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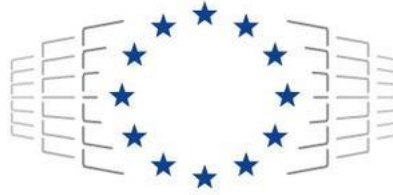


**Coordination & Support  
for National Competence Centres on a European Level Phase 2**

**Project Number: 101102047**

**D2.1**

**First year report on NCC/CoE Networking,  
Mapping of Competences, Codes and  
Services**



This project has received funding from the European High-Performance Computing Joint Undertaking (JU) under grant agreement No 101102047. The JU receives support from the Digital Europe Programme and Germany, Italy, Spain, France, Belgium, Austria.

<b>Work package:</b>	2	NCC/CoE Networking and Mapping of Competences, Codes and Services
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<b>Dissemination Level</b>	PU - Public	

Date	Author	Comments	Version	Status
2023-09-22	Laura Morselli	Initial draft	V0.0	Draft
2023-10-26	Laura Morselli	Draft Sent to WP2 partners	V0.1	Draft
2023-11-4	Laura Morselli	Initial comments of WP2 partners implements	V0.2	Draft
2023-11-13	Laura Morselli	Comments of WP2 partners implements and sent to reviewers	V1.0	Draft
2023-11-25	Laura Morselli	Started implementation of reviewers' comments	V1.1	Draft
2023-11-29	Laura Morselli	Reviewers' comments included	V1.2	Final
2023-12-06	Laura Morselli	Small refinements, sent to PMT	V1.3	Final
2023-12-13	Laura Morselli	Feedback from PMT included. Final version.	V1.4	Final

## List of abbreviations

<i>AI</i>	<i>Artificial Intelligence</i>
<i>BSCW</i>	<i>HLRS Social Workspace Server</i>
<i>C2ISS</i>	<i>CASTIEL 2 Information Sharing System</i>
<i>CoE</i>	<i>Centre of Excellence</i>
<i>CSA</i>	<i>Coordination and Support Action</i>
<i>EuroHPC JU</i>	<i>European High Performance Computing Joint Undertaking</i>
<i>GA</i>	<i>Grant Agreement</i>
<i>HPC</i>	<i>High Performance Computing</i>
<i>HPC3</i>	<i>HPC CoE Council</i>
<i>HPDA</i>	<i>High-Performance Data Analytics</i>
<i>KPI</i>	<i>Key Performance Indicator</i>
<i>NCC</i>	<i>National Competence Centre</i>
<i>PMT</i>	<i>Project Management Team</i>
<i>QC</i>	<i>Quantum Computing</i>
<i>TPR</i>	<i>Technical Progress Report</i>
<i>WP</i>	<i>Work Package</i>
<i>WPL</i>	<i>Work Package Leader</i>

## Executive Summary

This document provides information about the objectives, activities and results of Work Package (WP) 2 of CASTIEL 2 for the reporting period 01/01/2023-31/12/2023. CASTIEL 2 continues the mission of the CASTIEL H2020 project by coordinating and supporting the National Competences Centres (NCCs) and enlarges its activities to include the Centres of Excellence (CoE) in HPC. WP2 “NCC/CoE Networking and Mapping of Competences, Codes and Services” facilitates effective networking and collaboration between NCCs, CoEs and amongst NCCs and CoEs, and aims at mapping competences and codes of NCCs and CoEs, to make them known to the whole European HPC ecosystem. The main objectives of WP2 are: *i)* to host regular discussions between NCCs and CoEs on topics of mutual interest, with the support of HPC CoE Council (HPC3) and EuroCC2; *ii)* to interact with HPC3 to ensure fostering of collaborations between CoEs; *iii)* to contribute to the CASTIEL 2 Information Sharing System (C2ISS) design in terms of specifications and technical requirements for storing, indexing and referencing the HPC competences, codes & libraries; *iv)* to define and run workshops on non-HPC specific relevant topics and competences, based on the needs expressed by NCCs and CoEs; *v)* to guide WP2 activities by the improvements observed in competences.

In the first months of the project, WP2 focused the attention on onboarding CoEs with the activities of CASTIEL 2 and on creating opportunities to NCCs and CoEs to know each other's roles, objectives, areas of work. Examples of activities that were organised for this purpose are: the “NCCs-CoEs online meeting” and the summary document on CoEs requested by several NCCs. The creation of this document and the activities related to the milestone “Special Access Scheme” allowed WP2 to collect information about more than 60 codes managed by the CoEs.

The upgrade of the Competence Map on EuroCC Access (developed during phase 1 of EuroCC/CASTIEL) was the other focus of WP2 during the first year of the project. The need of an upgrade of the Competence Map produced by CASTIEL was expressed by NCCs on several occasions and WP2 supported the creation of a Task Force dedicated to such activity. The upgrade is currently ongoing, and the new structure of the Competence Map is planned for the end of the year 2023; the upgraded version will be used by WP3 to define the Mentoring and Twinning activities and to monitor the increase of competences in the CASTIEL 2 network. WP2 collaborated with WP5 for the questionnaire on the C2ISS, by preparing questions about codes and competences. The answers of NCCs and CoEs provided important input on how NCCs and CoEs wish to have their codes and competences collected and displayed in the C2ISS database. Finally, several webinars organized by WP2 or with the support of WP2 (and chosen based on the needs specified by NCCs and CoEs) took place in the reporting period.

The activities undertaken by WP2 during the first year of the CASTIEL 2 project were essential for establishing the basis for a successful collaboration of NCCs and CoEs with WP2 and among them. Several activities are currently being planned for the second year of the project, including a new series of monthly webinars on Energy Efficient Computing, the organization of development-oriented workshops and activities to address common issues of CoEs and NCCs related to code development and optimization, and the first collection of competences of NCCs and CoEs for the upgraded Competence Map and for C2ISS.

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# 1 Introduction

This document is the first periodic report of WP2 of CASTIEL 2 [1] and it provides information about the WP objectives and results for the reporting period 01/01/2023-31/12/2023. The Coordination and Support Action CASTIEL 2 continues the mission of the CASTIEL H2020 project [2] by coordinating and supporting the National Competences Centres and enlarges its activities to include also the Centres of Excellence in HPC (see list in Section 2). WP2 “NCC/CoE Networking and Mapping of Competences, Codes and Services” facilitates effective networking and collaboration between NCCs, CoEs and amongst NCCs and CoEs, and aims at mapping competences and codes of NCCs and CoEs, to make them known to the whole European HPC ecosystem.

In particular, the objectives of WP2 are to:

- Host regular discussions between NCCs and CoEs on topics of mutual interest, with the support of HPC CoE Council (HPC3 [3]) and EuroCC2.
- Interact with HPC3 to ensure fostering of collaborations between CoEs;
- Contribute to the Information Sharing System design in terms of specifications and technical requirements for storing, indexing and referencing the HPC competences, codes & libraries, and services offered by the NCCs and CoEs – focusing on the needs of the information providers (NCCs, CoEs) and academic/government end-users.
- Define and run workshops on non-HPC specific relevant topics and competences (soft skills, complementary competences), based on the needs expressed by NCCs and CoEs and make the materials available.
- Guide WP2 activities by the improvements observed in competences and the amount and kind of information made available through the EuroCC Access portal and provide input for WP1 (KPIs).

The activities of WP2 are divided into two tasks:

- T2.1 “Contribution to the C2ISS and the EuroCC Access Portal”, that focuses mostly on the mapping of competences and codes as inputs to the C2ISS and the EuroCC Access Portal;
- T2.2 “CoE/NCC Networking and Collaboration Support”, that aims at facilitating effective communication and collaboration among and between the set of NCCs and CoEs and at identifying and organising events (webinars, workshops, ...) on relevant topics.

As in phase 1, WP2 (and all the WPs of CASTIEL 2) interacts with NCCs and CoEs via WP2 “champions” and their deputies, e.g. people nominated by each NCC/CoE that are the contact points between CASTIEL 2 and the NCCs/CoEs and are in charge of reporting the CASTIEL 2 WP2 activities within their NCC/CoE. WP2 partners and the WP2 champions and deputies together constitute the WP2 Working Group.

In Section 2 of this Deliverable, the activities and events that supported the collaboration among NCCs, among CoEs and between NCCs and CoEs are reported, with a mention to the role of the HPC CoE Council (HPC3, Section 2.1), the Kick Off meeting of EuroCC2/CASTIEL 2 (Section 2.2), the NCCs-CoEs online meeting (Section 2.3) and the summary document on CoEs (Section 2.4).

Section 3 collects the activities of WP2 related to the competences and codes of NCCs and CoEs, in particular: the analysis of the questionnaire on C2ISS (questions concerning competences and codes) for NCCs and CoEs (Section 3.1), an analysis of the status of the current Competence Map of NCCs on EuroCC Access (Section 3.2) and the process of the



upgrade of the Competence Map on EuroCC Access that WP2 has been working on (and will continue to work on in the upcoming months). Section 3.4 focuses on the webinars that were organised by WP2 following the needs of NCCs and CoEs and aimed at fostering their collaboration. The activities related to the Special Access Scheme milestone are reported in Section 4. The codes and use cases of CoEs (for few of them referred to as “Grand Challenges”) are included in Section 5. Finally, Section 6 focuses on the activities of the Task Force “SME Assessment Tool”, Section 7 summarises the main achievements of WP2 in the first year of the project, and Section 8 includes the conclusions and an outlook on the activities of WP2 in the upcoming months.

