H2020-INFRAEDI-2018-2020

Concerted action for the European HPC CoEs

Project Number: 823964

D3.1– Report on the sectorial approach priorities

WP3 – CoE-Industry Interaction

Focus CoE has received funding from the European Union's Horizon 2020 research and innovation programme under the grant agreement Nº 823964

Workpackage:	WP3	CoE-Industry Interaction
Due Date	31.5.2019	
Author(s):	Marta Chinnici Andrea Quintiliani	ENEA
	Monica De Mier Torrecilla Maike Gilliot Jean-Francois Lavignon Hugh Martin Bastian Koller Michael Gienger	BSC Teratec Teratec UCL HLRS HLRS
Authorized by	Marta Chinnici	ENEA
Reviewer	Guy Lonsdale	Scapos
Reviewer	Lena Buhler	HLRS
Reviewer	Lilit Axner	KTH
Final Version Date	30-11-2020	
Dissemination Level	Public	

Executive Summary

This deliverable reports on activities performed in the period December 2018 to May 2019 and the bulk of the text provides analyses and planning as included in the version of the deliverable completed in May 2019.

The updated version of the deliverable completed in November 2020 provides additional or replacement material – which is clearly highlighted as such – that in part reflects changes to CoE interactions and cooperative procedures developed subsequent to the completion of the May 2019 version of the document.

This first deliverable of WP3 outlines the proposal of the FocusCoE project in the set-up of a work model to support the Centres of Excellence (CoEs) in the promotion of their offers and interactions with industry.

The approach is based, first of all, on the analysis of the offerings, in terms of services, competences and application domains, provided by the CoEs. This analysis was carried out in the first six months of the FocusCoE project (December 2018 - May 2019). The information used in this analysis was collected from published documents, websites, knowledge of FocusCoE partners who are also partners in some CoEs, direct interaction with CoE representatives.

The general approach in the analysis was to identify "commonalities" of the CoEs across different parameters, in order to put together and favour joint efforts and actions that can be of interest to several CoEs. To this end, common areas were identified in terms of industrial sectors/application areas, technical domains, computing techniques, application codes, services offered by the CoEs.

This analysis provides a "compass" to identify a promising set of events in which the CoEs' technological offer and, more generally, the HPC approach can be marketed and promoted.

This compass is used in a general strategy that aims at:

A. Leveraging existing contacts with industrial companies;
B. Creating contacts with new companies not yet strongly connected to the HPC ecosystem.

For the first axis, the idea is to leverage the portfolio of contacts with large companies and SMEs already developed by WP3 partners' past actions, the CoEs activities and in national and European projects, (e.g. PRACE SHAPE action; Fortissimo projects; Teratec SiMSEO project), without interfering with contacts and activities already under way.

For the second axis, the objective is the set-up of fruitful contacts with companies that could potentially benefit from the expertise of CoEs, through the participation in sectorial events. The selection of the most suitable events is of course crucial, and several alternatives will be assessed in the coming months in collaboration with the CoEs, with a particular regard to relevant events in the EU-13 countries[1]. Special attention will be given to contacts with

[1] Group of 13 EU countries: Bulgaria (BG), Croatia (HR), Cyprus (CY), Czech Republic (CZ), Estonia (EE), Hungary (HU), Latvia (LV), Lithuania (LT), Malta (MT), Poland (PL), Romania (RO), Slovakia (SK) and Slovenia (SI).

external organisations (such as Industrial associations) to evaluate industry-oriented events (such as Open days, brokerage events, etc.).

In the first phase (Oct.2019-July 2020) a set of around 5 events will be selected. Further events will be selected for the second phase (Sept. 2020 – Sept. 2021), after a thorough evaluation of the results of the first phase.

The aforementioned activities require a structured dialogue between the CoEs and WP3 to be established for the whole duration of the project. This will be organised through different channels. In the first instance, the European HPC CoE General Assembly is the body where the interaction among CoEs and FocusCoE takes place, and in which a general framework of the collaboration is put in place. Secondly, direct interaction of WP3 and CoEs will take place through periodic teleconferences dedicated to specific topics. More informal discussions may make use of the collaboration platform Slack, set up in WP5.

The actions described need to be monitored and evaluated, also in order to correct the course of action and maximise the results. The following tools were selected:

- Regular teleconferences of WP3 partners, for status reports and planning of actions;
- A selection of Key Performance Indicators (KPI), assessing data on industrial contacts and on events attended;
- Preparation of reporting materials on Success Stories, to be disseminated at events, conferences, and published on the web;
- Identification of Best Practices as a measure of the success of CoE's interaction with industry.

The criteria, activities, and evaluation mechanisms presented set the scene to perform an initial set of actions within WP3 in the first part of the project's lifetime. The evaluation of its results will allow us to potentially introduce corrections and changes in the second half of the project.

Table of Contents

Table of Tables

List of Acronyms and Abbreviations

CoE	Centres of Excellence for Computing Applications
CSA	Coordination and Support Action
D	Deliverable
DoW	Description of Work
EC	European Commission
ECMWF	European Centre for Medium-range Weather Forecasts
EESI	European Exascale Software Initiative
ENES	European Network for Earth System modelling
EPOS	European Plate Observing System
EsD	Extreme scale Demonstrators
EU	European Union
FET	Future and Emerging Technologies
FP7	Framework Programme 7
H2020	Horizon 2020 – The EC Research and Innovation Programme in Europe
HPC	High Performance Computing
ISV	Independent Software Vendor
KPI	Key-Performance Indicator
R&D	Research and Development
R&I	Research and Innovation
SME	Small and Medium Enterprise
SRA	Strategic Research Agenda
TRL	Technology Readiness Level
WG	Working Group
WP	Work Package

1 Introduction

This deliverable reports on activities performed in the period December 2018 to May 2019 and the bulk of the text provides analyses and planning as included in the version of the deliverable completed in May 2019.

The updated version of the deliverable completed in November 2020 provides additional or replacement material – which is clearly highlighted as such – that in part reflects changes to CoE interactions and cooperative procedures developed subsequent to the completion of the May 2019 version of the document.

The changes applied to the document can be summarised as follows:

- *Section 1.3 on the methodological approach*
- *Section 4 our approach for interaction with the CoEs (fully rewritten)*
- *Section 5.1 on Monitoring and KPI with a revised KPI table, that also indicates the target values*

The amendments and changes are clearly marked as such throughout the document.

1.1 Purpose of the document

The European HPC general strategy was put in place by the Commission since 2013, outlined in the ETP4HPC Strategic Research Agenda [1] and made operational through the following calls. It defined the role of the Centres of Excellence (CoE), as key actors that must ensure that applications are prepared for being executed on the future exascale systems, and to make sure that these applications are effectively taken up by industry and other stakeholders to address key challenges and translate the considerable effort put in place into tangible results.

In this framework, FocusCoE was promoted and funded by the European Commission to support CoEs in fulfilling their objective, and notably to put in place concerted outreach and business development actions capable of enhancing the interactions with industry and SMEs, in particular. More specifically, WP3 targets this latter objective and intends to set up actions, which are of interest to more than one CoE, thus bringing added value to the CoEs. These actions are understood as being complementary to the actions performed directly by the individual CoEs. The main principle of the action is to develop a sectorial approach and to present the potential services and products of all CoEs, related to each sector, to industrial stakeholders.

The present document describes the first analyses that were carried out to organise this activity and it outlines the approach and actions that will be put in place in order to achieve the foreseen result.

This document is organised as follows: in Chapter 1, a summary description of the scope and methodology approach is given. Chapter 2 describes the first analysis of the CoEs' offers and the industrial sectors covered by the projects. In Chapter 3 the identification of industrial sectorial events is provided. In Chapter 4 a presentation of the interaction between FocusCoE and CoEs is shown. The last chapter presents a set of parameters for monitoring and measure the level of CoE's success in terms of industrial interaction and also the monitoring activities.

1.2 Scope

FocusCoE interacts with a group of ten consortia that are currently running an extremely diverse set of CoE projects, with the common objective of developing extreme scale HPC technologies and applications and setting up, as much as possible, links and collaborations with industrial stakeholders to effectively carry out the transfer of these scientific results in the European economy.

This means that CoEs, as a whole, address a wide range of industrial sectors, employ the greater part of the most advanced computing codes currently available, and investigate many different cutting-edge technologies (cf. Section 2).

In order to select an appropriate course of action for FocusCoE, it was decided to investigate, which were the common areas among the CoEs, since addressing those areas will maximise the effects of our initiatives.

D3.1 builds on the first analysis of CoEs offerings that was carried out in the first six months of the FocusCoE project.

It shows common CoEs' offerings in terms of services, competences and application domains, also considering the individual CoE' strategies. It looks at the industrial sectors covered by CoEs' offerings, identifying a promising set of events to market them.

Through this analysis, FocusCoE will focus on a set of communication activities that will take the dissemination communication and exploitation plans of each CoE into account.

1.3 Methodological Approach

In November 2020, this section has been amended. The added parts are introduced in blue:

- *First, we provide some more details on the "Sectorial event selection and CoE participation", as well as the planned interaction with the CoEs (detailed in Section 4 of this deliverable).*
- *The added element on "Feedback on needs and expectation form industry" has been part of WP3's activities from the beginning of the project and is addressed by Task 3.3. We introduce this element now more explicitly.*
- *Regarding the Best Practices: upon recommendation, we strengthen this aspect. WP3 will provide insight on Best Practices mainly via Task 3.4, by focussing on the interaction with SMEs in particular.*

It is a great challenge to provide an assessment of sectorial industrial priorities in the field addressed by the ten CoEs, and to draw up the best possible course of action to maximise the effects of actions and resources put in place by FocusCoE. The reason is that the overall proposition of CoEs is extensive and that a wide range of technologies and strategies to reach their objectives is adopted.

FocusCoE adopts a methodological approach based on identifying the common factors (in terms of offers) within the CoEs to pinpoint a set of specific actions that can support the CoEs with their industrial interaction.

The methodological approach consists of the following elements:

- Assessment of the industrial sectors covered by CoEs' offerings: the objective is the identification of common ground and/or relevance, to maximise the impact of interactions

with industry: definition of a program of outreach and promotion of CoE competences and service offerings.

- Sectorial event selection and CoE participation: identification of events focussing on industrial sectors. Preference will be given to those events involving a large number of industrial stakeholders rather than those focussing primarily on research and academia. These sectorial events will be selected jointly with the CoEs. The CoEs will also be involved in defining by which means the CoEs are presented during these events (booth, presentations or talks, for example).
- Direct contact to potential industrial users: Actions towards industry for the promotion of the CoEs' competences and service propositions.
- Interactions with CoEs: definition of a plan to collaborate effectively with CoEs in order to support them. Regular telephone conferences will be set up between the CoEs and the partners of WP3 in order to assure smooth interaction on the WP's activities (cf. Section 4 for more details on this).
- Monitoring and assessment of the process: definition of KPIs and collection and illustration of Success Stories.
- Feedback on needs and expectation form industry: Via a dedicated question (cf. Task 3.3), we will gain insight into the needs and expectations from industry towards the CoE. This can help the CoEs in shaping their service offering accordingly.
- Sharing best practices: Amongst the CoEs, we will identify best practices for the collaboration with industry, and in particular for the collaboration with SMEs. These findings will be shared with all CoEs.

2 Identify the CoEs' competences and service offerings

The goal of the first actions in WP3 is to get an understanding of which are the common domains of CoEs' offerings in terms of technologies, expertise and services, and to evaluate the opportunities for FocusCoE to support the CoEs in their industrial interactions.

This analysis will be useful throughout the lifetime of the FocusCoE WP3 activities: it will be the basis for identifying relevant industrial sectorial events and potential clients for the CoEs.

This first analysis is based on the process of data collection carried out in the context of the CoEs and was presented in the Frankfurt CoE meeting (21th February 2019). It will be refined in a second step with the collaboration of CoEs during the project's lifetime.

This analysis is based on the following data:

- **Information about CoEs**
  Information was provided by the following 10 CoEs:

CoE' Acronym/Name	Website
1) **BioExcel** - Centre of Excellence for Computational Biomolecular	https://bioexcel.eu/
2) **ChEESE** - Centre of Excellence for Exascale in Solid Earth	https://cheese-coe.eu/
3) **CompBioMed** - Centre of Excellence in Computational Biomedicine	https://www.compbiomed.eu/
4) **E-CAM** - European HPC Centre of Excellence	https://www.e-cam2020.eu/
5) **EoCoE-II** - Energy oriented Centre of Excellence	https://www.eocoe.eu/
6) **ESiWACE** - For future exascale climate and weather predictions	https://www.esiwace.eu/
7) **HiDALGO** - HPC and Big Data Technologies for Global Challenges	https://hidalgo-project.eu/
8) **Max** - Material design at eXascale	http://www.max-centre.eu/
9) **POP2** - Performance Optimisation and Productivity 2	https://pop-coe.eu/
10) **EXCELLERAT** - The European Centre of Excellence for Engineering Applications	https://www.excellerat.eu/

- **Collected information about CoEs.**
  Data on CoEs was collected through a three-step process:

  - Within WP3, a template was jointly defined to describe relevant data on CoEs. This template covers all areas, which are relevant for the interaction of the

CoEs with industry. It includes information about their services, their contact points, their key codes, etc.

