functionalities include:

 Registration of users. For security and licencing purposes, all users must be registered and accepted by project representatives.

 Example of simulation definition that will show the basic functionality of the software and its usability.

 Definition of parameters for custom simulations. The set of available parameters can be limited to the most important ones.

 Submission and monitoring of test jobs

 Transfers of input data and output results.

The portal has not been developed from scratch, but uses a solution developed by EoCoE partner PSNC for their routine HPC services. It is installed in on PSNC's computing centers, where a limited number of resources are dedicated to run computational jobs submitted via this SaaS portal. It is notable that PSNC has agreed to maintain the Portal beyond the lifespan of EoCoE II, so this tool will remain in place and keep playing its part in the general framework of EoCoE's sustainability.

D. The EoCoE / EERA collaboration

Relying on trained researchers and intuitive demonstrators is a good basis for a sustainable endeavor, but a more effective approach to the problem of putting in place a program capable of having a significant impact on industrial users and, more generally, on communities that are external to the ones directly involved in the project, is to rely on one or more intermediate bodies. These should act as a vehicle for promotion and dissemination on information and opportunities that EoCoE can offer.

There is of course, both at national and international levels, a vast number of agencies, industrial associations, technology transfer organizations that could be contacted to discuss prospective opportunities of collaboration. Among these, the European Energy Research Alliance is of particular importance both for its characteristics and for its mode of operation.

EERA is an international non-for-profit Association incorporated in the Belgian law. The purpose of the Association is to strengthen and to expand Europe's capabilities in sustainable energy research by connecting and joining European energy research activities. It has the aim to optimize the research efforts and to overcome fragmentation in the European countries through a number of actions of coordination of different public research programs at regional, member state and European levels. The Association works in the context of the Strategic Energy Technology (SET) Plan.

EERA was founded in 2008 and currently involves over 200 European public research centers & universities from 24 EU member states plus Turkey, Norway and Switzerland. It involves over 50.000 researchers that participate in almost all the energy projects funded by the European Framework Programmes involved. It collaborates with European industry through platforms and partnerships.

EERA is organized around 18 Joint Programs (JP), created by interested organizations that define a joint research agenda. The EERA JPs coordinate research performed by the participating institutions based on their own resources, but can also obtain supplementary funding from national or EU sources.

Preliminary contacts have been carried out with EERA in 2018 and 2019, and several alternative possibilities of collaboration were discussed, in particular:

1. Set up of a new HPC Joint Program within EERA;

2. Set up of a HPC sub-program within one of the existing JPs;

3. Set up of an HPC coordination body across various existing JPs.

For different reasons, options 2 and 3 did not seem to be adequate or easy to organize, and therefore the preferred scheme was determined to be the creation of a specific JP dedicated to HPC, that can then communicate with the other JPs and identify/carry out common activities of promotion, dissemination and partnering in projects and collaborations.

The creation of a new JP was fostered by existing EERA partners. ENEA, as a member of EoCoE and a founding partner of EERA, was willing to participate in this action. Full participants in a JP must be EERA partners, have responsibilities and voting rights, and organize activities such as meetings and workshops. Associate participants can take part actively in the daily life of the JP, but do not have positions in its steering bodies.

As a result to the direct involvement of EoCoE and its partners in EERA, the Digitalization for Energy JP was launched at the end of 2020. It was conceived as a transversal (tJP) structure, constituting a new concept that could be later addressed by new initiatives, if the opportunity arises. The transversal Joint Programme Digitalization for Energy (tJP DfE) aims at defining key priorities for this field that will derive in research activities, as well as act as a contact point with major European initiatives on supercomputing, big data, artificial intelligence, open science, etc. It will also tackle the European Digital Strategy, which is strongly pushing these IT services.

The tJP DfE has a modular structure, i.e. profiting from ongoing EERA initiatives by keeping and integrating their structure as Subprogrammes (SPs) into the new tJP while also kicking-off specific SPs to the transversal Joint Programme focused on digital activities in a transparent and agnostic way. By doing so, in the future it will be straightforward to integrate new SPs and initiatives coming from either vertical JPs as they evolve in time, or coming from the tJP itself.

The transversal Joint Programme Digitalisation for Energy has organised its work in 2 sub-programmes (SP) and 4 transversal sub-programmes (tSP):

SP1: High Performance Computing (HPC)

SP2: Data Science & Artificial Intelligence

ESI tSP: Technology

AMPEA tSP: Multiscale modelling of materials, processes and devices

Hydropower tSP: Digitalisation

Nuclear Material tSP: Physical modelling, materials health monitoring and non-destructive microstructure examination for nuclear materials

This Joint Programme is both a major achievement for EoCoE, and a keystone to the project's long-term strategy, as it will facilitate contacts with prospective industrial companies and public organizations interested in the CoE's services and skills. It can convey information to selected partners, already well established in the field of energy R&D, capable of working in an international scientific environment, and potentially interested in the high-end services offered by EoCoE. Finally, it paves the way for future partnerships between the EoCoE consortium and EERA itself.

Conclusion

The long-term goal of EoCoE is to establish and maintain a sustainable network of experts both from the energy and the HPC fields, working closely together. This network should embrace the exascale challenge for the benefit of the energy transition and also foster the uptake of HPC within the energy ecosystem including SMEs and industries.

While the EoCoE project made sure it provided the training, tools, and collaborative framework to maximize its partners' exploitation of scientific results, the team's experience in various individual European countries and on the wider European scale led us to the conclusion that it seems rather unlikely that a pan-European structure of the size of the EoCoE consortium can be sustainable based on providing services to industry and SMEs. The EoCoE consortium will obviously have an impact on the energy sector, but this impact is a consequence of sustainability rather than an ability to source most of its funding there.

Building a sustainable structure within EERA, as was achieved with the launch of the Joint Programme on Digitalization for Energy, is the best option to maintain and develop the consortium and its impact. Public funding, from regional, national and European sources will remain a necessity to achieve the goal of EoCoE, especially regarding exascale computing.

This conclusion leads us to the issue detailed in D7.4 "Risk Assessment", which is to say that the EoCoE consortium applied to the EuroHPC call for "CENTRES OF EXCELLENCE FOR HPC APPLICATIONS (HORIZON-EUROHPC-JU-2021-COE-01)" in 2022, but was unsuccessful. This result is disappointing in itself, but it also means that EoCoE's sustainability will be put to the test in the short term, as public funding is about to dry up and the team will lose its non-permanent members, as well as a dedicated budget to set up the meetings, workshops, and collaborative sessions that were key to the project's dynamics. Nevertheless, the consortium is confident that the collaborations started and developed within the EoCoE framework, the high quality of the scientific results stemming from the project, as well as its integration within the European HPC and energy ecosystem, mean that the links built during EoCoE 1 and 2 are solid enough to withstand a period of time where the financial resources allocated to the project are not what they used to be.