## 2 Establishing the basis of the collaboration between NCCs and CoEs

Many of the activities of WP2 involve NCCs, CoEs and often other players of the European and worldwide HPC Ecosystem. CASTIEL 2 is per GA the CSA for the 10 JU-funded HPC CoEs who started in January 2023 ([4]), who also have the collaboration with CASTIEL 2 in their GAs. These CoEs are part of the CASTIEL 2 networking & competences working group managed by WP2 and of the inner “NCC & CoE network” and are:

- The BioExcel Centre of Excellence for Computational Biomolecular Research (BioEXCEL-3 [5]);
- The Centre of Excellence for Exascale CFD (CEEC [6]);
- The Centre of Excellence for Exascale in Solid Earth – Second Phase (ChEESE-2P [7]);
- The European Centre of Excellence for Engineering Applications on HPC and associated technologies (EXCELLERAT-P2 [8]);
- The Centre of Excellence for weather and climate phase 3 (ESiWACE-3 [9]);
- The HPC and Big Data Technologies for Global Challenges (HIDALGO-2 [10]);
- Materials Design at the Exascale (MaX-3 [11]);
- The Centre of Excellence in exascale-oriented application co-design and delivery for multiscale simulations (MultiXscale [12]);
- Plasma Exascale-Performance Simulations (Plasma-PEPSC [13]);
- Scalable Parallel and Distributed Astrophysics Codes for Exascale (SPACE [14]).

The 6 already running EC-funded CoEs (which will end between end 2023 and mid 2024) are considered the closest part of the HPC ecosystem, in view of their objectives close to those of the newly launched CoEs and their many, still ongoing, collaborations with NCCs stemming from the previous phase of CASTIEL. Thus, WP2 has strived to involve these CoEs wherever this was possible without the need for the more formalised relationship which is being established with the 10 new CoEs. For this reason, the interaction of CASTIEL 2-WP2 and HPC3 has played a key role in increasing the awareness of all the CoEs about the activities and objectives of CASTIEL 2, as outlined in Section 2.1. Other activities that saw the collaboration of WP2 with all the CoEs are the “NCCs-CoEs online meeting” in April 2023 (see Section 2.3) and the “Code of the Month” series of webinars (Section 3.4.1). Other activities were focused on the 10 CoEs started in January 2023, as the Kick Off meeting in Stuttgart (see Section 2.2), the summary document on CoEs (see Section 2.4) and the activities related to the Special Access Scheme milestone (see Section 4).

## 2.1 Interaction of CASTIEL 2 and HPC3

HPC3 was established with support from the CSA FocusCoE (December 2018 – March 2022 [15]) in May 2019 and was continued by the then active CoEs after the end of FocusCoE. HPC3 is run as an inclusive forum by the CoEs in order to exchange information, coordinate activities and identify common viewpoints. CASTIEL 2 WP2 is interacting with HPC3 and sees it as a very useful means of communication which is a good complement to the internal structures of CASTIEL 2 as HPC3 is driven by the CoEs themselves and permits to develop longer-term overarching views and positions in the context of application-oriented HPC research in Europe. Especially at the initial phase of CASTIEL 2, HPC3 was invaluable as a mean to make timely connection to all newly established CoE, as these had joined HPC3 already during their GA negotiation phase. HPC3 meets approximately on a monthly schedule.

## 2.2 The Kick Off Meeting in Stuttgart

The Kick Off meeting of CASTIEL 2 and EuroCC2 took place from the 7<sup>th</sup> to the 9<sup>th</sup> of February 2023 in Leinfelden near Stuttgart. During the meeting, WP2 had the chance to present to WP2 champions, and anyone else interested in attending the session, what was done during phase 1 of CASTIEL and to present its objectives and planned activities for phase 2. In preparation to the meeting, WP2 prepared an anonymous form to collect feedback from WP2 NCCs champions on what was done in phase 1 so to better address the activities of CASTIEL 2. The collected feedback as well as the open discussion that took place in the WP2 session during the Kick Off meeting underlined the following points:

- Need to have a better knowledge of the existing CoEs and of the opportunities for collaboration between NCCs and CoEs;
- Importance of setting up an efficient communication mechanism between NCCs and CoEs;
- Importance of having an easy-to-use Competence Map and to be informed of competences of other NCCs to set up possible twinning/mentoring activities, or other types of collaboration.
- Importance of keeping NCCs engaged and of planning 1-to-1 meeting as the “pitch-like” presentations done during phase 1.

This feedback was important to set up the activities of WP2 in the first year of the project. While some of the 10 CoE having started their activities in January 2023 were present at the Stuttgart kick off, it became clear that more opportunities to present the CoEs in some detail and to initiate discussions and interaction between NCCs and CoEs were needed. Thus, following the Kick Off meeting, WP2 decided to organise a 2-day online meeting focussing on the CoEs with the aim of (a) presenting all CoEs (including the 6 already running CoEs who were not present at the Kick Off) to each other and to the NCCs and (b) to fully onboard CoEs with the activities of CASTIEL 2 (see Section 2.3). This meeting also served as a starting point for subsequent activities directed at giving CoEs opportunities to present their work in more detail, such as the “Code of the Month” series of webinars (see 3.4.2). To address the feedback on the Competence Map, WP2 proposed to work on an upgraded version for the EuroCC Access and for the future C2ISS (see Sections 3.1, 3.2 and 3.3). Finally, to address the last point, WP2 decided to plan 1-to-1 meetings with NCCs and CoEs in the second year of the project, once the upgrade of the Competence Map is done.

## 2.3 The NCCs-CoEs online meeting

### 2.3.1 Overall organization

Following the feedback received during the EuroCC2-CASTIEL 2 Kick Off and during the activities related to the Special Access Scheme milestone at M3 (see Section 4), WP2 decided that a meeting was necessary to fully onboard the 10 CoE having started their activities in January 2023 with the CASTIEL 2 activities, as well as to present all the CoEs to the NCCs and vice versa. Thus, WP2 organised the “NCCs-CoEs online meeting” that took place on the 18<sup>th</sup> and 19<sup>th</sup> of April 2023 and was the chance for NCCs to get to know all the CoEs on HPC, for CoEs to better understand the role of CASTIEL 2, the structure and activities of NCCs as well as to get to know the other CoEs, an important aspect especially for the newly funded CoEs. The meeting was a great opportunity to foster future collaborations between NCCs and CoEs. Every CoE had the opportunity to present its aims and activities in a 15-minute presentation. During the second day, each WPL of CASTIEL 2 presented the aims, activities and plans of the respective WPs. The last hour of the second day was reserved for open discussion in the following break-out rooms, led by the WPLs of CASTIEL 2: 1. Competences/services mapping, workshops & NCC-CoE collaboration; 2. Training, twinning & mentoring; 3. Interaction with Industry; 4. Communication. Below the detailed agenda of the online meeting:

#### DAY 1 on 18th April from 11:00 to 13:30

- 11:00-11:05 Welcome
- 11:05-11:20 The National Competence Centers: structure & activities
- 11:20-11:50 Highlights from NCCs on past collaborations between NCCs and CoEs
- 11:50-13:20 CoEs presentations: EXCELLERAT-P2, CEEC, HiDALGO2, ChEESE-2P, MaX-3, SPACE
- 13:20-13:30 Q&A

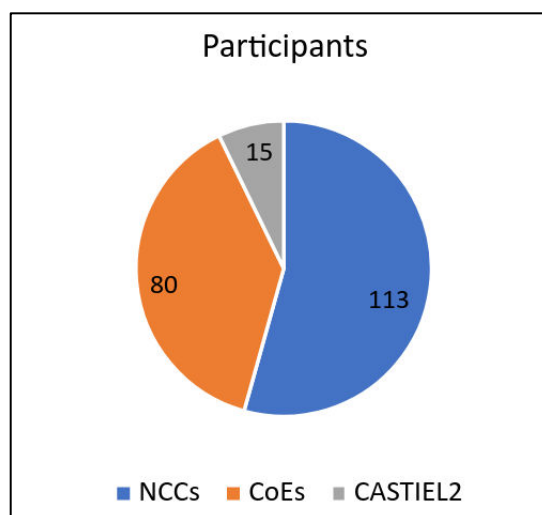
#### DAY 1 on 18th April from 14:30 to 16:10

- 14:30-16:00 CoEs presentations: NOMAD, TREX, RAISE, PerMedCoE, CoEC, CompBioMed
- 16:00-16:10 Q&A

#### DAY 2 on 19th April from 11:00 to 13:30

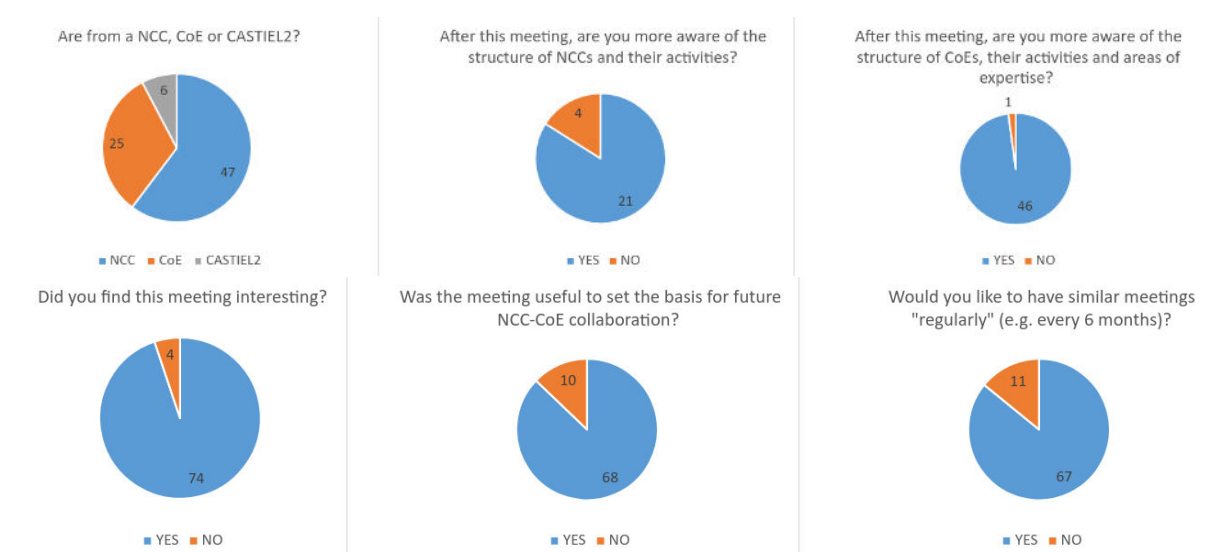
- 11:00-11:05 Welcome
- 11:05-11:30 The role of CASTIEL 2 and short presentations of WPs
- 11:30-12:30 CoEs presentations: MultiXScale, Plasma-PEPSC, BioExcel-3, ESiWACE-3
- 12:30-13:20 Open Discussion in break-out rooms
- 13:20-13:30 Final remarks & next steps

The registrations for the meeting were 208: 113 from NCCs, 80 from CoEs and 15 from CASTIEL 2 (see Figure 1).