- From each CoE, participants in WP3 collected data, based on public sources (such as websites, for example), and also in part on DoA extracts provided by some CoEs. This was used to prepare a first version of the description of CoE's activities and offers.
- In a second step, this data was validated by the CoEs themselves, and was also part of the discussion with the CoEs during the meeting in Frankfurt (21st February 2019).

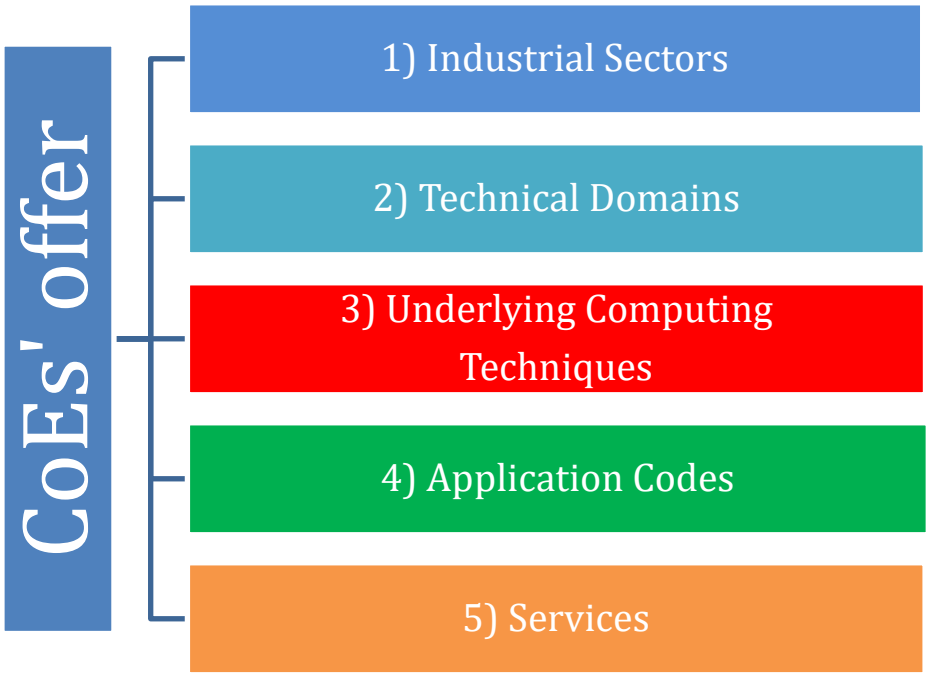
The templates with the descriptions of CoEs are included in Annex 1.

- **Approach used to find common activities, services and industrial sectors.**
  Data collected was analysed in terms of activities, services, sectors, application domains of the CoEs to identify appropriate common parameters useful to select SMEs and large companies that might be interested in, and benefit from, an interaction with CoEs, and appropriate sectorial events.

- **Approach used to assess the industrial sectors covered by CoEs' offer.**
  Through the collected data and information gathered at the Face-to-face meeting with the CoEs (21st February 2019), an assessment was carried out of the industrial sectors covered by the CoEs' competences and activities.

2.1 Analysis of CoEs activities, services, industrial sectors

In this section we provide the first analysis of the CoEs' technologies, application domains and skills. Their offer and their competences can be structured along different dimensions. The goal of this analysis is to identify sectors and domains, which are common to at least two CoEs for guiding our actions and activities in WP3 towards companies for the CoEs, and as such not exhaustive of all domains and all sectors covered by all the CoEs.



The first category differentiates according to the application areas of interest and hence the common industrial sectors. This category is defined taking into account the list of the industrial sectors provided by the European Commission [4]. The details of the analysis are shown in section 2.2 where an exhaustive table presents the common industrial sectors covered by the CoEs' provisions (see Table 5).

The second dimension looks at the common, underlying Technical Domains: Technical Domains, which are common to at least two CoEs.

Common Technical Domains	CoE
Computational Fluid Dynamics	CompBioMed, EoCoE2, EXCELLERAT, HiDALGO, ChEESE, ESiWACE
Molecular Modelling	EoCoE2, E-CAM, CompBioMed, Max, BioExcel
Structural Analysis	CompBioMed, EXCELLERAT, EoCoE2
Multiscale Modelling	CompBioMed, BioExcel, HiDALGO, ESiWACE

Table 1 Analysis of technical domains common to multiple CoEs

The third dimension focuses more on the common underlying Computing Techniques:

Common underlying Computing Techniques	CoE
Urgent computing	ChEESE (tsunami, earthquake), HiDALGO (pollution)
Uncertainty quantification	ChEESE, HiDALGO, CompBioMed, BioExcel, E-CAM, ESiWACE, EXCELLERAT, POP2
Machine learning	HiDALGO, EoCoE2, BioExcel
Performance optimisation	HiDALGO, CompBioMed, BioExcel, E-CAM, EXCELLERAT, POP2
Co-Design	HiDALGO, EXCELLERAT

Table 2 Analysis of underlying Computing Techniques common to multiple CoEs

Since CoEs can be innovative in this category and could represent an added value to the industrial companies working in these domains, this list could also include other potential topics of common interest such as:

- Container technologies
- Code coupling
- Model reduction
- Meshing technologies
- Workflow management

The fourth category includes the common Application Codes

Common Application Codes	CoE
Alya	CompBioMed, EoCoE2, EXCELLERAT
ESIAS	EoCoE2, ESiWACE
QMCPACK Abinitio code	EoCoE2, E-CAM
FEniCS	HiDALGO, EXCELLERAT
Quantum Expresso	MaX, E-CAM
Siesta	MaX, E-CAM
CP2K	MaX, E-CAM

Table 3 Analysis of Application Codes common to multiple CoEs

The last category includes the common services offered by CoEs:

Common Services	CoE
SaaS platform	EoCoE, BioExcel, HiDALGO
Codes Optimisation	POP2, CompBioMed, EoCoE, EXCELLERAT, HiDALGO
AiiDA - platform to enable automated high-throughput screening (workflows, turn-key solutions, curated data, analytics)	MaX, E-CAM

Table 4 Analysis of Services common to multiple CoEs

Following the discussion with the CoEs during the kick-off meeting in Frankfurt, we plan to consider also collaboration with Independent Software Vendors (ISVs). On the one hand the, CoEs may act as consultants to ISV on topics such as code optimization / code scalability; On the other hand, ISVs may become collaboration partners of the CoEs when it comes to code industrialisation, and even act as code providers to potential users.

During the FocusCoE kick-off meeting in Frankfurt, these different categories were discussed with the CoEs. It turns out that the CoEs consider their domain knowledge as the main entry point to start the collaborations with industrial partners. This applies to some extent also to the technical domains.

However, the CoEs pointed out that the other categories discussed (such as shared codes, common technical domains or common underlying computing domains) could be of interest for other actions, such as for the training activities from the CoEs towards industry or for training for the CoEs.

Regarding the activities of WP3 related to the interaction with industry, we will concentrate on the sectorial domains.

2.2 Assessing the industrial sectors covered by the CoEs offerings

In this section, we provide our insights and analysis about the industrial sectors addressed by the CoEs. The objective is to identify industrial sectors that are common to several CoEs in order to focus the project's efforts and maximise its impact.

As mentioned in the previous section, this analysis is based on the industrial sectors taxonomy made by the European Commission (EC) [4] where the authors have selected the most pertinent sectors and added the tertiary industries covered by the CoEs. The list represents the baseline for this analysis; indeed, the authors decided to improve this classification and adapted it to the project needs adding several categories (in red): Public services / Civil protection, Bank / Insurance, Energy industry, HPC system, services and software providers.

Mapping of the Sectors	CoE
Aeronautics industries	EXCELLERAT, ChEESE, ESiWACE2, E-CAM
Automotive industry	EXCELLERAT, MaX, E-CAM
Biotechnology	BioExcel, CompBioMed
Chemicals	MaX, E-CAM
Construction	EXCELLERAT
Cosmetics	MaX, E-CAM
Defence industries	EXCELLERAT
Electrical and electronic engineering industries	EXCELLERAT, MaX, E-CAM
Food and drink industry	EXCELLERAT, MaX, E-CAM
Healthcare industries	BioExcel, CompBioMed, E-CAM
Maritime industries	EXCELLERAT, ChEESE, ESiWACE2
Mechanical engineering	EXCELLERAT, EoCoE2, E-CAM
Medical devices	CompBioMed, Bioexcel
Raw materials, metals, minerals and forest-based industries	EXCELLERAT, ChEESE, EoCoE2
Space	EXCELLERAT, MaX, E-CAM
Textiles, Fashion and creative industries	MaX, E-CAM
Public services / Civil protection	ESiWACE2, HiDALGO, ChEESE
Bank / Insurance	HiDALGO, ChEESE
Energy industry	EoCoE2, EXCELLERAT, MAX, E-CAM
HPC system, services and software providers	POP2

Table 5 Analysis of Industrial Sectors common to multiple CoEs

3 Interaction with Industry

The work package "CoE-Industry interaction" (WP3) aims to disseminate and promote the CoE competence and service provisions to industry. The strategy for this objective is twofold:

A. Leveraging existing contacts with industrial companies;
B. Creating contacts with new companies not yet strongly connected to the HPC ecosystem.

A. The WP3 partners have been selected based on their expertise and collaboration with industrial HPC users. Through their past activities, they have developed industrial contacts with both large companies and SMEs. Moreover, an analysis of projects and initiatives, aiming to connect SMEs to HPC (such as the PRACE SHAPE programme; Fortissimo projects; Teratec SiMSEO project) will also provide contacts with companies that are already interested in using HPC. All this information will be gathered and will be used to create to a list of industrial companies that can easily be contacted through WP3 partners.

   This list may serve as a new source of industrial contacts for CoEs. The CoEs will be able to select the companies that they are interested to work with. With the help of the WP3 partners a "value proposition" for the targeted company will be prepared and then the contact will be established. The neutral intermediary position of the WP3 partners will help to find win-win situations and to avoid creating unwanted solicitations.

   This approach will not interfere with the contacts already in place between the CoEs and some companies. The CoEs will continue their collaborations with these companies without intervention of FocusCoE and they will select only the "targets" that are interesting and new for them. In this way, everyone is able to keep its contacts and new interactions are created only when there is a good chance of success.

B. For the second axis of the strategy, the idea is to select sectorial events where WP3 can develop new contacts interesting for the CoEs.

   Setting up new contacts is not easy and requires having a strong message to attract attention. This is one of the reasons for targeting sectorial events where one would expect to meet companies facing some common challenges that can be addressed by the CoE's activities. This reduction of scope can help to create the correct messages for the sector and to present "value propositions" that will be relevant for the industrial sector. The selection and the preparation of these events needs special care and is discussed in the following sections.

   This approach based on sectorial events was the one identified to create contacts with new companies at the time of writing the FocusCoE proposal. However, since then, several discussions between WP3 partners and with the CoEs have led to the idea of looking also at approaches based on

- Industrial associations
- Local industrial Open Days
- Brokerage events for SMEs
- Enterprise Europe Network platform (https://een.ec.europa.eu/)

These approaches will be investigated further and some small test ("pilots") could be made to assess their efficiency. These new directions will be implemented with respect to:

- the opportunities during the course of the project (i.e. industrial association could be present at sectorial events attended by WP3);
- the resources available to WP3 partners;
- the success of the "pilots" that will be conducted during the first phase of the execution of the project.

3.1 Identify industrial events: criteria

To maximise the success of the sectorial event approach, the selection of relevant events is crucial. As explained before, the objective is to attend events focused on an industrial sector in order to prepare with the relevant CoEs the right messages and "value proposition" that would be adequate to create contacts with new interesting companies.

We plan to target only events relevant for at least two CoEs. The interested CoEs may contribute to the event if willing.

The plan is to have two phases of events selection. This option has been chosen to allow some feedback from the first phase to the second phase. As most of the events are annual events, potentially very successful events could be selected again if continuity will increase the outreach or if evolution in the CoE offering opens new opportunities. The two-phase approach will also allow us to obtain feedback on the best way to organise the presence during the events.

To select the events, WP3 has put in place a process that aims to reach a consensus for this choice. The WP3 will prepare a list of potential events. For each event, several data will be gathered (see below for a description) to assess the relevance of the event. This list and the associated data will be discussed with the CoEs and the other FocusCoE WPs. After receiving the inputs from the CoEs and FocucCoE WPs, the WP3 will make the final choice.

For the first phase, we target events that will be held between October 2019 and mid-2020. For the second phase, the events will happen from September 2020 to September 2021.

The plan is to select around five events for the first phase. More events are expected for phase two, as not all the CoEs will have already developed industry-oriented propositions during the first year of their activity.

For the selection process, WP3 will gather information about the sectorial events to assess their relevance according to the following criteria:

A. Match with CoEs activities
B. Attractiveness of the attendees
C. Effective means to pass the message
D. Adequate timing of the event
E. Cost of the event

For each criterion, a set of relevant information will be gathered:

A. To assess to what extent the event matches with CoE's activities, we will look at:
   - Type of the event (trade fair, brokerage, industrial conference)
   - Targeted sector(s)
   - Targeted audience (research, business development, sales…)
   - Simulation and HPC focus
   - Language

B. To look at the attractiveness of the attendees, we will collect data on:
   - Number of participants
   - Number of exhibitors
   - Ratio industry/academy
   - Presence of relevant ISVs

C. To assess the means of passing on the message, we will check:
   - Booth opportunity, location and space
   - Presentation opportunity
   - Poster opportunity

D. Some timing information will be gathered to make sure the participation can be organised in a timely manner:
   - Date
   - Duration
   - Deadline for booth, poster, speech reservation
   - Time to prepare the event

E. For the financial criteria, the objective is to have enough data to make a budget estimate:
   - With respect to FocusCoE's budget: Costs for the event (booth fee, speaker fee…), as well as cost for corresponding communication material, such as flyers for example.
   - With respect to the budget of the attending CoEs: Travel cost for the CoE's personnel (travel, accommodation, registration fee).

All these data will be used to make the selection of the events, with special attention to relevant events within the EU13 countries. Scoreboards will be prepared to facilitate the comparison. The input from the CoEs will also be collected, and the decision on which event to attend will be taken jointly with the CoEs.

3.2 Communication strategy and support

Attracting industry can be challenging for organisations such as CoEs. CoEs can be viewed by industry as research projects with objectives that are too long term for them. To mitigate this risk, the messages that will be communicated will be prepared with great care. Several complementary dimensions will be followed to tailor a communication that can be successful towards industry:

> **Quantitative results**: whenever possible, quantitative data will be provided to make it easy for industries to assess the benefits. CoEs can propose valuable proposals for industry on topics such as speed-up of an application, scalability of an application, etc.

Quantitative data will also be important for the presentation of use cases or success stories (see below).

Hot topics: Industrial interests are often driven by "hot topics". An example of a current hot topic is the use of Machine Learning to increase the efficiency of HPC simulations (e.g. by reducing the search space, or tuning the simulation parameters, or helping to post-process the results). The experience of CoEs in these hot topics will be highlighted to attract the industries that seek partners to help them to deal with these new subjects.

Ease of access: More emphasis will be put on the CoEs' offerings and services that can be easily and quickly accessed by industrial users. For example, simulation as a service or access to an expert will be highlighted in the communication towards industry. The objective is to develop a first contact that the company can test and then build up on this to propose more complex solutions that the CoEs could have developed.

Connection with the value chain: HPC industrial users rely on a value chain in their usage of HPC. If we can show connections between the CoEs and the industry value chain it will be easier to develop contacts. Examples of connections with the value chain are: work done on codes used by the industry; collaboration with ISVs that are industry providers, work done with HPC cloud providers. Again, emphasis will be put on CoEs' connections with other players that participate in the value chain of industrial HPC users.

Based on examples: industries will better appreciate examples close to their business than general achievements. Thus, communication based on use cases and success stories will be developed for industrial outreach.

Trusted relationship: it is key to establish a professional and trusted contact. Thus, for each proposed service or proposition it is important to identify the name of a point of contact that will handle the development of the collaboration in a timely and professional manner. Before communication of a message towards industry, we will analyse and prepare the process that will be put in place if industries would like to follow-up after the first interaction.

In order to support this communication, we will develop different materials jointly with WP5. Currently we plan for the following industry outreach:

Booths: for sectorial events with an exhibition, we plan to have a booth that will be the means to create contacts with the visitors. The communication material and the design of the booth will be decided jointly with the FocusCoE WP5 and the CoEs that will be interested in the event. The idea is to reuse as much as possible the material developed for the WP5-2 tasks (HPC events communication material) but to keep in mind that we need to convince industries of the values brought by the CoEs.

Flyers: to present how CoEs can address industry issues. We will start from the materials developed by the CoEs and the WP5 and work to extract the good messages that have the potential to attract the attention of industries (see below).

Presentations: where possible, we plan for presentations during the conferences of the sectorial events. We will also use presentations that will be displayed at the booth during an exhibition at the sectorial events.

Posters: upon opportunity, e.g. in the frame of poster sessions, posters can be used during sectorial events to present some achievements or research of the CoEs. They

will be designed to convey messages targeting industry in order to optimise the communication.

By implementing this approach, a successful communication toward industry can be achieved.

4 Interactions with CoEs

In November 2020, this section has been fully rewritten. The updated text follows, marked in blue.

To effectively perform the activities in WP3, a structured dialogue between the CoEs and WP3 for the duration of the project is needed.

This dialogue will take place mainly via regular, joint telephone conferences with the CoEs, organised and moderated by WP3. Analogous to the approach taken by WP2 and WP4, WP3 has identified within each CoE a contact point for "industrial collaboration". Three to four telephone conferences are planned per year, each dedicated to a specific topic, such as:

- Presentation of the "Direct Approach to Industry" (as part of the activities in Task 3.1)
- Sectorial events: presentation of our approach, the selection process we suggest and some first ideas for sectorial events (related to Task 3.2)
- Update on WP3's event strategy in Task 3.2 (in reaction to the crisis caused by the Covid-19 pandemic): discussion on how to overcome the issue and joint definition of webinars relevant to the industrial collaborations of the CoEs.
- Discussion on how to involve partners from industry in the EU13 countries (concerning all tasks in WP3)
- Joint elaboration of a questionnaire towards industry in order to understand their needs and expectations (Task 3.4)
- Feedback to the CoEs on the information gathered via this survey (Task 3.4)
- Contact towards SMEs: discussion of the activities planned (as part of the activities in Task 3.3)

On top of this, WP3 makes use of the HPC CoE Council for discussing WP3 activities with the CoEs, and supports such through invited participation in their meetings and workshops.

5 Follow-up on WP3 activities

The actions described in the previous sections need to be monitored and also the most interesting findings need to be extracted from them. This is why we plan to:

- Monitor the process in order to keep the WP3 actions on track. A list of KPIs will also be defined for quantitative measurement;
- Gather success stories to highlight the achievements;
- Summarise best practices to extract what really works in the interaction between industry and CoEs.

5.1 Monitoring and KPIs

The activities of the work package "CoE-industry interaction" (WP3) are be monitored mainly via the monthly WP3 synchronisation meetings. These meetings are usually held online, with the participation of all WP3 partners. During these meetings, we monitor the work done in each task and plan the actions for the coming months. The overall schedule for the WP3 is also discussed to be sure that the activity will be completed in a timely manner. If

serious issues arise within WP3, this will be escalated to the Project Coordination committee (PCC).

Secondly, a selection of Key Performance Indicators (KPI) has been made to keep track of the results of the WP3. For the time being, the selected KPI will assess the level of success of the WP3 in two domains:

A. Contacts created within WP3 between a CoE and an industrial company;
B. Dissemination of information on CoE propositions to industry.

A third dimension: "feedback from industry toward CoEs" has been envisioned but the decision to select or not a KPI for this dimension has been postponed. The decision will be taken when the precise plan for gathering the point of view of the industry on the CoE activities will be established.

A. For the first dimension, the KPI will simply be the "number of new industrial contacts" created through the activity of WP3. To allow more in-depth analyses, some attributes of each contact will be documented:

    - Company
    - CoE
    - Sector of the company
    - Size of the company (SME or large company)
    - Nature of contact (discussion, cooperation, common project, funding…)

    The first four attributes are straightforward and will allow some statistical analysis on different criteria:

    - What are the sectors with the most CoE-industry interactions?
    - Are there more contacts with SMEs or large companies?
    - How has WP3 helped each CoE?

    The attribute on the nature of contact is qualitative and will be more difficult to analyse. This attribute could evolve during the time-frame of the project and the WP3 partners might no longer be in the loop when the nature of the contact changes (the plan is to be active in establishing the contact but the CoEs and the industry will not have any obligation to keep the WP3 partners informed of the way their relationship evolves). Hence, we are aware of the uncertainty and of the risk regarding the quality of this attribute. Nevertheless, we decided to keep it, as it is important to qualify the degree of "success" of an industrial interaction for a CoE.

    Another way to measure the success of an interaction would have been to quantify the "gain" for the industrial company and for the CoE. Some contacts could lead to contracts from the company to the CoE with eventually funding for products/services or for PhD students. The interaction could also generate "gains" at the level of the company by improving its business (shorter time to market, cost saving, new innovation increasing market share…). The option to collect information on the "gain" of both CoE and companies has been discarded for several reasons. The first is that it is difficult and costly to collect this kind of information. Secondly, often one is obliged to make estimations or guesses and the quality of the data is questionable. Thirdly, most of the time the information is confidential and even if it is communicated it is not allowed to be used.

However, for the description of success stories (see below) this kind of information will be gathered with the agreement of the CoE and of the industrial company.

B. The second dimension is related to the activity of the WP3 that aims to raise the awareness of the industry about the CoE propositions. This will mainly be the presence of FocusCoE at sectorial events. These events will serve to get in touch with new industrial companies that are not yet in contact with the CoEs or the WP3 partners. We hope that through these events we will create new contacts that will be listed in the previous KPI. We also expect that some information about the CoEs and their offerings will be disseminated during these events. We want to keep track of how many people have been in touch even if they did not seek to develop contact with one of the CoEs at this stage. These people will at least be aware of the existence of the CoEs and of what they can offer to their company. In the future, this awareness can lead to contact with CoEs or to participation in events organised by the CoEs.

   The KPI selected to measure this activity is the "number of industrial individuals" that will have received information about the CoEs and their offerings. Here as well some attributes will be collected to allow a more in-depth analysis, such as the name of the company, its size and its sector.

The KPIs selected to measure the activity of WP3 are summarised in the following table, including the targets[2]:

WP3 KPIs		
KPIs	**Attributes**	**Target (in total)**
Number of new industrial contacts for the CoEs	- Company - CoE - Sector of the company - Size of the company (SME or large company) - Level of contact (discussion, cooperation, common project, funding…)	100
Number of industrial individuals having received information about CoEs	- Company - Sector of the company - Size of the company (SME or large company)	5000

Table 6 WP3 KPIs ***(updated in November 2020)***

[2] *This table is an update of that in the previous version of the report, including the concrete targets, consistent with the periodic progress report for the first project period.*

WP3 will put in place tools to keep track of the information needed to follow the KPIs. For the first KPI, we will use a table internally in WP3 as a "Customer Relationship Management Tool" that will record information on:

- Company (name, size, sector, people involved);
- CoE (name, people involved);
- WP3 partner involved;
- Contact information (how it has been created, what actions have been put in place…).

For the second KPI a simpler tool will be used to collect information about the industries that have been met during the sectorial events. In both cases, the tools will help to document the activity of WP3 and to measure the KPIs.

5.2 Success Stories and Best Practices

Success stories based on the outcomes of the CoEs will be prepared for dissemination of the benefits of using HPC in industry. The success stories will contain the following information:

- Organisations involved: brief description of the end user company and the CoE involved
- Challenge: description of the technical challenge solved by means of HPC
- Solution: description of how the challenge has been solved
- Business impact: description of the current situation and how using HPC is improving or is expected to improve it
- Benefits: bullet points summarising the time/cost savings, product optimisation, waste reduction, etc.
- Software and hardware used
- Industry sector
- Images of the challenge and of the solution (if possible)

Together with WP5, we will monitor success stories of the CoEs and disseminate them through appropriate channels (sectorial events, social networks, etc.).

The analysis of the success stories will lead to the identification of a selection of Best Practices, i.e. procedures and approaches that were found particularly effective and beneficiary for the companies involved.

The objective is to produce a formal description of Best Practices that are capable of:

- Facilitating the match between offer and demand for HPC technologies, services, and expertise;
- Achieving a market added value by the CoEs' action.

The best practices will be analysed and described along different characteristics, such as:

- how to identify researchers who will understand company practices and technology goals;
- how to set up specific collaborations that can provide value to the company;
- how to set up long-term relationships capable of yielding effective results.

The results of the analyses on Success Stories and Best Practices will be discussed and jointly validated together with the CoEs.

6 Conclusions

This deliverable reports on activities performed in the period December 2018 to May 2019 and the bulk of the text provides analyses and planning as included in the version of the deliverable completed in May 2019.

The updated version of the deliverable completed in November 2020 provides additional or replacement material – which is clearly highlighted as such – that in part reflects changes to CoE interactions and cooperative procedures developed subsequent to the completion of the May 2019 version of the document.

The changes applied to the document can be summarised as follows:

- *Section 1.3 on the methodological approach*
- *Section 4 our approach for interaction with the CoEs (fully rewritten)*
- *Section 5.1 on Monitoring and KPI with a revised KPI table, that also indicates the target values*

The amendments and changes have been clearly marked as such throughout the document.

In the previous chapters a combination of criteria, activities, and evaluation mechanisms was presented that allow the identification of the priorities that the work package must address in developing its action. It can be envisioned as a set of tools to select an appropriate course, perform a first set of actions, evaluate its results, and eventually introduce corrections and changes later in the project's lifetime. With this "toolbox" at hand the project can now start performing its role of promotion of the Centres of Excellence.

The soundness of this approach will be tested in practice, and in this sense the need for a constant interaction of FocusCoE with the ten CoEs must not be forgotten. An effective collaboration must be put in place, avoiding on the one hand all interference of FocusCoE with the initiatives already put in place by the CoEs, on the other hand leveraging on their experience to maximise its effects, promote the transfer of technologies across different companies, industrial sectors, and countries.