**Figure 1: Registered participants to the “NCCs-CoEs online meeting”.**

The average attendance to the meeting was around 170 people in the first day and 130 attendees on the second day. All the slides shown during the meeting were collected and shared with all the NCCs and CoEs via BSCW and HPC3. Finally, a short questionnaire was prepared by WP2 and shared with the registered participants at the end of the meeting to assess the effectiveness of the event. 78 attendees answered the questionnaire: 47 from NCCs, 25 from CoEs and 6 from CASTIEL 2. Of the 25 respondents from CoEs, 21 answered positively when asked “After this meeting, are you more aware of the structure of NCCs and their activities?”. Of the 47 respondents from NCCs, 46 answered positively when asked “After this meeting, are you more aware of the structure of CoEs, their activities and areas of expertise?”. Finally, of the 78 overall respondents, 74 found the meeting interesting, 68 declared that the meeting was useful to the basis for future NCC-CoE collaborations and 67 declared that they would like to have similar meetings regularly. Figure 2 summarises the results of the final questionnaire.



**Figure 2: Summary of the final questionnaire on the “NCCs-CoEs online meeting”.**

When analysing the input received during the meeting as well as through the final questionnaire (especially the last open question “Would you like to leave us any feedback / observations that

could be useful for us to set up the activities of CASTIEL 2?”), WP2 realised the recurrent request, especially coming from NCCs, to have a summary document on CoEs including sector, objectives, partners, contacts, technologies area, and tools. For this reason, WP2 decided to proceed with creating such document, as detailed in Section 2.4.

### 2.3.2 Inputs for WP2 in the breakout room

During the last session of the second day of the NCCs-CoEs online meeting, WP2 led the open discussion in the break-out room “Competences/services mapping, workshops & NCC-CoE collaboration”. To guide the discussion and collect the input, WP2 prepared a concept board that was shared with participants (around 20 people).

When asked “*What are your ideas, expectations, needs for networking with NCCs / CoEs?*” the following aggregated input were collected:

- Organize common activities/events/hands-on sessions with CoEs to know more about the work and find common goals in which CoEs can support NCCs;
- Focused meetings on selected topics, with some CoE and NCC representatives.

When asked “*What topics would interest you most?*” the following input were collected:

- Applications of AI;
- CFD Software and Applications in the Exa-scale era;
- Possible integrations of HPC simulation ("physics-based") and AI methods;
- Code Optimization;
- Quantum Technologies and Quantum Computing Software.

When asked “*NCC & CoEs are information providers for a common information system (C2ISS): codes, libraries, competences, services. Do you have any input/thoughts on this?*” the following aggregated input were collected:

- Importance of providing examples, as success stories of additional material, to showcase competences.
- Importance of navigating the information hierarchically, from general concepts to details.
- Importance of keeping in mind the differences between NCCs and CoEs. Thus, the system should be general enough to accommodate the diverse set of competences and codes.
- The system should reuse "as much as possible" technologies and know-how already developed previous projects.

When asked “*WP2 needs to collect periodic samples of competences/services of NCCs&CoEs to share with them, PMT and JU. For NCCs: what are your thoughts on introducing levels of competences & verification means and sample competences periodically? For CoEs: do you have suggestions/ideas /starting points on how to carry out these periodic samples of competences and services?*” the following aggregated input were collected:

- Importance of agreeing on definition of competences before starting a collection.
- Importance of gathering competences using the existing portals of CoEs and NCCs and all the information already available.



- It is considered useful to provide templates and forms to NCCs and CoEs to fill in as starting points. Then periodically (each year) ask them to send updates.
- Introducing levels of competences and verification means to ensure that certain standards are met. Periodic sampling of competences would help maintain these standards and thus foster collaboration.

Finally, few questions were posed to better collect the needs around meetings of WP2 with its champions. These are the questions and the results:

- *Would you like to attend regular meetings of WP2 Working Group?* YES: 12 ; NO: 3.
- *How frequently would you prefer the WP2 Working Group to meet?* MONTHLY: 4; BI-MONTHLY: 10.
- *Which communication channel do you prefer?* MAIL: 11; SLACK: 6.

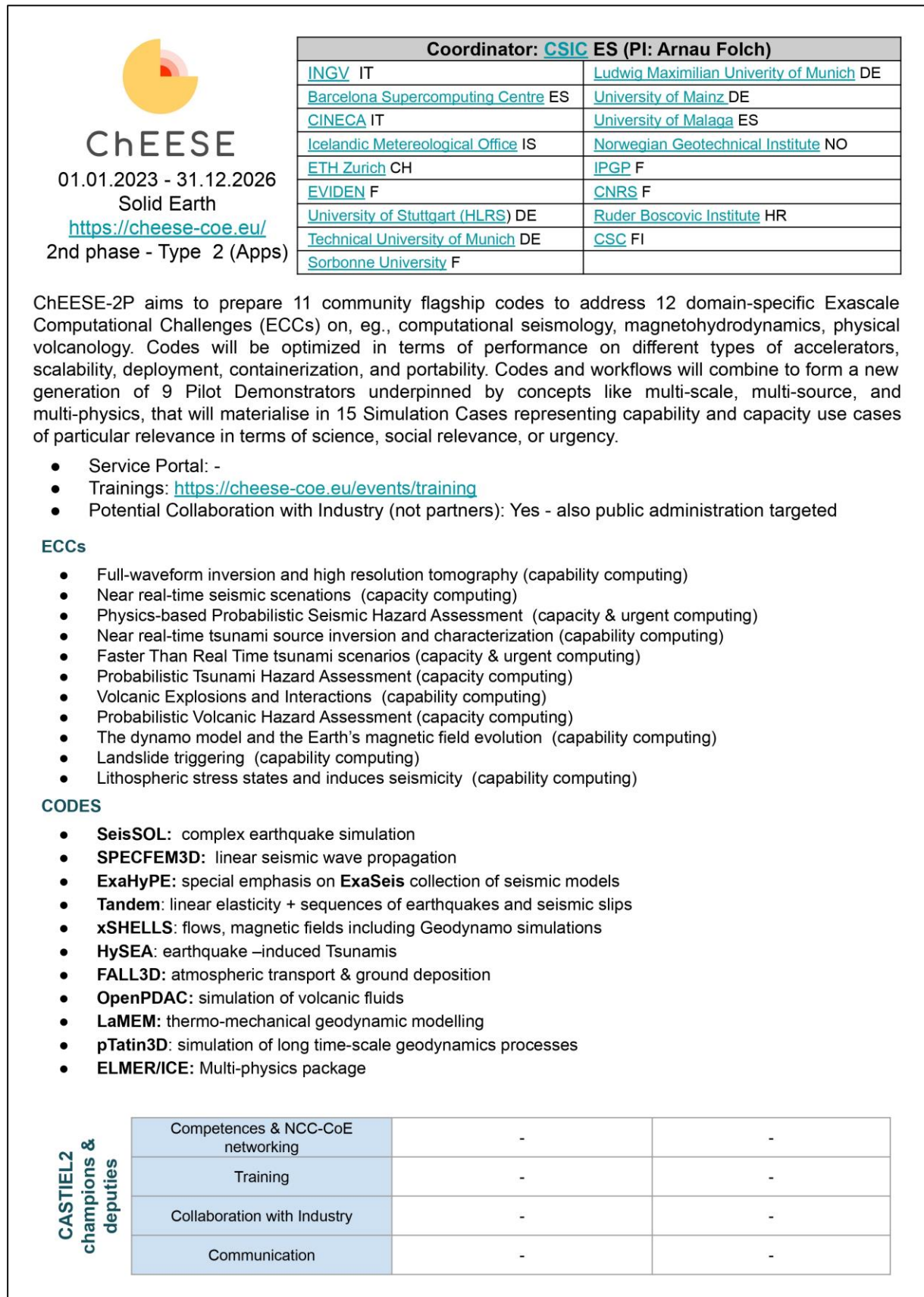
The open discussion held in the break-out room and the input received were important to set up the strategy for the upgrade of the Competence Map on EuroCC Access (Section 3.3) and design the future Competence Map included in the C2ISS (Section 3.1), as well as to start organise webinars for NCCs and CoEs around topics of interest (Section 3.4).

## 2.4 The Summary Document on CoEs

As mentioned in Section 2.3, during the “NCCs-CoEs online meeting” organised by WP2 and that took place on the 18<sup>th</sup> and 19<sup>th</sup> of April 2023, several NCCs expressed the need to have at their disposal a summary document on CoEs containing their objectives, codes / workflows, tools, use cases, partners, contacts, etc. Thus, WP2 decided to be the author of such document, that was prepared during May and June 2023. For each of the 10 CoEs anticipating a collaboration agreement with CASTIEL 2, WP2 collected the following information:

- Coordinator (name, country and name of PI)
- Partners (name and country)
- Duration of the project
- Webpage
- Type (I or II)
- Phase (1 if newly funded, 2 if in the second funding round, 3 if in the third funding round)
- Brief description with objectives
- Link to service portal (if present)
- Link to training portal (if present)
- Possibility of collaboration with industry
- Use cases
- Codes
- Contacts of CASTIEL 2 champions and deputies for each WP of CASTIEL 2.

Figure 3 shows an example of the summary for the ChEESE CoE (contacts of champions and deputies for each WP have been removed). The draft of the document was initially shared with the WP2 champions during the WP2 Working Group Meeting that took place on the 1<sup>st</sup> of June 2023. As positive feedback on the draft was received, WP2 completed the document, which was shared with CoEs at the beginning of July with the request to check the collected information. Finally, the document was shared internally with NCCs and CoEs on the 11<sup>th</sup> of July 2023 (and uploaded to BSCW).