This is not an easy task, given the manifold scenarios, with dozens of participants in the CoEs, a variety of addressed industrial sectors, a large number of cutting-edge computing codes still under development, and therefore a constant effort will have to be put in place maintain a fruitful and constructive interaction and ensure success in this important objective of FocusCoE.

7 References

[1] https://www.etp4hpc.eu/pujades/files/SRA%203.pdf
[2] FocusCoE project, http://www.focus-coe.eu/
[3] FocusCoE Deliverable D1.2, “Management Report”, Project Month 19 (June 2020)
[4] https://ec.europa.eu/growth/sectors_en

8 Annex I

8.1 CoE Description (1): BioExcel

BioExcel, Centre of Excellence in biomolecular research	
Consortium Partners	1. KUNGLIGA TEKNISKA HOEGSKOLAN 2. THE UNIVERSITY OF EDINBURGH 3. EUROPEAN MOLECULAR BIOLOGY LABORATORY 4. THE UNIVERSITY OF MANCHESTER 5. MAX-PLANCK-GESELLSCHAFT ZUR FORDERUNG DER WISSENSCHAFTEN EV 6. UNIVERSITEIT UTRECHT 7. FORSCHUNGSZENTRUM JULICH GMBH 8. FUNDACIO INSTITUT DE RECERCA BIOMEDICA (IRB BARCELONA) 9. BARCELONA SUPERCOMPUTING CENTER - CENTRO NACIONAL DE SUPERCOMPUTACION 10. FORWARD TECHNOLOGIES AB 11. IAN HARROW CONSULTING LTD
Duration and effort	36 months
Mission-Main topics-Codes-Sectors	
Mission	Enabling better science by improving the most popular biomolecular software and spreading best practices and expertise among the communities through consultancy and training.
Main scientific topics	BioExcel is a Centre of Excellence for provision of support to academic and industrial researchers in the use of high-performance computing (HPC) and high-throughput computing (HTC) in biomolecular research. Much of the current Life Sciences research relies on intensive biomolecular modelling and simulation. As a result of this, both academic and industrial researchers are facing significant challenges when it comes to applying best practices for optimal resource usage and workflow productivity, and to finding a faster path to achieve results. High-performance computing (HPC) and high-throughput computing (HTC) techniques have now reached a level of maturity in widely used codes and platforms, but taking full advantage of these requires training and guidance by experts. The services ecosystem required for that is presently inadequate, so a suitable infrastructure needs to be set up in a sustainable way. The BioExcel Center of Excellence (CoE) was thus established to provide the necessary solutions for long-term support of the biomolecular research communities: fast and scalable software, user-friendly automation

	workflows and a support base of expert core developers. The main services offered by the center include hands-on training, tailored customization of code and personalized consultancy support.
Addressed industrial sectors	• HPC • HTC • Biomolecular research
Services – Training	
Services	• Support Forums: ask.bioexcel.eu - forum to support the community for computational biomolecular research in academia and industry, with particular focus on biomolecular simulation and modelling. • Webinars: bioexcel.eu/category/webinar/ - covering broad topics related to the latest development of the supported software packages; their application to modelling and simulation; best practices for performance tuning and efficient usage on HPC and novel architectures; introductory tutorials for entry level users and much more • Knowledge resource centre: krc.bioexcel.eu/ - repository for computational biomolecular training resources aggregated from BioExcel partners and third party providers • Training: bioexcel.eu/services/training/ - The BioExcel Training Programme. • Chat channels: general chat topic, gitter.im/bioexcel/general, and workflows, data integration, platforms, etc topics, gitter.im/bioexcel/workflows.
Training	As part of Bioexcel services, the BioExcel Training Programme has been developed from a competency-based training needs analysis. A list of things individuals need to know or be able to do to interact efficiently with the BioExcel services has been created as a first step.
Interaction with industry	
Interaction with industry	• BioExcel Strategic Partnership Scheme • BioExcel Webinars (series of educational webinars for computational biomolecular research, covering broad topics related to the latest development of the BioExcel supported software packages) • BioExcel Training Programme (competency-based training for interacting efficiently with the BioExcel services) • Media outreach (press kit, interviews, social media, YouTube channel)
Types of interaction	• BioExcel Innovation Advisory Board
Contacts already established	The following have been established through the Bioexcel Strategic Partnership Scheme. • Open PHACTS Foundation • ELIXIR • Molecular Sciences Software Institute (MolSSI) • Vrije Universiteit Amsterdam(VUA) • HPCE3 Europa

	• Scuola Normale Superiore (SNS) • Multiscale Complex Genomics Virtual Research Environment (MuG VRE) • VI-SEEM Virtual Research Environment Portal
Contacts	
• Software Scalability &Usability contact	Mark Abraham <mark.j.abraham@gmail.com>
•	
• Project Manager	Rossen Apostolov <rossen@kth.se>
• Training contact	Vera Matser <matser@ebi.ac.uk>
• Portable Environments for Computing and Data Resources	Adam Hospital <adam.hospital@irbbarcelona.org>
• Consultancy and User Groups	Arno Proeme <a.proeme@epcc.ed.ac.uk>
• Dissemination contact person	Vera Matser <matser@ebi.ac.uk>

8.2 CoE Description (2): ChEESE

ChEESE **Centre of Excellence for Exascale in Solid Earth**	
Consortium Partners	OVERVIEW: • PRACE Centers (BSC, HLRS, CINECA) • other academic partners (INGV, ETHZ, TUM, LMU, UM, IPGP, CNRS) • 2 private partners (NGI, BULL) • others (VI) IN DETAIL: • Barcelona Supercomputing Center (ES) • Istituto Nazionale di Geofisica e Vulcanologia (IT) • Vedurstofa Islands (Iceland) • Eidgenoessische Technische Hochschule Zuerich (CH) • Universität of Stuttgart – HLRS (DE) • CINECA (IT) • Technische Universitaet Muenchen (DE) • Ludwig-Maximilians-Universitaet Muenchen (DE) • Universidad de Malaga (ES) • Stiftelsen Norges Geotekniske Institutt (NO) • Institut de Physique du Globe de Paris (FR) • Centre National de la Recherche Scientifique CNRS (FR) • Bull SAS (FR)
Duration and effort	36 months, starting in Nov. 2018, overall budget € 7 683 241,25
Mission-Main topics-Codes-Sectors	
Mission	• Prepare 10 flagship codes to address Exascale Computing Challenging problems on computational seismology, magnetohydrodynamics, physical volcanology, tsunamis, and data analysis and predictive techniques for earthquake and volcano monitoring. • Develop Pilot Demonstrators for scientific problems requiring of Exascale computing on near real-time seismic simulations and full-wave inversion, ensemble-based volcanic ash dispersal, faster than real-time tsunami simulations and physics-based hazard assessments for seismics, volcanoes and tsunamis. • ChEESE aims at acting as a hub to foster HPC across the Solid Earth Community and related stakeholders and to provide specialized training on services and capacity building measures. • ChEESE gatherss European institutions in charge of operational monitoring networks, tier-0 supercomputing centers, academia, hardware developers and third-parties from SMEs, Industry and public-governance.
Main scientific	• Computational Seismology • Magnetohydrodynamics

topics	• Physical volcanology • Tsunami modelling
Codes of interest	• ExaHyPE https://exahype.eu/ • Salvus https://salvus.io/ • SeisSol https:seissol.org/ • SPECFEM3D https://geodynamics.org/cig/software/specfem3d/ • PARODY_PDAF • XSHELLS https://bitbucket.org/nschaeff/xshells • ASHEE https://www.geosci-model-dev.net/9/697/2016/ • FALL3D http://datasim.ov.ingv.it/models/fall3d.html • T-HySEA https://edanya.uma.es/hysea/index.php/models/tsunami-ysea • L-HySEA https://edanya.uma.es/hysea/index.php/models/landslide-hysea
Addressed industrial sectors	Main • Civil protection organizations • Oil & Gas companies with exploration activity • Insurance companies • Natural risk assessment companies • Earth Science associations and networks Secondary • Aeronautics industries • Maritime industries
Services – Training	
Services	Potential services in Urgent Computing: • Urgent seismic simulations • Faster than real-time tsunami simulations • High-resolution volcanic ash dispersal forecast Potential services in Hazard Assessment: • Physics-based probabilistic seismic hazard assessment • Probabilistic volcanic hazard assessment • Probabilistic tsunami hazard assessment Potential services in Early Warning: • Probabilistic Tsunami Forecast for early warning and rapid post event assessment Other potential services: • Seismic tomography
Training	A minimum of 4 training courses will be organized with the PRACE Advanced Training Centers (PATC) infrastructure. Different webinars will also be considered and defined in the Training Plan (deliverable in M6).
Interaction with industry	
Interaction	The project has an Industry and User Board (IUB) composed of 12

with industry	companies and organizations.
Types of interaction	IUB participates in the general assemblies of the project. Provides feedback on the services.
Already done	Personalized interviews with the IUB members
Contacts already established	IUB members: • Italian Civil Protection Department (DPC) • Icelandic Civil Protection (NCIP) • Spanish Geographic National Institute (IGN) • International Association of Seismology and Physics of the Earth's Interior (IASPEI) • International Association of Volcanology and Chemistry of the Earth's Interior (IAVCEI) • European Plate Observing System (EPOS) • GW4 ISAMBARD (Isambard) • Geohazard Supersites and Natural Laboratory (GEO-GSNL) • REPSOL • Schlumberger • INTEL • MITIGA Solutions
Innovation	
List of Project IP	The flagship codes listed above
Contacts	
• Principal Investigator	Arnau Folch (arnau.folch@bsc.es)
• Project Manager	Isabel Martinez (isabel.martinez@bsc.es)
• Training contact	Renata Gimenez (renata.gimenez@bsc.es)
• Innovation contact	Monica de Mier (monica.demier@bsc.es)
• Dissemination contact	Renata Gimenez (renata.gimenez@bsc.es)

8.3 CoE Description (3): CompBioMed

CompBioMed **Centre of Excellence in Computational Biomedicine**	
Consortium Partners	• University College London (UCL) – Lead • University of Amsterdam (UvA) • University of Edinburgh (EPCC) • Surfsara • Barcelona Supercomputing Centre (BSC) • University of Oxford • University of Geneva • University of Sheffield • CBK Sci Con Ltd • Universitat Pompeu Fabra • LifeTec Group • Acellera • Evotec • Bull (Atos) • Jannsen
Duration and effort	CompBioMed1 – 3 years ending 30 Sep 2019 CompBioMed2 – 4 years starting 1 Oct 2019
Mission-Main topics-Codes-Sectors	
Mission	CompBioMed's mission is to foster a community in Computational Biomedicine while advancing that domain to the Exascale.
Main scientific topics	CompBioMed is a European Commission H2020 funded Centre of Excellence focussed on the use and development of computational methods for biomedical applications. We have users within academia, industry and clinical environments and are working to train more people in the use of our products and methods.
Addressed industrial sectors	• HPC • Computational Biomedicine
Services – Training	
Services	• Training Hub (see below) • Software Hub - https://www.compbiomed.eu/services/software-hub/ • Visitor Programme - https://www.compbiomed.eu/innovation/visitor-programme/ • HPC Allocation Requests (to be added shortly)
Training	• Training Repository and listing of events shown here: https://www.compbiomed.eu/training-3/ Detailed training plan available on request.
Interaction with industry	
Interaction	CompBioMed Associate Partner scheme

with industry	CompBioMed Visitor Programme CompBioMed Training Programme CompBioMed Innovation Advisory Board
Types of interaction	• EU Incubators: - https://ec.europa.eu/easme/en - https://een.ec.europa.eu/ - https://cordis.europa.eu/project/rcn/194234/factsheet/en - https://cordis.europa.eu/project/rcn/213086/factsheet/en - https://dispatcheseurope.com/start-it-build-it-grow-it-dispatches-2018-list-of-europes-best-accelerators-incubators/ - http://www.bambi-medical.com/ - https://www.crunchbase.com/hub/european-union-incubators#section-overview - https://www.etondigital.com/guide-to-european-incubators-and-accelerators/ - http://www.inits.at/en/ - https://ec.europa.eu/regional_policy/sources/docoffic/2007/working/innovation_incubator.pdf - https://opendataincubator.eu/resources/ • Potentially new UK Incubators for our list: - https://www.gov.uk/government/organisations/department-for-business-energy-and-industrial-strategy - https://www.youtube.com/channel/UCyGwamm_eoM69zC1wO9qVDg?reload=9 - https://www.gov.uk/government/organisations/innovate-uk - https://www.gov.uk/government/publications/business-incubators-and-accelerators-the-national-picture - http://data.parliament.uk/DepositedPapers/Files/DEP2009-2118/DEP2009-2118.pdf - https://edinburgh-innovations.ed.ac.uk/2018/09/25/data-driven-innovation-programme-launched/ - https://www.ed.ac.uk/local/city-region-deal/data-capital-of-europe - https://www.ed.ac.uk/data-science/health-informatics/innovation-community/partner-with-us - https://www.meetup.com/Health-2-0-Edinburgh-Scotland/events/233203498/ - https://pdfs.semanticscholar.org/dcbc/fb98ea7b7ac0e58dd5c4dd5328299145b85e.pdf - https://www.mygov.scot/incubators-accelerators/west-of-scotland/ - http://edinburghbioquarter.com/ - https://www.stratmed.co.uk/
Contacts already established	- LifeTec Group - CBK SciCon - Evotec AG - Janssen - Bull (Atos) - Acellera - Shell - Thoroughly modern media - Francis Crick Institute - Amgen - AnaBios Corporation - UCB Biopharma

	- Convergence Pharma - GSK - DNA Nexus - Alces Software - Microsft Research - Schrodinger - Boehringer - Merck - Karthik Innovation - Sri Padmavathi Solutions - Norton Straw - Amazon Web Services - Cadfem - Ansys - Rosetta HUB - Diamond Light Source - Sardina Systems - Intel - OCF - Velocient - ParTec - Genomics England - Polymaths - Tiara Solutions - QuintilesIMS - Alten Group - The HCI Group - Intelligent Voice - Cyfronet - Verne Global - SPARC-E Ltd - Sygnature Discovery - Medtronic - iVascular - IHT - Leibniz Rechenzentrum - Science Museum London - Materialise - Deep Science Venture - Janet - MedCity HQ - HiTs - InsilicoMedicine - Abbvie - Biotrial - Clyde Biosciences - Eli Lilly & Co - Chugai Pharma Europe - Lipz - Pfizer - QT Informatics - Vala Sciences - LumiraDX - Aridhia - Fios Genomics - Scotland's DNA - PhysioMedics - MathResolutions - Oxford Nanopore Technologies - RSRCH BV - Phillips Research - The Hyve - Castor DC - Base Clear - MicroLife Solutions - PacMed - Quaero Systems BV - Electric Ant Lab - Astrocyte - Institute of Cancer Research - EA - Astra Zeneca - Avicenna Alliance - Pozlab - Hamad - Diavita - Dassault Systemes - Lightox - Insilico Trials - Ensemble MD - Ansys - Pie Medical Imaging
Innovation	
List of Project IP	IP shown here: https://www.compbiomed.eu/services/software-hub/
Innovation Strategy	Innovation Plan Deliverable available on request Sustainability Operations Procedure due in month 30 of CompBioMed1 CompBioMed Innovation Advisory Board CompBioMed2 contains a task dedicated to commercialisation

Contacts	
• Principal Investigator	Peter Coveney <p.v.coveney@ucl.ac.uk>
• Project Manager	Emily Lumley <e.lumley@ucl.ac.uk>
• Training contact	Manuela Corsini M.Corsini@uva.nl
• Innovation contact	Gaving Pringle gavin@epcc.ac.uk
• Dissemination contact	Hugh Martin <h.martin@cbkscicon.com

8.4 CoE Description (4): E-CAM

E-CAM **The European Centre of Excellence for Calcul Atomique et Moléculaire**	
Consortium Partners	OVERVIEW: • 16 CECAM Nodes (Centre Européen de Calcul Atomique et Moléculaire) • 12 industrialists • 3 PRACE centres • 1 centre for industrial computing (Hartree)) IN DETAIL: • École Polytechnique Fédérale de Lausanne, Switzerland (CECAM HQ) – Coordinator • University College Dublin, Ireland (CECAM-IRL Node) • Freie Universität Berlin, Germany (CECAM-DE-MMS Node) • Universita degli Studi di Roma La Sapienza, Italy (CECAM-IT-SIMUL Node) • Centre national de la recherche scientifique, France (CECAM-FR-MOSER Node) • Technische Universität Wien, Austria (CECAM-AT Node) • University of Cambridge, United Kingdom (CECAM-UK-JCMAXWELL Node) • Max-Planck-Institut für Polymerforschung, Germany (CECAM-DE-SMSM Node) • École Normale Supérieure de Lyon, France (CECAM-FR-RA Node) • Forschungszentrum Jülich, Germany (CECAM-DE-JUELICH Node) • Universitat de Barcelona, Spain (CECAM-ES Node) • Daresbury Laboratory, Scientific and Technology Facilities Council, United Kingdom (CECAM-UK-HARTREE Node) • Scuola Internazionale Superiore Di Trieste, Italy (CECAM-IT-SIDE Node) • Universiteit van Amsterdam, Netherlands (CECAM-NL Node) • Scuola Normale Superiore Pisa, Italy (CECAM-IT-SMART Node) • Aalto University, Finland (CECAM-FI Node) • CSC-IT Centre for Science Ltd, Finland • Irish Centre for High-End Computing, Ireland
Duration and effort	5 years from October 2015 to September 2020 48 staff years' effort, overall budget € 4 836 896,25
Mission-Main topics-Codes-Sectors	
Mission	• E-CAM is an e-infrastructure for software development, training, and industrial discussion in simulation and modelling.
Main scientific topics	• Classical Molecular Dynamics • Electronic Structure • Quantum Dynamics

	• Meso- and Multi-Scale Modelling
Codes of interest	WP1 Molecular dynamics: - LAMMPS - GROMACS - OPS - DL-POLY WP2 Electronic structure - Electronic Structure Library Project (ESL) - ELSI - Wannier90 - QMCPACK - QuantumEspresso - SIESTA - Aiida WP3 Quantum Dynamics - PaPIM - Quantics - CP2K - Q-Chem - CPMD WP4: Meso and multi scale modelling - MP2C - ESPResSo++ . - Ludwig - DL_MESO_DPD - GC-AdResS Optimizations efforts have been done for - Classical Molecular Dynamics: benchmark of OPS using LAMMPS and GROMACS - Electronic Structure: LibOMM and Wannier90 - Quantum Dynamics: PaPIM code and Quantics - Meso- and Multi-scale Modelling: performance improvements of DL_MESO_DPD on multi-GPU and benchmark of ESPResSo++ with Easybuild and JUBE
Addressed industrial sectors	Main • Pharmaceutical • Chemical (including personal care i.e. cosmetics and industrial care i.e. detergent) • Oil and Gas • Manufacturing Secondary • Food • Simulation software
Services – Training	

Services	• Software development Repositories for codes Pilot projects Porting and performance analysis • Training (see section 4) • Discussion with industry (see section 5)
Training	E-CAM is focus on workshops, called Extended Software Development Workshops (ESDW). The objectives: - they are a mechanism for generating software modules for inclusion in the E-CAM repository - they are an integral part of the E-CAM training programme and represent "training by doing" Participation is free of charge for academic participants and for industrial participants from one of the current or future industrial partners of E-CAM. An attendance fee of up to 1000 Euro may be charged to industrial trainees from outside the E-CAM partnership. E-CAM has developed a training portal at https://clowder.e-cam2020.eu/
Interaction with industry	
Interaction with industry	- **state-of-the-art workshops**, that serve to monitor software developments, identify new directions and transfer knowledge into industry and academia - **scoping workshop**, where industrialists can expose their software needs; and interact with the academic and software developers community - possibility to engage industry in discussions with experts in E-CAM, that can 1. assist on business decision as to whether computational methods can be effectively applied to a given problem with good cost/benefit ratio 2. define of the most appropriate modelling strategy for a given problem within and across the scientific areas of E-CAM 3. survey existing methods to establish whether a given modelling strategy requires new developments or can be enacted with existing tools 4. evaluate the accuracy of available methods for a given problem 5. develop, document, validate and benchmark of new software, for packages structured by combining modules already present in the E-CAM repositories or of interfaces with community codes belonging to the E-CAM partnership 6. assist in selecting the most appropriate hardware architecture
Already done	Scoping workshops: - E-CAM Scoping Workshop: "Solubility prediction", 14 – 15 May 2018, Ecole Normale Supérieure de Lyon, France, - E-CAM Scoping Workshop: "Dissipative particle dynamics: Where do we stand on predictive application?", 24 – 26 April 2018, Daresbury

	Laboratory, United Kingdom, - E-CAM Scoping Workshop "From the Atom to the Material" 18 – 20 September 2017, CECAM-UK-JCMAXWELL, University of Cambridge, United Kingdom - E-CAM Scoping Workshop "Industry Partnerships", 7-9 September 2016, CECAM-SMSM, MPI Mainz, Germany Workshop reports publicly available at https://www.e-cam2020.eu/scientific-reports/
Contacts already established	BASF SE, Germany: - Bachmann, Stephan - Köhler, Stephan PROCTER AND GAMBLE, USA - Koenig, Peter UNILEVER, UK - Warren, Patrick - Stott, Ian - Massimo Noro Pfizer Limited - Docherty, Robert - Klimentina Pencheva Astra Zeneca, Sweden - Lindfors, Lennart Sanofi-Aventis: - Marc Bianciotto Servier: Pierre Ducrot Novartis: Richard Lewis Merck Darmstadt - Steffen Gnauck - Leo Weegels Johnson Matthey - Misbah Sarwar APC Ldt (Pharmaceutical) Ireland - Martis, Alessandro SHELL - Detlef Hohl - Pratamesh Shenai BP: - Filip Sorin - Benjamin DENNIS-SMITHER - Ian Collins

	Total - Lozano, Sylvain ROLLS ROYCE, UK: - David Rugg HYUNDAI: Woomin Kyoung Michelin - Dronet, Severin - Schnell, Benoît ISVs CULGI (ISVs) The Netherlands: - Fraaije, Hans DASSAULT SYSTEM, Biovia - Stephen Todd - Victor Milman - Johan Carlsson ATOMERA, US (quantum engineered material) - Marek Hytha - Ukrainczyk, Marko Scienomics ISV France - Xenophon Krokidis Biki Technologies ISV Italy: - Giuseppina La Sala - Sergio Decherchi Schrödinger ISV: - Davide Branduardi Simune Atomistic Simulations, ISV - Mónica García Mota

Contacts

• Principal Investigator	Luke Drury, University College Dublin
• Project Manager	Ana Catarina Mendonça, École Polytechnique Fédérale de Lausanne **<ana.mendonca@epfl.ch>**
• Training contact	Ana Catarina Mendonça, École Polytechnique Fédérale de Lausanne **<ana.mendonca@epfl.ch>**

8.5 CoE Description (5): EoCoE-II

EoCoE-II Energy oriented Centre of Excellence	
Consortium Partners	1. COMMISSARIAT À L'ÉNERGIE ATOMIQUE ET AUX ÉNERGIES ALTERNATIVES (CEA), France, Project Coordinator 2. FORSCHUNGSZENTRUM JULICH GMBH, Germany 3. MAX PLANCK GESELLSCHAFT ZUR FOERDERUNG DER WISSENSCHAFTEN E.V, Germany 4. AGENZIA NAZIONALE PER LE NUOVE TECNOLOGIE, L'ENERGIA E LO SVILUPPO ECONOMICO SOSTENIBILE (ENEA), Italy 5. CENTRE EUROPEEN DE RECHERCHE ET DE FORMATION AVANCEE EN CALCUL SCIENTIFIQUE (CERFACS), France 6. INSTITUT NATIONAL DE RECHERCHE EN INFORMATIQUE ET EN AUTOMATIQUE (INRIA), France 7. CENTRE NATIONALE DE LA RECHERCHE SCIENTIFIQUE (CNRS), France 8. INSTYTUT CHEMII BIOORGANICZNEJ POLSKIEJ AKADEMII NAUK (PSNC), Poland 9. UNIVERSITÀ DEGLI STUDI DI TRENTO (UNITN), Italy 10. FRAUNHOFER-GESELLSCHAFT ZUR FOERDERUNG DER ANGEWANDTEN FORSCHUNG E.V., Germany 11. FRIDERICH-ALXEANDER-UNIVERSITAET ERLANGEN NUERNBERG (FAU), Germany 12. UNIVERSITY OF BATH (UBAH), UK 13. CONSIGLIO NAZIONALE DELLE RICERCHE (CNR), Italy 14. UNIVERSITE LIBRE DE BRUXELLES (ULB), Belgium 15. BARCELONA SUPERCOMPUTING CENTER - CENTRO NACIONAL DE SUPERCOMPUTACION (BSC), Spain 16. CENTRO DE INVESTIGACIONES ENERGETICAS MEDIOAMBIENTALES Y TECNOLOGICAS (CIEMAT), Spain 17. INSTITUT FRANÇAIS DU PETROL ET DES ENERGIES NOUVELLES (IFPEN), France 18. DATA DIRECT NETWORKS France (DDN), France
Duration and effort	36 months (January 2019 – December 2021) Overall budget € 8,622,000 €
Mission-Main topics-Codes-Sectors	
Mission	The mission of the Energy-oriented Centre of Excellence (EoCoE) is to contribute to accelerate the transition towards the production, storage and management of clean, decarbonized energy through the application of cutting-edge computational methods.
Main scientific topics	The present project is the 2nd round of project EoCoE, a proof-of-principle phase in which a large set of diverse computer applications from four such energy domains achieved significant efficiency gains thanks to its multidisciplinary expertise in applied mathematics and supercomputing. During this 2nd round EoCoE-II will channel its efforts into 5 scientific Exascale low-carbon Application Sectors: Energy Meteorology, Materials, Water, Wind and Fusion.

Below is the project Workpackage layout.

Work package No	Work Package Title
1	Exascale Science Challenges in energy research
2	Programming models
3	Scalable Solvers
4	IO & Data Flow
5	Ensemble Runs
6	Dissemination & networking
7	Management

The project adopts a matrix structure in which the 5 Technical Workpackages (WP1-5) intersect the 5 Applications Sectors mentioned above.