**Figure 3: Example of the information collected in the “Summary Document on CoEs” produced by WP2 and shared with all NCCs and CoEs. Contacts of CASTIEL 2 champions and deputies have been removed.**

## 2.5 Summary of NCCs Services

The 33 NCCs in the EuroCC2/CASTIEL 2 network play a crucial role for technology and knowledge transfer towards industry, academia and the public sector. They offer an extremely rich variety of services for different types of users and thus it is beneficial for the whole ecosystem to have these services known and easily accessible (as it will be in the future thanks to LinkHPC, previously referred to as Marketplace, and developed by WP4 with a specific focus on industrial users. More information on LinkHPC can be found in D4.1 of WP4).

This point is of interest also for the CoEs, as NCCs could act as intermediaries between users and the CoEs, for example for projects exploiting one of the codes or software stack developed/maintained by the CoEs. For this reason, and to address the inputs coming from CoEs and collected during the WP2 Working Group Meeting that took place in June 2023, WP2 discussed the possibility of working on a summary document like the one produced on CoEs (Section 2.4) but on NCCs and their services. The preparation of the document is currently planned for the first half of the second year of the project, and some initial collection of materials on NCC services has started, using as starting point the Deliverable 1.19 of EUROCC2 titled “NCC Services”. Some general conclusions can be drawn from the information provided by NCCs:

- Services of NCCs cover four types of users: industry, SMEs, public administration and academia;
- Almost all of the NCCs offer trainings (online or face-to-face) for the four types of end users, ranging from introductory to advanced level, and covering from few hours to few days of teaching. In general, NCCs provide trainings covering topics related to HPC (e.g. on code parallelization) or AI (e.g. on deep learning). Some NCCs provide software trainings also in the field of Quantum Computing;
- Several NCCs offer services for awareness creation and for dissemination, as workshops, information days, seminars and conferences;
- Some NCCs offer a maturity level assessment for users;
- The majority of NCCs offers consulting services for the successful development of a project or of a Proof of Concept, that cover both code consultation and technology consultation.

NCCs services are described in detail in D1.19 of EuroCC. In the upcoming months WP2, in collaboration with WP4 and the EuroCC PMT, will aggregate and harmonize the several services provided by each NCC. The aim is to achieve a homogeneous list of service types per end-user (e.g. academia, industry, public administration) that is planned to be made public. NCCs services will also be included in the summary document on NCCs.

## 3 Competences of NCCs and CoEs

### 3.1 Designing the C2ISS Questionnaire

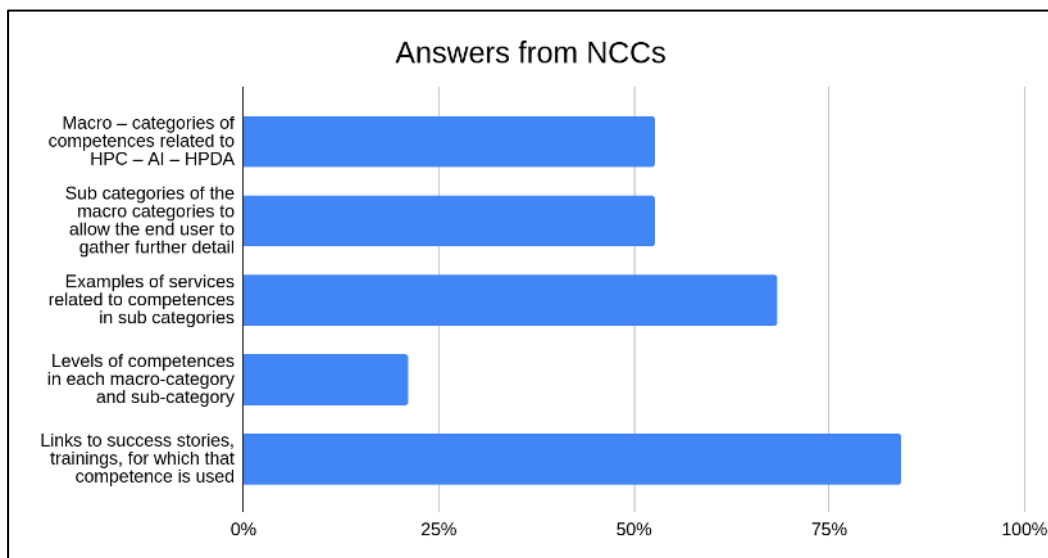
During a meeting that took place in Barcelona on the 22<sup>nd</sup> of February 2023, all the WPs of CASTIEL 2, led by WP5, carried out an initial brainstorming on the functionalities and design of C2ISS and the roadmap for its implementation. Following the meeting in February, in spring 2023 WP2 prepared the questions related to codes and competences to include in the “C2ISS questionnaire” for NCCs and CoEs. These are the questions included in the questionnaire shared with NCCs and CoEs:



- What information would be needed to describe your code? (multiple answers possible)
  1. Links to available training, support, success stories, use cases
  2. General Description
  3. Application Area/Areas
  4. Scalability Information
  5. Availability on JU systems
  6. Legal / Licensing info
  7. TRL
  8. Other
- What information would be needed to describe the competences of your CoE/NCC? (select all that apply)
  1. Macro – categories of competences related to HPC – AI – HPDA
  2. Sub-categories of the macro categories to allow the end user to gather further detail
  3. Examples of services related to competences in sub-categories, to help the end user in addressing his/her needs.
  4. Levels (just as an example: not available - available but not used - available and used) of competences in each macro-category and sub-category
  5. Links to success stories, trainings, for which that competence is used
  6. Other
- What kind of information do you want to find in an information system on CoEs, NCCs, and potentially other players in the HPC ecosystem?
  1. Finding collaboration partners
  2. Finding sources for support, best practices
  3. Other

The questionnaire was shared by WP5 in June 2023 with NCCs and with the 10 CoEs anticipating a Collaboration Agreement with CASTIEL 2.

Figures 4 and 5 summarise the answers provided by NCCs on the question about competences and expectations on C2ISS. 19 NCCs out of 32 answered the questionnaire.

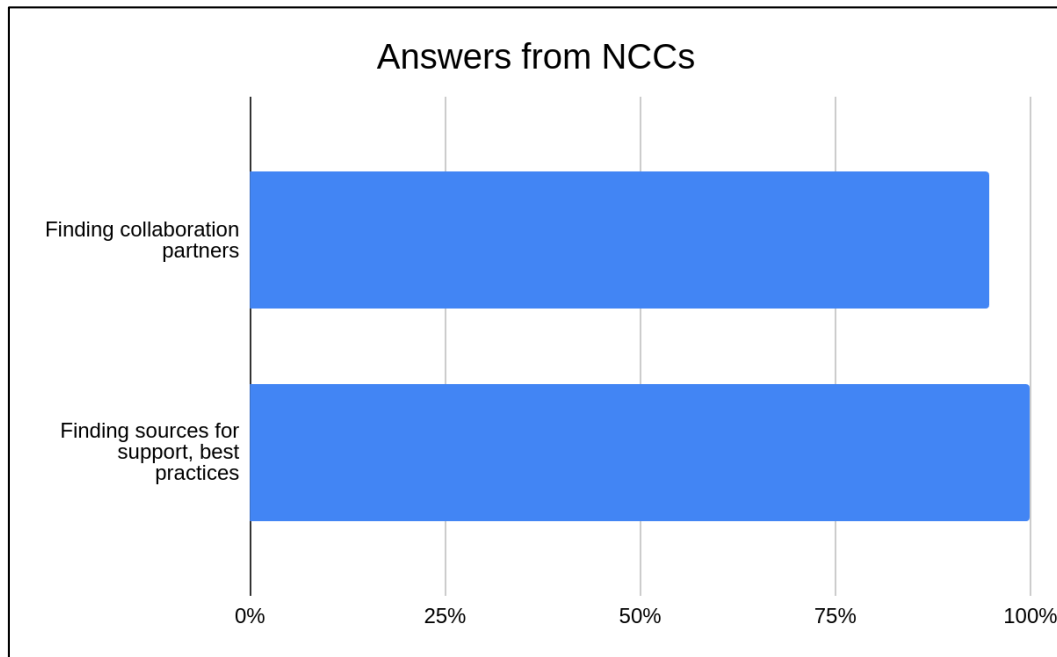


**Figure 4: Answers by NCCs to the question on competences for C2ISS.**

16 out of 19 NCCs consider important to include in a competence map links to success stories and trainings for which a particular competence is used. Also examples of services provided thanks to a given competence in a subcategory are considered important (voted by 13 out of 19

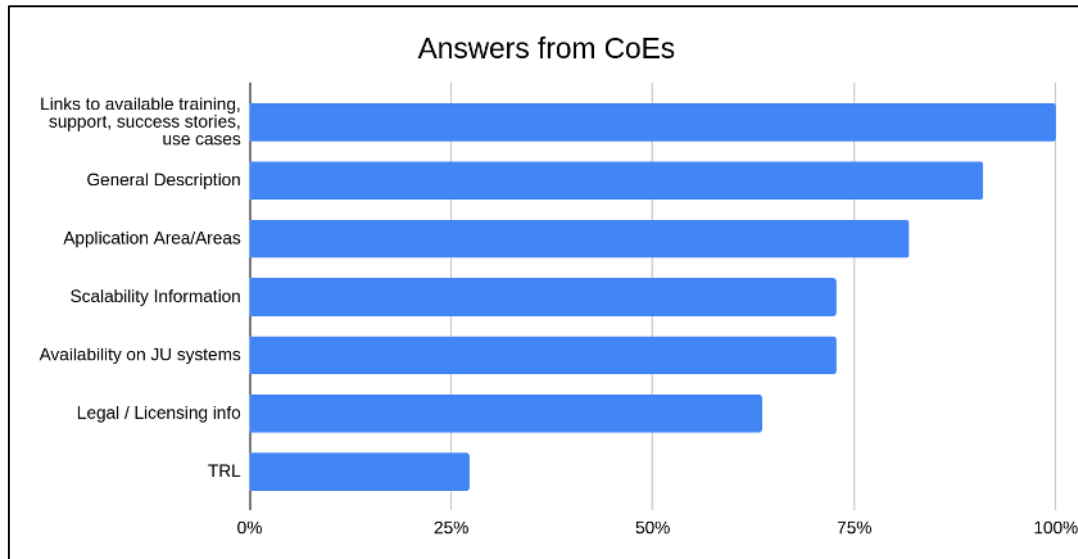
NCCs). Interestingly, only 4 NCCs selected “Levels” as information that would be useful to add to describe a given competence. On the second question, NCCs clearly voted that they hope C2ISS can help them find collaboration partners and sources for best practices and support. In the “Other” option the following inputs were received by NCCs:

- Open-source code, events and training, hardware infrastructure, active academic or business projects;
- All events, provided by NCCs, CoEs, EU projects, other EU entities and HPC relevant events (also commercial ones), useful links of e.g. ongoing EU HPC-related projects, list of EU HPC entities, list of Industry associations in each country



**Figure 5: Answers by NCCs to the question on expectations for C2ISS.**

Figure 6 summarises the answers provided by CoEs on the question about codes. All the provided options, with the exclusion of TRL, were selected by most of the respondents. Links to available training, support, success stories and use cases are considered important by all the CoEs when presenting their codes on C2ISS, together with the general description and the application areas.