Codes of interest

Scientific challenge	Code name	Description
Wind	Alya	Alya (website) is a high performance computational mechanics code that solves complex coupled multi-physics problems.
Meteorology	ESIAS-Chem	ESIAS-Chem is a tool for generating and controlling ultra-large ensembles of chemistry transport models for stochastic integration.
	ESIAS-Meteo	ESIAS-Meteo is a tool for generating and controlling ultra-large ensembles of numerical weather forecast models for stochastic integration.
	EURAD-IM	EURAD-IM (Elbern (1997), Elbern et al. (2007)) simulates chemistry particle transportation in local atmospheres coupled with a weather forecast application WRF.
Materials	QMCPACK	QMCPACK (website) is an open-source production level many-body ab initio Quantum Monte Carlo code for computing the electronic structure of atoms, molecules, and solids..
	PVnegf	PVnegf (Aeberhard (2011), Aeberhard (2016)) describes photon-carrier dynamics (generation, transport and recombination) in nanostructured regions and at complex interfaces in advanced high-efficiency solar cell devices.
	KMC/DMC	Kinetic Monte Carlo (KMC, Kimber et al. (2012)) simulates charge and energy transport in organic solar cells.

<table>
<tr><td></td><td>
<table>
<tr><td rowspan="2">Water</td><td>ParFlow</td><td>ParFlow (Kollet et al. (2010)) is a physics-based 3D parallel hydrologic model, which simulates surface and 3D subsurface flow.</td></tr>
<tr><td>SHEMAT-Suite</td><td>SHEMAT-Suite (Clauser (2003), Rath et al. (2006)) is a code for simulating single- or multi-phase heat and mass transport in porous media.</td></tr>
<tr><td>Fusion</td><td>Gysela</td><td>Gysela (Bigot et al. (2013), Grandgirard et al. (2016)) is a 5D full-f (regarding Vlasov eq.) and flux-driven gyrokinetic Fortran parallel code that solves Vlasov (ions and electrons) and Poisson (electric potential) equations to simulate plasma turbulence and transport in Tokamak devices.</td></tr>
</table>
</td></tr>
<tr><td>Addressed industrial sectors</td><td>The project addresses the Energy industry, and in particular companies operating in the abovementioned Application Sectors.</td></tr>
<tr><td colspan="2">Services – Training</td></tr>
<tr><td>Services</td><td>EoCoE-II provides the following services:

- Improvement of third-party applications
o Code auditing, performance assessment and optimization
o Porting
o Software integration, special purpose algorithms
- Usage of developed/provided codes and numerical tools
- Consultancy and training</td></tr>
<tr><td>Training</td><td>The general plan in organizing Education activities within EoCoE II is to ensure a strong collaboration with PRACE/PATC and other organisations and partners training facilities to leverage on existing programs, courses, and facilities. This will be complemented with the set-up of focused courses and materials to address problems and topics specific to EoCoE.
The program will be aimed to a wide range of potential targets, including doctoral, post-doctoral and master students, researchers, and professionals working in private enterprises and or public administrations. Specific training is envisaged for the PhD & Master students that will be incorporated to work in the project and for the industrial and academic partners in the use of computational methods, specific application and optimisation tools of EoCoE II.
EoCoE-II will disseminate the acquired knowledge and expertise through:
• 9 workshops and an international conference;
• Participation to the main international conferences, including Supercomputing (SC) and the International Supercomputing Conference (ISC);
• The development of a large network to promote the tools and best practices as well as gather needs, especially through a tight collaboration with EERA;
• Education and training modules/workshops to help laboratories and industry to access and use HPC methods and code.</td></tr>
</table>

Interaction with industry	
Interaction with industry	Based on the experience gained during the first phase of the project and our vision of similar actions carried out at national or European levels, EoCoE will try to propose new means to develop relationships with SMEs/industries: more focused services, and a proper balance will have to be established between very specific research activities where EoCoE-II would provide unique added value and 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 Software as a Service (SaaS) platform is foreseen. This platform will propose access to EoCoE-II, and third parties, software in a very targeted and simple way. It will allow engineers from SMEs/industries to easily test and see potential benefit from simulation tools on concrete examples. These simple use cases will eventually provide the opportunity to develop more ambitious collaborations between interested users and scientific teams of EoCoE. Moreover, the following actions are foreseen: • Enlarge the network of EoCoE with industry and SMEs building on existing collaborations with industrial partners (e.g. EDF R&D, Iberdrola Renovables, Amprion, TenneT TSO, 50 Hertz Transmission, Vestas and Vortex Bladeless, just to name a few) and develop further collaboration links. • Enlarge the visibility of EoCoE's services: via connections to over 30 other complementary organisations active on policy/strategic networking on energy research and on HPC in Europe and elsewhere in the world. • Participate in events organised by public administration sponsoring research in either Energy or HPC related domains or organise side events to large networking conferences: to lobby for the adoption of world-class simulation tools for cleaner energy solutions (e.g. Supercomputing conference, International Supercomputing conference, EU Sustainable Energy Week, PRACE days). • A direct involvement of EoCoE-II and its partners in EERA (European Energy Research Alliance) is deemed to be very effective in facilitating contacts with prospective industrial companies and public organizations interested in the CoE's services and skills. 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 special 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. It currently involves over 200 European public research centers & universities with over 50.000 researchers. It collaborates with European industry through platforms and partnerships. EERA is organized in 17 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.
Contacts	
• Principal Investigator	Edouard Audit (CEA): edouard.audit@cea.fr
• Training contact	Marcin Plociennik (PSNC): marcinp@man.poznan.pl
• Dissemination contact	Massimo Celino (ENEA) massimo.celino@enea.it

8.6 CoE Description (6): ESiWACE2

ESiWACE2 **Centre of Excellence in Simulation of Weather and Climate in Europe**	
Consortium Partners	1. Deutsches Klimarechenzentrum GmbH 2. Centre National de la Recherche Scientifique 3. European Centre for Medium-Range Weather Forecasts 4. Barcelona Supercomputing Center 5. Max-Planck-Gesellschaft zur Förderung der Wissenschaften e.V./ Max-Planck-Institut für Meteorologie 6. Sveriges meteorologiska och hydrologiska institut 7. Centre Européen de Recherche et de Formation Avancée en Calcul Scientifique 8. National University of Ireland Galway (Irish Centre for High End Computing) 9. Met Office 10. Fondazione Centro Euro-Mediterraneo sui Cambiamenti Climatici 11. The University of Reading 12. Science and Technology Facilities Council 13. BULL SAS 14. Seagate Systems UK Limited 15. ETH Zürich 16. The University of Manchester 17. Netherlands eScience Center 18. Federal Office of Meteorology and Climatology 19. DataDirect Networks 20. Mercator Océan
Duration and effort	48 months: 1 January 2019- 31 December 2022 Indicative PMs: 808
Mission-Main topics-Codes-Sectors	
Mission	Two overall objectives: 1. Enable leading European weather and climate models to leverage the available performance of pre-exascale systems with regard to both compute and data capacity in 2021. 2. Prepare the weather and climate community to be able to make use of exascale systems when they become available.
Main scientific topics	• The path towards exascale computing holds enormous challenges for the community of weather and climate modelling regarding portability, scalability and data management that can hardly be faced by individual institutes. ESiWACE2 will therefore link, organise and enhance Europe's excellence in weather and climate modelling to: (1) enable leading European weather and climate models to leverage the performance of pre-exascale systems with regard to both compute and data capacity as soon as possible; and (2) prepare the weather and climate community to be able to make use of exascale systems when they become available. To achieve this goal, ESiWACE2 will: - Improve throughput and scalability of leading European weather and climate models and demonstrate the technical and scientific

	performance of the models in unprecedented resolution on pre-exascale EuroHPC systems, - Evaluate and establish new technologies such as domain specific languages and machine learning for use in weather and climate modelling, - Enhance HPC capacity via services to the weather and climate community to optimize code performance and allow model porting, - Improve the data management tool chain from weather and climate simulations at scale, - Foster co-design between model developers, HPC manufacturers and HPC centres, and - Strengthen interactions of the community with the European HPC Eco-system. - ESiWACE2 will deliver configurations of leading models that can make efficient use of the largest supercomputers in Europe and run at unprecedented resolution for high quality weather and climate predictions. This will be a beacon for the community in Europe and around the world. ESiWACE2 will develop HPC benchmarks, increase flexibility to use heterogeneous hardware and co-design and provide targeted education and training for one of the most challenging applications to shape the future of HPC in Europe.
Codes of interest	Codes: Leading European Weather & Climate Models (coupled models of atmosphere and ocean) • ICON (German weather service and MPIM) • IFS (ECMWF and EC-Earth consortium) • NEMO (European community ocean model) • Dynamico (Next generation French model by IPSL) Support to other models, e.g. UM from UK Met Office
Addressed industrial sectors	HPC vendors (software and hardrware), storage industry.
Services – Training	
Services	Our WP2 "Establish and watch new technologies for the community" plans to establish, evaluate and watch new technologies to prepare climate and weather simulation for the exascale era. Direct services: Create a prototype for open services to the Earth system modelling community in Europe. The goal of the services is to create collaborations that provide guidance, engineering, and advice to support exascale preparations for weather and climate models. All groups developing and maintaining weather and climate codes - not only the ESiWACE2 partners - can apply. Proposals for such collaboration projects will be peer-reviewed and when found eligible, will be granted in-kind support by one of the partners involved. Indirect Services: - Establish DSLs in the community. - Evaluate Concurrent Components to improve performance. - Evaluate Containers to port Earth system models to new hardware.

	- Watch emerging technologies.
Training	Trainings are going to be organized in our WP6 "Community engagement and Training". WP6 links ESiWACE2 to the weather and climate community it serves on the one hand and to the European HPC ecosystem on the other hand. Training and Schools - IO and HPC awareness - DSL - C++ for HPC - OASIS3-MCT - High performance Data Analytics - Docker - Summer school in HPC for weather and climate
Interaction with industry	
Interaction with industry	ESiWACE2 will improve access to computing applications and expertise that enables industry to be more productive, leading to scientific excellence and economic and social benefit.

Types of interaction	• Improved competitiveness for European companies and SMEs through access to CoE expertise and services: Giving industry the opportunity to build technology prototypes that are suited for the weather and climate community and verticals, the time-to-market for upcoming products will be positively affected – not only for this community, but also for other related verticals in data-intensive computing
	• Widening the access to codes and fostering transfer of know-how to user communities, including specific and targeted measures for industry and SMEs through:
	  • Enhanced sharing of code, best practices and corresponding expertise through ESiWACE2 community services.
	  • Knowledge transfer on evolving new technologies (exascale hardware, heterogeneous computing, machine learning, containerisation) via workshops and white papers.
	  • Sharing improved tools, such as OASIS and XIOS, by the entire community.
	  • Fostering exchange of know-how on data management requirements between the weather and climate community and storage vendors (SEAGATE, DDN).
	  • Selected measures for industry provided through key performance indicators.

Already done	Our community already engaged with the industrial sector in the previous project (ESiWACE): Exchange with HPC vendors has been sought through discussions at the major HPC events/exhibitions SC/ISC. We further invited speakers from EXDCI, PoP, EoCoE, EuroEXA to the ENES HPC workshop in Lecce, Italy, and fostered fruitful exchange at the workshop. Discussions with Altair were held regarding their attendance at a workflow workshop to seek community interest in the Altair Cylc/PBS integration initiative with a particular focus on the weather community. Several international vendors (Fujitsu, NEC, Sugon) were visited, with the visits featuring talks

	and discussions on ESiWACE goals. Looking ahead, due to ESiWACE interactions, a new industrial partner (DDN) will join the ESiWACE2 project and NEC and CRAY will serve on the ESiWACE2 Scientific Advisory Board.
Contacts already established	• Partners ESiWACE2: BULL/ATOS, DDN, Seagate. • Addtl Partner ESiWACE: ARM. • Further: NEC, nVIDIA, ALTAIR, CRAY.

Contacts

• Principal Investigator	Project Coordinator: Joachim Biercamp biercamp@dkrz.de
• Technical Manager/Scientific Manager	Philipp Neumann (interim) neumann@dkrz.de
• Project Manager	Chiara Bearzotti (interim) bearzotti@dkrz.de
• Dissemination contact	Michael Boettinger (boettinger@dkrz.de) and Chiara Bearzotti (interim) bearzotti@dkrz.de
• Exploitation contact	Chiara Bearzotti (interim) bearzotti@dkrz.de

8.7 CoE Description (7): HiDALGO

HiDALGO **HPC and Big Data Technologies for Global Challenges**	
Consortium Partners	OVERVIEW: • PRACE Centers (USTUTT HLRS, PSNC) • Academic Partners (ICCS, BUL, KNOW, SZE, PLUS, ECMWF) • Industrial Partners (ATOS, MOON, ARH) • Others (MK, DIA) IN DETAIL: • ATOS Spain SA, Spain (ATOS) – Coordinator • University of Stuttgart - The High Performance Computing Center, Germany (USTUTT) • Instytut Chemii Bioorganicznej Polskiej Akademii Nauk - Poznań Supercomputing and Networking Center, Poland (PSNC) • Institute of Communication and Computer Systems, Greece (ICCS) • Brunel University London, United Kingdom (BUL) • KNOW-Center GmbH - Research center for data-driven business & big data analytics, Austria (KNOW) • Széchenyi István University, Hungary (SZE) • University of Salzburg, Austria (PLUS) • European Centre for Medium-Range Weather Forecasts, United Kingdom (ECMWF) • MoonStar Communications GmbH, Germany (MOON) • DIALOGIK, Germany (DIA) • Magyar Közút Nonprofit Zrt., Hungary (MK) • Adaptive Recognition Hungary Inc., Hungary (ARH)
Duration and effort	36 months, starting in Dec. 2018, overall budget € 7 991 500
Mission-Main topics-Codes-Sectors	
Mission	Developing evidence and understanding concerning Global Challenges and their underlying parameters is rapidly becoming a vital challenge for modern societies. Various examples, such as health care, the transition of green technologies or the evolution of the global climate up to hazards and stress tests for the financial sector demonstrate the complexity of the involved systems and underpin their interdisciplinary as well as their globality. This becomes even more obvious if coupled systems are considered: problem statements and their corresponding parameters are dependent on each other, which results in interconnected simulations with a tremendous overall complexity. Although the process for bringing together the different communities has already started within the Centre of Excellence for Global Systems Science (CoeGSS), the importance of assisted decision making by addressing global, multidimensional problems is more important than ever. Global decisions with their dependencies cannot be based on incomplete problem assessments or gut feelings anymore, since impacts cannot be foreseen without an accurate problem representation and its systemic evolution. Therefore, HiDALGO bridges that shortcoming by

	enabling highly accurate simulations, data analytics and data visualisation but also by providing knowledge on how to integrate the various workflows and the corresponding data.

Main scientific topics	• Global Challenges Simulations
	  ○ Agent-based Modelling
	  ○ Coupled Social Sciences Simulation
	• Data Analytics
	  ○ Real-world Data Flow Integration
	• Machine Learning
	  ○ Intelligent Workflow Composition

Codes of interest	• Agent-based Modelling
	  ○ AMOS
	  ○ RepastHPC
	  ○ MASON
	  ○ SUMO
	  ○ FLEE
	  ○ MUSCLE2
	• Data Analytics
	  ○ Apache Spark
	  ○ Apache Flink
	  ○ Apache Storm
	• Machine Learning
	  ○ TensorFlow
	  ○ Torch
	• Visualization
	  ○ COVISE
	  ○ VISTLE
	• Computational Fluid Dynamics (CFD)
	  ○ FEniCS

Addressed industrial sectors	The user groups for HiDALGO are twofold. First, the High Performance Data Analytics and Artificial Intelligence methods are cornerstones for efficient High Performance Computing. HiDALGO develops and integrates novel approaches in order to simply pre- and post-processing and entire workflow compositions that will be of importance each resource demanding application. Consequently, this project addresses end users, scientists, professionals, vendors and HPC providers. In contrast, Global Challenges cannot be addressed by small-scale industries. Therefore, only decision makers, stakeholders, politics or non-governmental organizations can directly benefit from HiDALGO.
Services – Training	

Services	• Software development
	  ○ Repositories for codes
	  ○ Pilot projects
	  ○ Porting and performance analysis
	• Data access and management
	• Training
	• Portal as a single access point

Training	HiDALGO will offer training services to its users and customers. Those will encompass HPC, HPDA, AI and Global Challenges simulation trainings with different community foci. The training services will be based on the well-established PATC Centers and furthermore, self-developed courses and materials. Nevertheless, the training activity will start in M12 of the project, further details need to be determined.
Interaction with industry	

Interaction with industry	As already described, the Global Challenges of HiDALGO can't be addressed by small-scale industries. Nevertheless, HiDALGO is in close cooperation with global decision makers, such as the European Commission or the UN Refugee Agency (UNHCR), in order to forecast refugee movements all over Europe (the Migration pilot applications of HiDALGO). Furthermore, contacts with the Municipality of Gyor have been established that focus the simulation of urban air pollution and their countermeasures (the Urban Pollution pilot application of HiDALGO).
Types of interaction	• HiDALGO established an exploitation and innovation advisory board that reviews the business strategy and provides insights in further business and marketing opportunities. • During the first phase of the project, each interaction shall provide new challenges, arising from the usage of the HiDALGO service portfolio. • Community events and stakeholder meetings are planned throughout the project's lifetime in order to advertise the project, but also to collaborate with stakeholders.
Contacts already established	Not industries, but our target stakeholders: • Medecins Sans Frontieres • UNHCR • Imperial College London • Municipality of Gyor • University of Deusto
Innovation	
List of Project IP	Project IP needs to be developed first.
Innovation Strategy	The project focuses contributions and improvements to well-established community codes. This ensures the uptake and simplifies community building. Furthermore, HiDALGO follows a strict Open Source policy in order to foster the access to codes, whenever possible.
Contacts	
• Principal Investigator	**Francisco Javier Nieto de Santos, ATOS** francisco.nieto@atos.net
• Project Manager	**Michael Gienger, HLRS** gienger@hlrs.de
• Training contact	**Michael Gienger, HLRS** gienger@hlrs.de
• Innovation contact	**Gert Breitfuss, KNOW** gbreitfuss@know-center.at
• Dissemination contact	**Robert Elsaesser, PLUS** elsa@cs.sbg.ac.at
• Exploitation contact	**Lara Lopez Muniz, ATOS** lara.lopez@atos.net

8.8 CoE Description (8): MAX

Max Material design At eXascale	
Consortium Partners	1. CONSIGLIO NAZIONALE DELLE RICERCHE – ISTITUTO NANOSCIENZE (CNR), Italy, Coordinator 2. COMMISSARIAT À L'ÉNERGIE ATOMIQUE ET AUX ÉNERGIES ALTERNATIVES (CEA), France 3. FORSCHUNGSZENTRUM JUELICH GMBH, Germany 4. BARCELONA SUPERCOMPUTING CENTER - CENTRO NACIONAL DE SUPERCOMPUTACION (BSC), Spain 5. CINECA, Italy 6. ETH Zurich, Switzerland 7. SCUOLA INTERNAZIONALE SUPERIORE DI STUDI AVANZATI (SISSA), Italy 8. INSTITUT CATALA DE NANOCIENCIA I NANOTECNOLOGIA (ICN2), Spain 9. ECOLE POLYTECHNIQUE FEDERALE DE LAUSANNE (EPFL), Switzerland 10. ARM, UK 11. E4 COMPUTER ENGINEERING SPA, Italy 12. INTERNATIONAL CENTRE FOR THEORETICAL PHYSICS (ICTP), Italy 13. GHENT UNIVERSITY, Belgium 14. PSI-K, UK 15. TRUST-IT SERVICES, Italy 16. CENTRE EUROPEEN DE CALCUL ATOMIQUE ET MOLECULAIRE (CECAM), France
Duration and effort	36 months (December 2018 – November 2021)
Mission-Main topics-Codes-Sectors	
Mission	MAX (Materials design at the eXascale) is a user-driven European Centre of Excellence (ECoE) established to support developers and end-users for materials simulations, design and discovery. MAX is focused at enabling the best use and evolution of HPC technologies by creating an ecosystem of knowledge, capabilities, applications, data workflows, analytic tools and user-oriented services.
Main scientific topics	MaX is in the domain of material modelling. Materials are crucial to scientific and technological change and industrial competitiveness, as well as to tackle key societal challenges – from energy and environment, to health care, information and communications, industrial processes and manufacturing, safety and transportation. The increasingly high accuracy and predictive power of computer simulations combined with the increasingly higher levels of computing power and large amounts of storage capacity of High-Performance Computing (HPC) technologies, nowadays enables a paradigm shift in material design and discovery, in which every increasingly complex material behaviour will be addressed by easily accessible, interdisciplinary, easy-to-use computational experiments.

<table>
<tr><td></td><td>Below is the project Workpackage layout.

<table>
<tr><th>WP #</th><th>Work Package Title</th></tr>
<tr><td>WP1</td><td>Exascale-enabling software architectures</td></tr>
<tr><td>WP2</td><td>Performance portability: European codes at the exascale</td></tr>
<tr><td>WP3</td><td>Code evolution: exploiting algorithmic advances</td></tr>
<tr><td>WP4</td><td>Exascaling and codesign technologies</td></tr>
<tr><td>WP5</td><td>Ecosystem for HPC, HTC and HPDA convergence</td></tr>
<tr><td>WP6</td><td>Demonstration</td></tr>
<tr><td>WP7</td><td>High level domain-specific support</td></tr>
<tr><td>WP8</td><td>Training and User Uptake</td></tr>
<tr><td>WP9</td><td>Engagement, Communication, Dissemination & Uptake</td></tr>
<tr><td>WP10</td><td>Management</td></tr>
</table></td></tr>
<tr><td>Codes of interest</td><td>
<table>
<tr><td>codes</td><td>Quantum Espresso, Yambo, Fleur, Siesta, BigDFT, CP2K</td></tr>
<tr><td>framework</td><td>AiiDA</td></tr>
<tr><td>Domain Specific Libraries</td><td>Sirius, FFTXLib, LAXLib</td></tr>
</table></td></tr>
<tr><td>Addressed industrial sectors</td><td>MAX is designed and managed to support the needs and the visions of a number of players:
• End-users in research and innovation, both in industry and academia, who explore materials discovery and rely on computer experiments.
• Domain scientists who develop new methods, algorithms and tools in materials simulations.
• Software engineers and vendors who optimise hardware and software performance and usability together with analytical tools for increasingly efficient computer-assisted materials design.
• HPC centres and industry who are interested in empowering the most advanced and ambitious solutions and in hardware-software co-design</td></tr>
<tr><td colspan="2">Services – Training</td></tr>
<tr><td>Services</td><td>MaX implementation strategy consists of developing a new application and data ecosystem, and to serve its industrial and academic community through end-user oriented actions. MAX key actions include:

• Implementing a Sustainable Programming Platform properly designed</td></tr>
</table>

	quantum engine kernels and low-level domain specific libraries, to facilitating quantum engines advanced functionalities and to share libraries with other communities/domains. • Building a Dynamic Data Framework to manage the automation of high-throughput calculations, automatic data storage, workflows interchange where data provenance, preservation, reproducibility, and reuse are guaranteed. • Promoting the Exascale Transition Enabling Action through the development of novel algorithms, domain-specific libraries, in-memory data management, and software/hardware co-design. • Establishing the User Needs and Solutions Integrating Protocol by aligning the technological offer with leading end-users requirements. • Developing a Catalogue of Services accommodating end-users help-desk and support, communities' integration, industrial outreach, custom development and consulting. • Contributing to the diffusion of material simulations by addressing the skills gap through an integrated offer of Training and Education programs in HPC and computational material science. **MaX Pilot Projects** Four Pilot Projects have been identified to demonstrate the use of data produced by flagship codes in the context of HPDA, HPC and HTC calculations: i. Predicting Code Performance. ii. Configuration explorer/data explorer toolkit. iii. Dissemination of highly-curated computational materials data. iv. Edge computing: Deployment of data analysis solutions co-located with experiments. **MaX Demonstrators** One of the core objectives of MaX is to define and plan the onboarding of new demonstrators, and has a dedicated task to identify additional demonstrators over the lifespan of the project addressing specific scientific challenges that would not be possible without the technology developments of the codes which are as follows: • Pre-exascale-ready Demonstrators. • Reduction of the complexity in very large-scale systems. • Full DFT simulation of new, particle-like objects in chiral magnets. • RPA and double hybrid-based MD simulations of condensed phase systems. • Coupled electrons and phonon dynamics within NEQ–MBPT in technologically relevant materials.
Training	
Interaction with industry	

Interaction with industry

#	Priority Stakeholder Group and dissemination vehicles	Main outcomes of interest	Resulting benefits and impacts
1	**European and member states institutions** *Online reports with fresh insights* *Policy recommendations* MAX *plans and roadmaps*	Pre-exascale and exascale computing capabilities. Scalable and sustainable parallel codes (wider use across science, industry and to address societal challenges). Sustainability Plan. Less fragmentation across member states through collaboration.	Boosting industrial, economic and societal innovation. A complete HPC value chain in EU with applications as a lever for leadership. Key steps towards EuroHPC strategy for stronger EU leadership. Priority frameworks for smart specialisation strategies. Meeting new and future training needs, filling skills gaps.
2	**European HPC ecosystem (HPC centres, Prace, Eudat, . . .).** *Joint promotion on common goals, training, technical and results showcase events. Common approaches.*	Codes portable to & scalable on future HPC computing platforms. Joint contributions to the EuroHPC strategy. Training package for re-use. Avoided duplication and increased impacts. Open source codes.	Advanced use cases; showcases of performance, energy efficiency, scalability based on new benchmarks. Optimised use of HPC resources Shared best practices and common co-design processes. Enlarged pool of skilled young people as testimonials to the benefits of HPC.
3	**Hardware Manufacturers.** *Co-design reports.* *Roadmaps and SW/Data plans.* *Technical reports*	Shared co-design cycle and strategies for the design of new products. Demonstrated new benchmarks, e.g. performance, energy efficiency, scalability.	Showcases of advances in the field. Enlarged market, opportunity to consolidate HPC market position for next generation machines, including SME providers.
4	**Industrial & academic end-users.** *Collaboration with the CSA for targeted outreach and dedicated info packs.* *Downloadable OS SW & documentation.* *Dedicated technical workshops, hands-on training/hackathons/summer schools with online re-usable content for self-paced skills development.*	Flagship codes ready for use. User-friendly adoption packages and documentation for HPC & HTC. Easy access to research data, SW, reports. User-oriented workflows and turn-key solutions with potential for bespoke support.	Scientific & technological breakthroughs for new usages. Evermore robust access to efficient materials simulation software, rapidly incorporating scientific advances and running effectively on evolving architectures. Sustainable environment to manage calculations, high-throughput and data. Containerisation for easy access, especially for SMEs. High-level domain-specific support. Enlarged pool of skilled young people, equipped for industry work environments.
5	**Independent software vendors (ISVs), code developers** *Downloadable OS SW & documentation.* *Individual code forum, mailing lists.* *Dedicated training events and re-usable materials.* *Briefings/1-2-1 meetings at events*	OS code, modules, libraries, where code modularisation central to the MAX strategy is a key ISV asset. Extensions in-code documentation.	High-quality open source code modules and libraries, rapidly incorporating scientific advances and ensuring performance portability, code documentation. High-level domain-specific support. New skill sets developed.New opportunities in value chain identified.
6	**Large scale experimental facilities** *Downloadable OS SW & documentation. Dedicated technical workshops, hands-on training and online re-usable content.*	Containerisation for easy use by experimental teams. Integrated data strategies, moving codes to data. New benchmarks.	Enabled the design of new experiments in scientific or industrial settings. Supported interpretation of experiments, computational spectroscopy.
7	**Education system.** *Teaching and training events; material to suit different trainee and HR needs.* *Ready-to-use workflows.* *Downloadable OS SW & documentation.*	Education and teaching materials (undergrad and graduate students level), including for hands-on modules based on open source codes Easy access to open source codes (containers) and documentation.	Sustainable environment to manage calculations & data and retrieve information. Highly effective and re-usable resources.