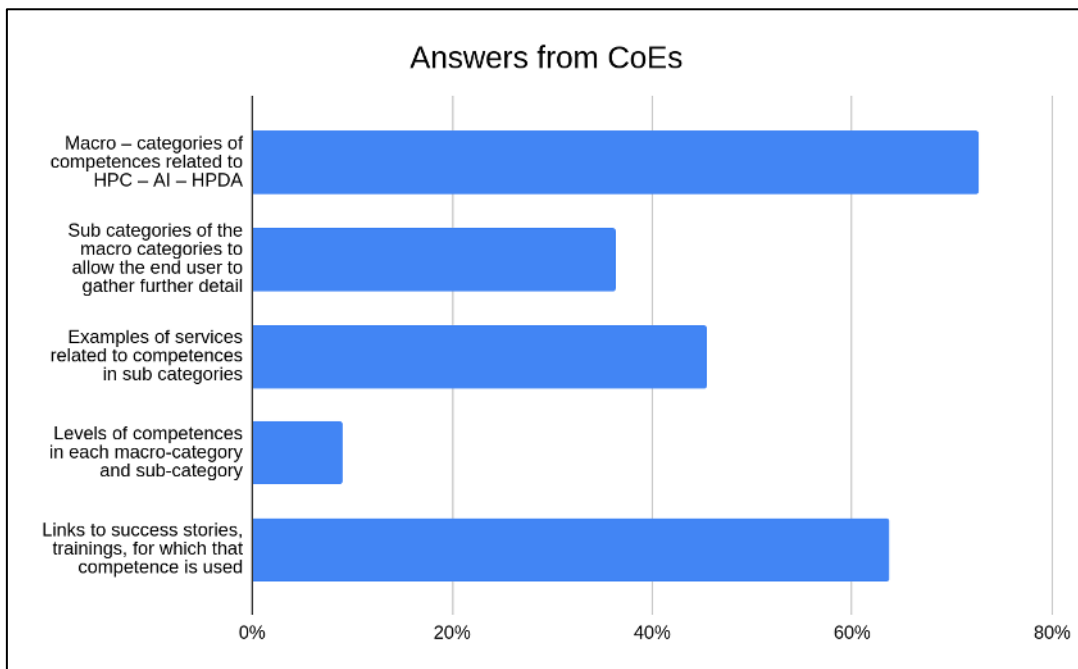


**Figure 6: Answers by CoEs to the question on codes for C2ISS.**

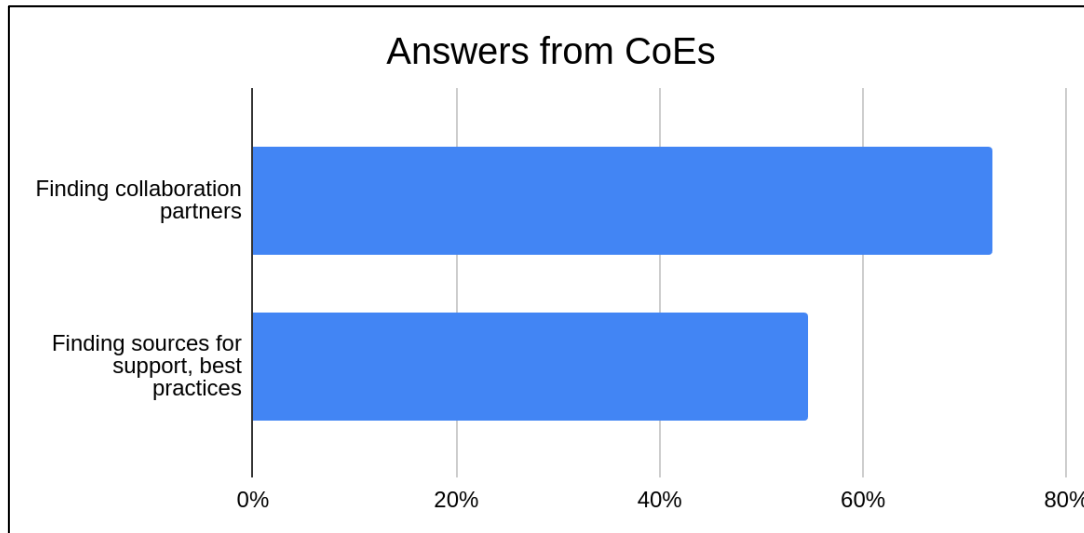
Figure 7 and 8 summarise the answers provided by CoEs on the question about competences and expectation on C2ISS. Similar to the NCCs, most CoEs consider important to include in a competence map links to success stories and trainings where a particular competence is used, along with macro-categories of competences. As for the NCCs, the least voted option is “Levels”, thus pointing towards the fact that levels are not considered necessary in a competence map by both NCCs and CoEs.

For what concerns expectations on C2ISS, “Finding collaboration partners” was the most voted option. In the “Other” option the following input were collected:

- “Links to all public deliverables”;
- “Matchmaking, expert database”.



**Figure 7: Answers by CoEs to the question on competences for C2ISS.**



**Figure 8: Answers by CoEs to the question on expectations for C2ISS.**

The inputs provided by NCCs and CoEs via their answers were and are currently being addressed by WP2 when designing the inclusion of codes and competences in the C2ISS and for the upgrade of the Competence Map (Section 3.3).

### 3.2 The current status of the NCCs Competence Map on EuroCC Access

The CASTIEL (phase 1) project produced the Competence Map [15] shown in Figure 9 and available online on EuroCC Access (deliverables D2.1, D2.2 and D2.3 of CASTIEL).

The structure of the map is the following:

- Competences in HPC, HPDA and AI organised the following 4 macro-categories:
  - Awareness Creation
  - Expert Technical Consultancy
  - Business and Project Consultancy
  - Products & Services
- Each macro-category is divided into the following sub-categories:
  - Awareness Creation
    - Informative Events & communication of opportunities
    - Dissemination of Results & Networking Events
  - Expert Technical Consultancy
    - Technological Scouting and assessment
    - Technology Transfer
  - Business and Project Consultancy
    - Feasibility & impact assessment (Proof of Concept)
    - Finding Partners & Projects - Matchmaking
    - Call Application and Fundraising Support
    - Project Design
    - Project Management
  - Products & Services
    - High Performance Computing Service Offering
    - Workflows Development & Optimization
    - High Performance Data Analytics Service Offering
    - Cloud Service Offering

- Quantum Service Offering
- Software Development & Optimization
- User Support
- Additionally, there is the possibility for the end user to select his/her HPC level between 5 categories, to better identify those NCCs that can provide a “competence” for a specific level of end user. These are the 5 experience levels:
  - Digitalization Needed
  - Digitally Ready
  - HPC Ready
  - HPC Users
  - HPC Champions

The current structure of the Competence Map reflects the strategy adopted during CASTIEL to merge competences and services in a single tool. Nevertheless, the competences/services categories listed are very broad and could fail in providing useful information for the HPC Ecosystem (NCCs, CoEs, end-users, other HPC-related projects). The broadness of the categories also makes it difficult to track the improvement of competences in the CASTIEL 2 network. In addition, as the Grant Agreement of CASTIEL 2 includes the creation of a separate information system for services, the now-called LinkHPC platform (formerly referred to as “Marketplace”). Another aspect to keep in mind is that the additional categorization based on the “HPC readiness” of end users resulted in some cases in incoherent information being portrayed in the Map.

Thus, considering all these aspects, as well as keeping the focus on a tool able to portray the richness of knowledge available in the network of NCCs and CoEs, **it became clear that a restructuring of the Competence Map was needed**, also with the aim of including the CoEs in the map. The aim of such an upgrade is to produce a tool able to showcase to the entire HPC Ecosystem the abundance of competences, knowledge and expertise in HPC, HPDA and AI, also when no services are in place to put a given competence at work. For this reason, WP2 launched the upgrade of the Competence Map, as detailed in the following Section.