Innovation

Contacts

- Training contact — Daniele Varsano, daniele.varsano@nano.cnr.it
- Dissemination contact — Silvana Muscella (Dissemination), s.muscella@trust-itservices.com; Luisa Neri (Exploitation), luisa.neri@nano.cnr.it

8.9 CoE Description (9): POP2

POP2 **Performance Optimisation and Productivity 2**	
Consortium Partners	OVERVIEW: • PRACE Centers (BSC, HLRS, JUELICH, IT4I) • other academic partners (RWTH AACHEN, UVSQ) • 2 private partners (NAG) • others (Teratec, association) IN DETAIL: • Barcelona Supercomputing Center (ES) • Universität of Stuttgart – HLRS (DE) • Forschungszentrum Julich GMBH (DE) • Numerical Algorithms Group Ltd (UK) • Rheinisch-Westfälische Technische Hochschule Aachen (DE) • TERATEC (FR) • Universite De Versailles Saint-Quentin-En-Yvelines (FR) • Vysoka Skola Banska - Technicka Univerzita Ostrava (CZ)
Duration and effort	36 months, starting in Dec. 2018, overall budget € 7 605 998,75
Mission-Main topics-Codes-Sectors	
Mission	• Continue and improve the POP project operating a Centre of Excellence in Computing Applications in the area of Performance Optimisation and Productivity with a special focus on very large scale towards exascale. • Continue the service oriented activity, giving code developers, users and infrastructure operators an impartial external view that will help them improve their codes.
Main scientific topics	• Performance Tools and analysis • Code optimization • Parallel programming models • Productivity

Codes of interest	Open-source toolsets (developed by POP partners and collaborators)
	• BSC performance tools
	  ○ Extrae http://tools.bsc.es/extrae
	  ○ Paraver http://tools.bsc.es/paraver/
	  ○ Dimemas http://tools.bsc.es/dimemas
	• JUELICH performance tools
	  ○ Scalasca http://www.scalasca.org/
	  ○ Cube http://www.scalasca.org/software/cube-4.x/
	  ○ Extra-P http://www.scalasca.org/software/extra-p/
	  ○ Score-P http://www.score-p.org/
	  ○ Vampir (via collaboration partner Technical University of Dresden) http://www.vampir.eu/

	○ TAU (via collaboration partner University of Oregon) http://tau.uoregon.edu/ • UVSQ performance tools ○ MAQAO http://www.maqao.org/ • MUST and Thread Sanitizer / ARCHER https://pruners.github.io/archer/ Commercial tools (if available at customer site): • Intel tools ○ Trace Analyzer and Collector https://software.intel.com/en-us/intel-trace-analyzer ○ VTune Amplifier https://software.intel.com/en-us/intel-vtune-amplifier-xe • Cray Performance Measurement and Analysis Tools (or CrayPAT) https://pubs.cray.com/content/S-2376/7.0.0/cray-performance-measurement-and-analysis-tools-user-guide/ • ARM tools ○ MAP https://www.arm.com/products/development-tools/server-and-hpc/forge/map ○ Performance Reports https://www.arm.com/products/development-tools/server-and-hpc/performance-reports
Addressed industrial sectors	Main • The addressed industrial sector is any with need of code-optimisation • The target customers are code developers, code users, infrastructure operators and vendors
Services – Training	
Services	POP2 provides performance optimisation and productivity services for academic and industrial code(s) in all domains. It offers a portfolio of services designed to help users optimise parallel software and understand performance issues. 1. Parallel Application Performance Assessment • Initial analysis measuring a range of performance metrics to assess quality of performance and identify the issues affecting performance 2. Proof-of-Concept • Experiments and mock-up tests for customer codes (after initial performance assessment) • Kernel extraction, parallelisation, mini-apps experiments to demonstrate the actual benefits of proposed optimisations
Training	The main training activities offered by POP are: • Performance analysis of parallel applications: processes and tools • Webinars https://www.youtube.com/playlist?list=PLDPdSvR_5-GhR1OWQW3ovK_qGg09tmNuq The fundamental focus will continue on well-targeted training events,

	focused as much as possible on real code examples of the customers. It will also continue the gathering and production of new material on tools, programming models and practices that have been done within POP1. In the training workshops, attendees bring their application code and POP teaches them about using the tools and do a preliminary performance analysis of their codes. The spectrum of activities ranges from half- or one-day conference tutorials to tuning workshops lasting up to a week. BSC, HLRS, IT4I, JUELICH and UVSQ are part of their national PRACE (Advanced) Training Centres. In addition, the project partners BSC, HLRS, JUELICH, RWTH, and UVSQ bundle their training activities in the framework of the Virtual Institute – High Productivity Supercomputing (VIHPS, www.vi-hps.org), which offers effective advertisement channels, including a website, a mailing list, a "VI-HPS Tools Guide", and flyers. VI-HPS is an initiative of currently twelve HPC tool builders in Europe and the USA, including universities, national labs, and companies. Next to the development of state-of-the-art productivity tools for high performance computing, VI-HPS also provides training in the application of these tools.
Interaction with industry	
Interaction with industry	Providing the services mentioned above
Types of interaction	Interactions with code developers: • Assessment of detailed actual behaviour • Suggestion of most productive directions to refactor code With users: • Assessment of achieved performance in specific production conditions • Possible improvements modifying environment setup • Evidence to interact with code provider With infrastructure operators: • Assessment of achieved performance in production conditions • Possible improvements from modifying environment setup • Information for time computer time allocation processes • Training of support staff With vendors: • Benchmarking • Customer support • System dimensioning/design
Already done	More than 120 assessment services provided to customers in academia, research and industry (https://pop-coe.eu/target-customers/success-stories)
Innovation	
List of Project IP	POP2 contributes to the development of several free and open-source software solutions:

	• Scalasca [3-clause BSD License] (JUELICH) - Trace Tools - Cube • BSC performance tools [GNU Lesser General Public License] (BSC) - Paraver - Extrae - Dimemas - Basic analysis - Clustering - Tracking - Folding • Score-P [3-clause BSD License] (JUELICH, RWTH) • MAQAO [GNU Lesser General Public License] (UVSQ)
Contacts	
• Principal Investigator	Jesús Labarta (BSC) , jesus.labarta@bsc.es Judit Gimenez (BSC), judit.gimenez@bsc.es
• Project Manager	Yara Duverger (BSC) , yara.duverger@bsc.es
• Training contact	Bernd Mohr (Juelich), b.mohr@fz-juelich.de
• Innovation contact	Mike Dewar (NAG), mike.dewar@nag.co.uk
• Dissemination contact	Bernd Mohr (Juelich), b.mohr@fz-juelich.de

8.10 CoE Description (10): EXCELLERAT

EXCELLERAT **The European Centre of Excellence for Engineering Applications**	
Consortium Partners	OVERVIEW: • PRACE Centers (HLRS, CINECA, BSC, EPCC) • other academic partners (KTH, CERFACS, Fraunhofer, DLR, RWTH) • 3 private partners (SICOS, SSC, Arctur) • others (Teratec, association) IN DETAIL: • Universität of Stuttgart – HLRS (DE) • The University of Edinburgh (UK) • CINECA (IT) • Sicos BW GmBH (DE) • Kungliga Tekniska Hoegskolan – KTH (SE) • Arctur (SL) • DLR: DEUTSCHES ZENTRUM FUER LUFT- UND RAUMFAHRT (DE) • Centre Européen de la Recherche et de la Formation avancée en Calcul Scientifique (FR) • Barcelona Supercomputing Center (ES) • SSC-Services GmBH (DE) • Fraunhofer Gesellschaft (DE) • Teratec (FR) • Rheinisch Wesfaelische Technische Hochshule Aachen (DE)
Duration and effort	36 months, starting in Dec. 2018, overall budget € 7 884 757,50
Mission-Main topics-Codes-Sectors	
Mission	• Engineering applications will be among the first exploiting Exascale, not only in academia but also industry. In fact, the industrial engineering field is the industrial field with the highest Exascale potential. • All of this to support strongly the engineering community and to pave the way for the evolution of applications towards Exascale. • EXCELLERAT brings together Europe's leading HPC centres, application specialists and supporting partners who have worked with and offered their expertise and knowledge to engineering companies and researchers from across industry and academia for the past three decades. • Ensuring that innovations produced are applicable to other engineering codes.

Main scientific topics	• Engineering applications
	• Exascale technologies & methodologies
	  ○ Node Level Performance Optimization
	  ○ System-Level Performance Optimization

	○ Advanced Meshing ○ Data Handling • High Performance Data Analytics
Codes of interest	• **Nek5000:** https://nek5000.mcs.anl.gov/ a fast and scalable high-order solver for computational fluid dynamics • **Alya**: https://www.bsc.es/es/computer-applications/alya-system/ Large Scale Computational Mechanics • **AVBP**: http://www.cerfacs.fr/avbp7x/ software tool for Computational Fluid Dynamics • **Fluidity:** http://fluidityproject.github.io/ open source, general purpose, multiphase computational fluid dynamics code • **FEniCS:** https://fenicsproject.org/ FEniCS is a popular open-source computing platform for solving PDEs • **Flucs:** FLexible Unstructured CFD Software For each of the codes, at least one developers and users have committed to the project. To each code are associated a couple of use cases, which will serve to "test" the improved codes.
Addressed industrial sectors	Main • Aerospace, • Automotive • Combustion Engines Secondary • Energy • Renewables • Marine • Environmental modelling
Services – Training	
Services	• Support in porting/optimising code • Development of dedicated "general purpose tools/ plug-ins", who are of interest to the community • Expertise on the ecosystem, network consulting • Support services for the entire life cycle of engineering applications (e.g., visualization, data management, data transfer)
Training	Not determined yet
Interaction with industry	
Interaction with industry	For each of the codes, (at least one of) the key developers, the key users have committed to the project. Data from website: • **Nek5000:** Scania, Tetra Pak, Agusta Westland • **Alya**: Idiada, EM Combustion, iVascular, IHT, Seat, Repsol, Iberdrola, Medtronic, Siemens AG General Electric • **AVBP**: SAFRAN Group, TOTAL, CNES, Ariane Groupe • **Fluidity:** Flo-wave, Rio Tinto, Alstom Group, Meygen Ltd, Renewable Energy Systems Ltd, HR

	Wallingford Ltd • **FEniCS:** Augusta Westland • **Flucs:** Airbus
Types of interaction	• Industry provides new challenges arising from their usage to "test" the EXCELLERAT services (feeding back into business model) • ISVs and industrial users are gathered around EXCELLERAT via "special interest groups"
Already done	Does not apply yet
Contacts already established	Some industrial users have already indicated strong interest to participate in EXCELLERAT's interest groups – information on this will be shared later on.
Innovation	
List of Project IP	Project IP needs to be developed first.
Innovation Strategy	EXCELLERAT relies on a mixture of Open Source and proprietary codes. Hence, a thorough IPR strategy is required, which needs to ensure that ownership of results is clearly defined. All innovative developments follow the module concept as much as possible, so that individual combinations and code contributions are provided.
Contacts	
• Principal Investigator	**Bastian Koller, HLRS** koller@hlrs.de
• Project Manager	**Ralf Schneider, HLRS** schneider@hlrs.de
• Training contact	**Claudio Arlandini, CINECA** c.arlandini@cineca.it
• Innovation contact	**Andreas Wierse, SICOS** wierse@sicos-bw.de
• Dissemination contact	**Lena Buehler, HLRS** buehler@hlrs.de