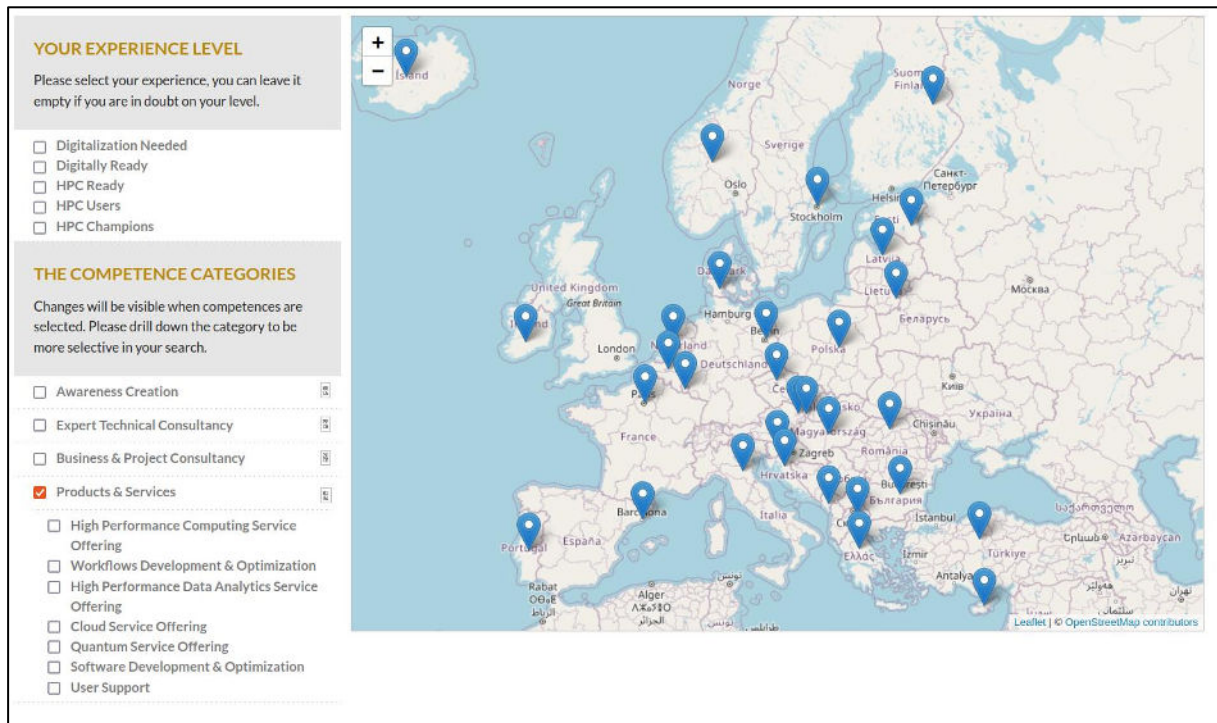


Figure 9: The current status of the NCCs Competence Map on EuroCC Access.

### 3.3 The upgrade of the Competence Map

#### 3.3.1 Setting the basis for a successful upgrade

From the beginning of CASTIEL 2 it was evident that a successful mapping of competences of NCCs and CoEs could happen only after converging on a clear and shared definition of what competences are. Such question was raised on several occasions by both NCCs and CoEs (e.g. during the Kick Off meeting in Stuttgart, through the C2ISS questionnaire, during open discussion during the NCCs-CoEs online meeting in April). For this reason and considering that the Competence Map produced by CASTIEL-phase 1 is a mixture of competences and services, WP2 decided to first coordinate with the other CASTIEL 2 WPs (especially WP4, who is focused on services to industry) to clearly define the boundaries of the Competence Map and its visualisation on EuroCC Access and inclusion in the future C2ISS database.

During an initial meeting on C2ISS that took place in Barcelona in February 2023 as well as follow up telcos with WPLs from WP4 and WP5, it was better defined that the competences of NCCs and CoEs will be included in the C2ISS and not in the Marketplace (now called LinkHPC) that will instead focus on services.

Following this initial coordination with the CASTIEL 2 WPs and the collection of inputs that took place in the NCCs-CoEs online meeting in April, WP2 prepared a presentation on the upgrade of the Competence Map, including a clear definition of competences, a collection of possible visualizations of competence maps, a proposition for the roadmap to be followed to upgrade the existing competence map. This presentation was shared with the WP2 champions during the Working Group meeting that took place on the 1<sup>st</sup> of June 2023. The points below summarise the contents of the presentations.

- **General purpose of the competence map**
  - **For the ecosystem**, to give a global overview of HPC-related competences (technical and related non-technical) in the network;



- **For NCCs and CoEs**, to find experts for specific areas to ask for collaborations (e.g. training, use cases, projects..);
- **For other EU projects**, to find experts for specific areas to ask for collaborations (e.g. training, use cases, projects..);
- **For end users**, to find who can provide a competence they are looking for and then look for their services;
- **For the PMT and the JU**, to monitor the evolution of competences within the network.
- **A common definition of competences**
  - The ability to do something successfully or efficiently.
  - Competence indicates sufficiency of knowledge and skills that enable someone to act in a wide variety of situations.
  - The combination of training, skills, experience and knowledge that a person has and their ability to apply them to perform a task safely
  - The quality of being competent; adequacy; possession of required skill, knowledge, qualification, or capacity
  - **Competences are a requirement to provide a service**: I can provide a service only if I have the competence needed in that topic!
  - Example: I have a competence on “Porting codes on GPUs” because I know how to do it. **I can decide if providing a service on it** (e.g. consultancy on porting codes on GPUs) or a training, **or not because I do not have the available resources!**
- **The current state of the Competence Map on EuroCC Access**
  - Categories include both competences and services.
  - No verification means or link to success stories / trainings is available when selecting a competence.
  - It is unclear whether the distinction on end-user expertise helps the users of the Competence Map or makes the Competence Map less easy to use.
- **Proposition of WP2**
  - Keeping in mind the points discussed and the distinction between competences and services, **WP2 proposes to upgrade the Competence Map and aim at a collection of competences of NCCs while starting a collection of competences of CoEs**;
  - **WP2 launched a Task Force** to work on the upgrade of the Competence Map (more details in the next Section).

### 3.3.2 The Task Force for the upgrade of the Competence Map

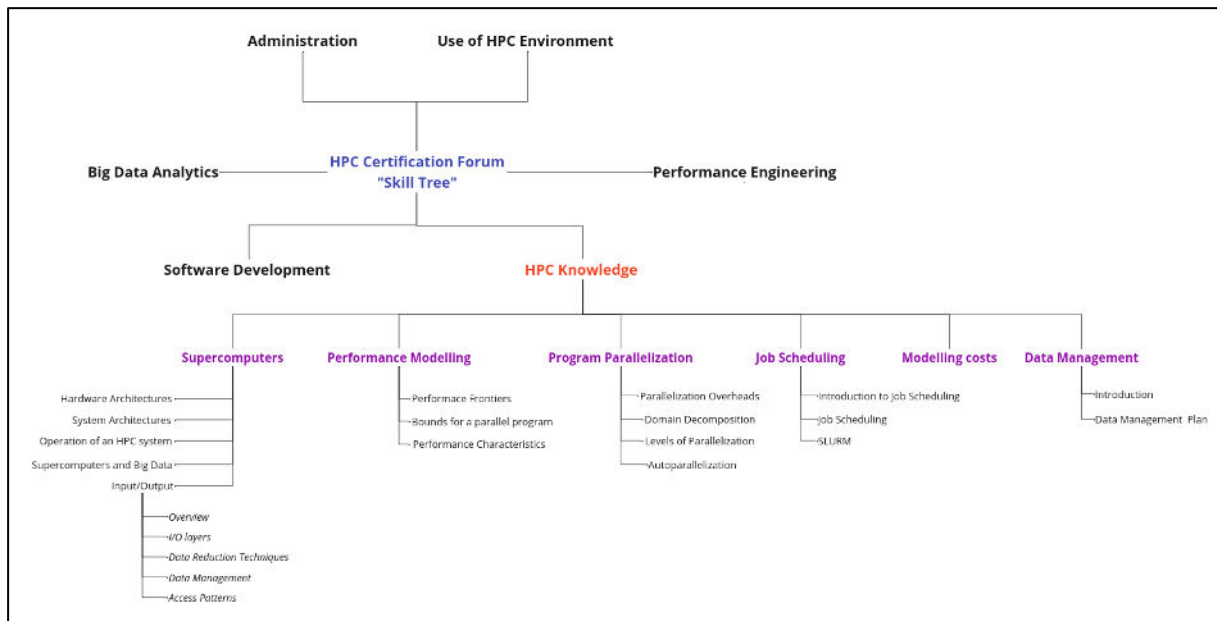
Following a positive discussion with the WP2 champions during the WP2 Working Group and the general agreement on the definition of competences as well as on the proposition of upgrading the Competence Map on EuroCC Access, WP2 asked for volunteers from NCCs to join the Task Force “Upgrade of the Competence Map”.

The following 7 NCCs volunteered: NCC Cyprus, NCC Türkiye, NCC Sweden, NCC Spain, NCC Poland, NCC Italy and NCC Serbia. NCC Germany also joined the Task Force in Autumn 2023.

The first meeting of the Task Force took place on the 18<sup>th</sup> of July 2023. During this meeting, WP2 presented two “Competence Maps” that could be used as starting point and as inspirations for the upgrade of the NCCs Competence Map:

- The “Skill” Tree of the HPC Certification Forum [16];
- The European Competence Framework for Quantum Technologies [17].

The structure of the “Skill Tree” of the HPC Certification Forum is shown in Figure 10. The “Skill Tree”, which is built from a training perspective, divides HPC-related knowledge into 6 macro categories: “Administration”, “Big Data Analytics”, “HPC knowledge”, “Performance Engineering”, “Software Development” and “Use of HPC Environment”. Each of these macro categories is divided further into categories, as visible in Figure 10 (all the six macro-categories mentioned above are further split into subcategories, but Figure 10 shows the details only for the “HPC Knowledge” category for visualization purposes).



**Figure 10: Structure of the HPC Certification Forum “Skill Tree” highlighting the 6 macro-categories of competences and sub-categories (only for the “HPC Knowledge” category for visualization needs).**

After analysing the “Skill Tree” during the Task Force meeting, the volunteers agreed that it represented a good starting point to define categories of competences for the upgrade of the Competence Map of NCCs.

On the other hand, the European Competence Framework for Quantum Technologies produced a competence map for Quantum Technologies that is extremely rich and comprehensive. After analysing this mapping (version of April 2023), the Task Force agreed that it represents a good starting point to define categories of competences in Quantum Computing that are relevant for NCCs.

Following this initial brainstorming of the Task Force, WP2 prepared a unique file including seven total macro categories: the six of the “Skill Tree” of the HPC Certification Forum and the seventh category “Quantum Technologies” where the structure of the Competence Framework for Quantum Technologies was reproduced. WP2 then asked the Task Force members to select at least two macro categories each and to discuss internally within their NCCs if the structure of subcategories is efficient in describing their competences, and which of them should be merged/deleted/added. The Task Force members had around 6 weeks' time to work on the assignment. During a meeting that took place on the 2<sup>nd</sup> of October 2023, the Task Force members reported back to WP2 the comments on the structure of the 7 macro-categories, their suggested modifications and general impressions. WP2 merged their feedback into a new Competence Map structure that was presented to the Task Force in November 2023 and



received positive feedback. At the time of writing, the macro-categories that have been identified for the upgraded Competence Map are the following:

- CLUSTER INFRASTRUCTURE & MANAGEMENT
- BIG DATA & ARTIFICIAL INTELLIGENCE
- BUILDING & DEPLOYING PARALLEL PROGRAMS
- QUANTUM COMPUTING
- DOMAIN SPECIFIC SOFTWARE

Each macro-category is currently being additionally divided into two levels of subcategories. WP2 aims at presenting it to all the champions in a WP2 Working Group meeting that is scheduled to take place on the 12<sup>th</sup> of December 2023. The planned next steps on the upgrade of the Competence Map are:

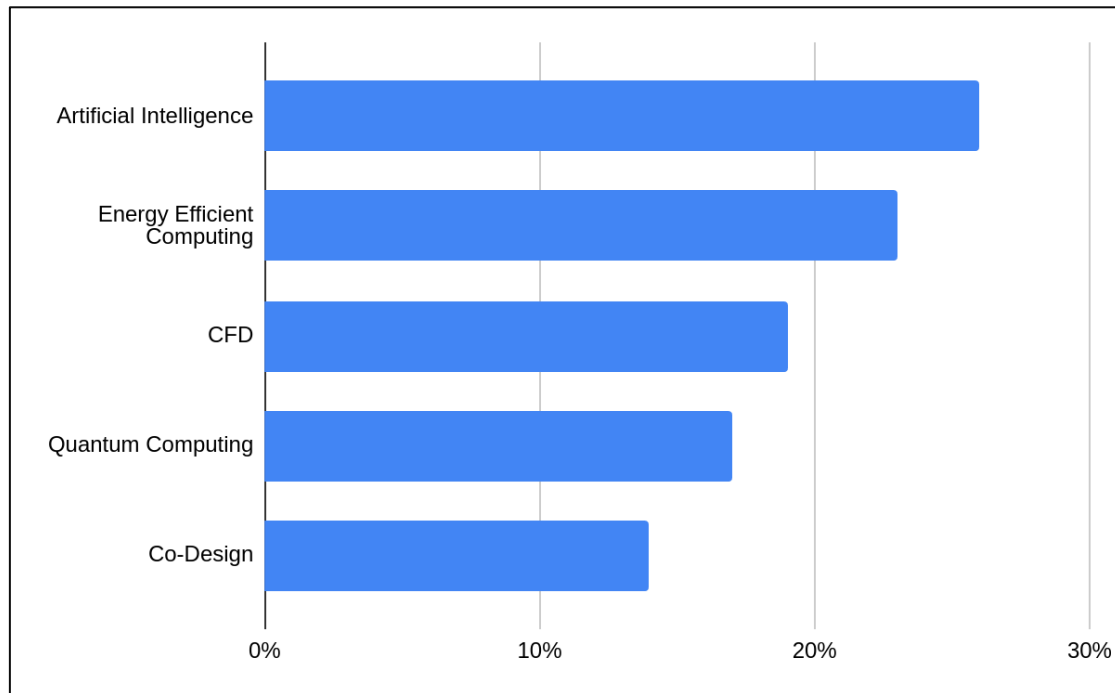
- Present the upgraded structure to WP2 champions and collect and implement their feedback;
- Present the upgraded structure (with the feedback from the previous step implemented) to EuroCC2 WPLs (beginning of 2024);
- Start the collection of competences following the upgraded structure (beginning of 2024);
- Have the upgraded Competence Map online during Spring 2024.
- Track the improvement of competences of NCCs (and CoEs, when applicable) for the remaining part of 2024 and 2025 via periodic reporting. Special focus will be put in tracking the motivations behind the improvement of competences.

Additionally, WP2 plans to address the inputs received via the C2ISS questionnaire on adding links to success stories and available training for a given competence category, to deliver a complete picture of the knowledge and opportunities within the CASTIEL 2 network.

Finally, WP2 and WP3 agreed that the upgraded Competence Map will be used in the second year of the project as an input for the Mentoring and Twinning program of WP3. This tool will be used to suggest combinations of NCCs (and in the future also CoEs) to conduct activities related to Mentoring and Twinning. This is an important example of coordination of efforts and collaboration.

### **3.4 Sharing, fostering and enriching the competences of NCCs and CoEs**

One of the objectives of CASTIEL 2 WP2 is to define and run workshops on non-HPC specific relevant topics and competences (soft skills, complementary competences), based on the needs expressed by NCCs and CoEs, and make the materials available (sometimes internally to all NCCs and CoEs, sometimes to the wider ecosystem, depending on the webinar). For this reason, both during the NCCs-CoEs online meeting and the WP2 Working Group meeting, WP2 collected input from NCCs and CoEs on topics of common interest to organise future relevant information-sharing workshops. During the first WP2 Working Group meeting that took place on the 1<sup>st</sup> of June 2023, WP2 prepared a short poll to have WP2 champions from NCCs and CoEs vote (and suggest) topics of interest. The results of the poll are shown in Figure 11 and show that Artificial Intelligence and Energy Efficient Computing are the two most voted topics, followed by CFD, Quantum Computing and Co-Design.



**Figure 11: Results of the poll prepared by WP2 to define the topics of common interest to organise workshops on.**

In additions to webinars identified thanks to the input from NCCs and CoEs, other were organised following the needs expressed by one CoE/NCC when WP2 considers it of potential interest for the network (see Section 3.4.1). Finally, the “Code of the Month” new series of webinars was addressed as a common effort between CASTIEL 2 WPs to foster collaboration between NCCs and CoEs (see Sections 3.4.2).

### 3.4.1 Webinars organised by WP2

The following is a summary of the webinars that were organised by WP2 or with the support of WP2 during the first year of the project.

- **The “HiDALGO-2 in-depth introduction” webinar**

In May 2023, WP2 was contacted by the HiDALGO-2 coordinator who wished to have support in the organization of a public webinar to present in depth the use-cases of the CoE and its goals. The webinar took place on the 15<sup>th</sup> of June 2023, and the details about the event were shared with the NCCs and CoEs champions and deputies of CASTIEL 2-WP2 and WP4, with the invitation to spread the information to their network as the event was public. The webinar had an average attendance of around 40 people. The slides used by the speakers were shared with WP2 and WP4 champions and uploaded to BSCW for all NCCs and CoEs to use.

- **The “GVM Software by Arc Compute” webinar**

During Spring 2023, WP2 was contacted by the Canadian company “Arc Compute”. They expressed their interest in presenting their GVM Server Software solution to NCCs and COEs. According to Arc Compute, GVM addresses administrative code and infrastructure inefficiencies enabling increased GPU performance, reduced compute times, and ‘true’ utilization. Through low-level utilization management, GVM Server users can achieve 100% GPU utilization. After an internal alignment with WPLs, WP2 presented this possible webinar during the WP2 Working Group meeting on the 1<sup>st</sup> of June. As positive feedback was collected, WP2 proceeded with the organization of the

webinar. The webinar took place on Monday, the 3<sup>rd</sup> of July, from 12:00 to 12:45 and had an average participation of 20 people.

- **“Large Language Models: a challenge called scalability”**

As Large Language Models become more and more prevalent in the Artificial Intelligence landscape worldwide, and as the rhythm at which this technology is changing is very high, WP2 decided that it would be beneficial to organise a webinar to summarise the situation on LLMs, the European efforts and the main challenges when trying to train and optimize such models. This was done also to address the need to have more webinars focused on AI. The webinar was led by Giuseppe Fiameni, Data Scientist at NVIDIA and responsible for the NVIDIA AI Technology Centre in Italy, and it was held on the 24<sup>th</sup> of October 2023, from 11 am to 12.30 pm. In total, 78 people registered to the webinar, of which 58 from NCCs, 12 from CoEs and 8 from CASTIEL 2. The slides of the meeting were shared internally to NCCs and CoEs and made available on BSCW.

- **The “Energy Efficient Computing” monthly webinars**

During the WP2 break-out session of the NCCs-CoEs online meeting and the WP2 Working Group meeting, the topic “Energy Efficient Computing” was one of the most requested topics for the organizations of webinars/workshops. To address this need of NCCs and CoEs, WP2 contacted the ETP4HPC project and proposed to them the organization of a new series of monthly webinars titled “Energy Efficiency Computing Webinars”. As the first proposition was successful, WP2 and ETP4HPC collaborated to collect the possible topics for the webinars, find the speakers, as well as drafting an agenda. It was decided that the webinars will last 1-hour and will take place on the first Friday of the month, starting from December 2023. At the moment of writing, this is the proposed agenda:

- 1<sup>st</sup> December 2023: *Introduction to Energy Efficient Computing and Thermal Control in today's HPC systems*
- 12<sup>th</sup> January 2024: *Introduction to energy and performance profiling techniques in HPC systems*
- February 2024: *Introduction to low-level processor architectural information on power saving techniques*
- March 2024: *ExaMon & COUNTDOWN*
- April 2024: *Energy analysis and optimization with EAR*

These webinars will be public and NCCs and CoEs will be requested to spread the news on the events to their networks.

- **“The EBRAINS Project: A Gateway to Collaborative Neuroscience”**

During the break-out session of WP2 in the “NCCs-CoEs online meeting” WP2 received the input to collaborate with the EBRAINS project. This initial request by NCC Sweden was then explored by WP2, that decided to support the organization of a webinar, as some of the open-source tools developed by EBRAINS could be exploited by NCCs, for example when interacting with public administrations. The webinar aims at introducing EBRAINS, a digital research infrastructure that is accelerating collaborative brain research across neuroscience, brain health, and brain-related technologies. The session is set to commence with an overview of EBRAINS by Prof. Petra Ritter (EBRAINS coordinator), followed by a detailed presentation on the platform’s tools and datasets. The webinar wants to explore potential collaborations

with interested NCCs and CoEs and demonstrate how EBRAINS' commitment to Responsible Research and Innovation practices can shape research in ethical ways that serve the public interest. The webinar, initially scheduled for the 13<sup>th</sup> of December 2023, was moved to February 2024.

In the upcoming months, WP2 will continue to collect the needs of NCCs and CoEs for topics of interest and will continue to organize and support the organization of webinars that are of interest to NCCs and CoEs.

### 3.4.2 The “Code of the Month” monthly webinars

The codes on which CoEs are working represent an important entry point for collaboration between NCCs and CoEs. For this reason, WP2, WP4 and WP5 decided to set up a new series of webinars called “Code of the Month” during which each month a CoE presents one of its codes in two different seminars: one internal for NCCs and CoEs (“industrial Code of the Month”) and one open to the public. These are the “Code of the Month” that took place during Summer and Autumn 2023:

- 14<sup>th</sup> of June (internal) and 28<sup>th</sup> of June (public): EXCELLERAT-P2 presented the code AVBP.
- 19<sup>th</sup> of July (internal) and 26<sup>th</sup> of July (public): RAISE CoE presenting the Unified Artificial Intelligence Framework.
- 20<sup>th</sup> of September (internal) and 27<sup>th</sup> of September (public): CoEC presented NekRS.
- 8<sup>th</sup> of November (internal) and 15<sup>th</sup> of November (public): PerMedCoE presented PhysiCell-X.
- 28<sup>th</sup> of November (internal) and 5<sup>th</sup> of December (public, organised by CASTIEL 2-WP3 as a 2-hour tutorial): MultiXscale presented the European Environment for Scientific Software Installations (ESSI).

As co-organizer of these events with WP4 and WP5, WP2 contributed to the organization of the webinars by pre-selecting potentially interesting codes, by contacting the CoEs and asking for their availability to present their code in the proposed dates. Additionally, WP2 shared the information about the webinars to the WP2 NCCs and CoEs champions and deputies. As the older, EC-funded CoEs are reaching the end of their run time soon, and many codes of the newly established CoE have not yet reached a high maturity level, there was a certain preference on these older CoE presenting some of their codes to enable NCCs to still benefit from these CoEs' work. The public webinars were recorded, and the recordings made publicly available. Detailed information on the “Code of the Month” webinars can be found in Deliverable 4.1 of CASTIEL 2-WP4 “Initial Report on the Actions performed to support the NCCs and the CoEs' Interactions with Industry”.

## 4 The Special Access Scheme for CoEs

WP2 was tasked with managing a joint application of the 10 CoEs starting in January 2023 for the JU special access scheme to the JU supercomputing systems. Such task was summarized in a milestone (number 9) of CASTIEL 2 to be reached by the end of M3, thus March 2023.

To familiarize the CoEs with the milestone, given the short time available and considering that most CoEs were still not familiar with the activities and requests of CASTIEL 2, WP2 prepared a short presentation that was given to CoEs during webinar that took place in February 2023

and organized by WP5 to kick-off the CI/CD activities. WP2 proposed to collect the requirements from CoEs about the estimated resources needed to install, test, benchmark and development of their codes/pilots on the different EuroHPC systems. The collection started in February 2023 via a document provided by WP2 to every CoE, that was also presented during the meeting. In parallel, WP2 collected information on the status of access to EuroHPC supercomputers and summarized them in the following Figure 12 (status of access in March 2023).

	BENCHMARK		DEVELOPMENT		REGULAR ACCESS		EXTREME SCALE		
	node-hour	core-hour	node-hour	core-hour	core-hour	minimum request in core-hour	core-hour	node-hour	minimum request in core-hour
Vega CPU	5.000	640.000	10.000	1.280.000	150.000.000	10.000.000	N/A	N/A	N/A
Vega GPU	400	51.200	1.000	128.000	4.100.000	1.000.000	N/A	N/A	N/A
Karolina CPU	7.000	896.000	15.000	1.920.000	60.000.000	10.000.000	N/A	N/A	N/A
Karolina GPU	1.000	128.000	3.000	384.000	6.000.000	1.000.000	N/A	N/A	N/A
Meluxina CPU	7.100	908.800	15.300	1.958.400	65.500.000	10.000.000	N/A	N/A	N/A
Meluxina GPU	1.000	64.000	3.000	192.000	11.100.000	2.000.000	N/A	N/A	N/A
Discoverer	7.000	896.000	15.000	1.920.000	104.000.000	10.000.000	N/A	N/A	N/A
LUMI-C	7.000	896.000	15.000	1.920.000	306.000.000	20.000.000	826.700.000	6.500.000	80.000.000
LUMI-G	20.000	1.280.000	N/A	N/A	N/A	-	689.000.000	10.800.000	80.000.000
LEONARDO Booster	N/A	N/A	N/A	N/A	N/A	-	189.000.000	5.900.000	20.000.000
TOTAL	55.500	5.760.000	77.300	9.702.400	706.700.000	-	1.704.700.000	23.200.000	-

**Figure 12: For each of the JU systems available in March 2023, maximum resources allocated per project per cutoff for different access calls (benchmark, development, regular and extreme) in core-hours and node-hours (if given).**

The CoEs were asked to provide details for all their codes/pilots, including information (per code) on which systems they are already known to run, which of the above access categories they foresee for each of the systems, and which resources are required for each access category. In addition, specific hardware and tool chain requirements could be specified, and contact information for each code was collected. Estimates of requests were asked for all 4 years of the lifetime of the CoEs, albeit it is evident that numbers and planned access for the coming years can only be indicative.

WP2 has collected input from these CoEs, regarding known installability of their codes on individual systems, as well as their plans for accessing these systems and their corresponding computing resource requests for different access schemes. Much of this relies on initial estimates. Also, some details on the individual codes were collected, including main developer contacts. This information was extremely useful when planning the “Code of the Month” and as a starting point for this deliverable and D2.4.

In general, the requested core/node hours were in line with the limits / ceilings mentioned above for individual applications. The largest number of core-hours was requested in the regular access mode.

The final document that was shared with EuroHPC JU included:

- The hours requested for Y1 by each CoE in the 4 different access modes (regular, development, extreme and benchmark);
- The overall hours requested by each CoE in years 1, 2,3 and 4;
- Several recommendations for designing a Special Access Scheme, grouped by type of access (regular, development, extreme and benchmark).

Overall, the document that was produced by WP2 provided a first overview of the CoEs’ plans and requests for using the JU systems, including a complete list of the CoEs’ codes with descriptions, contact details and known or expected installability on the JU systems. Due to the early stage and missing first-hand experience on many of those systems, much of the information, however, was preliminary and subject to changes. Furthermore, given the size and



novelty of the task to assign resources on such a large scale, CASTIEL 2 WP2 proposed to define and continually optimize a process meeting the needs of all parties involved. The follow-up to this activity depends on if and what level of special access will eventually be granted to the CoEs (which is unclear at the time of writing).

## 5 The codes and use cases/grand challenges of CoEs

In this Section, the codes, workflow engines, tools and use cases (sometimes referred to as Grand Challenges or Exascale Computational Challenge by some CoEs) that are the focus of CoEs are reported. Most of this information was collected during the activities related to the Special Access Scheme (Section 4) and to the Summary Document on CoEs (Section 2.4). More details on these codes will be reported in D2.4 “Legacy Code Report” also due in M12 by WP2.

### 5.1 BioExcel

BioExcel’s mission is to provide applications, tools, support, and networking opportunities to Life Science researchers, enabling them to address grand scientific challenges by fully exploiting the power of data and computing e-infrastructure. Powerful and sophisticated software packages are critically important for fundamental and applied research, including industrial development, in particular in the areas of drug design, biotechnology, food and chemical industries.

These are the 4 use cases of BioExcel:

- Antibody Design through Biomolecular Interactions Engineering
- High-Throughput Modelling of Interactomes
- Electronic Interaction Phenomena: Proton Dynamics and Fluorescent Proteins
- Rational Drug Design

These are the 4 codes and workflow engines on which BioExcel is working on:

- GROMACS [18]: one of the most used molecular dynamics codes. Highly tuned assembly kernels with hybrid CPU/GPU execution.
- HADDOCK [19]: used for integrative modelling. Python wrapper to execute a series of CNS (Crystallography and NMR system) scripts that also run pre and post-processing analysis.
- PMX [20]: used to automate the free energy calculations and assess binding between drug and protein. It uses GROMACS as a backend engine.
- BioBB [21]: Python library consisting of a collection of wrappers on top of biomolecular tools (e.g. GROMACS, HADDOCK, PMX), adding interoperability between them, and allowing an easy creation of biomolecular simulation workflows. The library combined with BSC PyCOMPSs workflow manager can be used to launch the workflows in HPC systems using thousands of cores.

### 5.2 CEEC

CEEC’s ambition is to enable the use of exascale computers for key CFD applications and demonstrate their capabilities through key light-house cases. Understanding the turbulent behaviour of gases and liquids has direct societal impact. In fact, it will be key for enabling the

transition to a carbon-free economy through optimizations like more fuel-efficient airplanes and cargo ships or wind turbines that can be more easily and sustainably installed on the ocean floor. CEEC aims at: implement exascale-ready workflows to solve grand scientific challenges, develop new or improves algorithms that can efficiently exploit exascale systems, improve energy efficiency of simulations and demonstrate workflows on lighthouse cases that are relevant for academia and industry.

These are the 6 use cases of CEEC:

- Shock – Boundary layer interaction and buffet on wings at the edge of the flight envelope – FLEXI [22]
- High fidelity aeroelastic simulation of the SFB 401 wing in flight conditions – ALYA [24]
- Topology optimization of static mixers – Neko [23]
- Localized erosion of an offshore wind-turbine foundation – waLBerla [25]
- Simulation of Atmospheric Boundary Layer (ABL) flows - NekRS/Nek500 [26]
- Merchant ship hull – Neko [27]

These are the 5 codes on which CEEC is working on:

- ALYA: Multi-physics / multi-scale simulation framework
- FLEXI: DG-Spectral element based CFD code
- Nek5000 & NekRS: Spectral element based CFD Codes
- Neko: Spectral element based CFD code
- waLBerla: Lattice Boltzmann based multiphysics framework

### 5.3 ChEESE-2P

ChEESE-2P aims to prepare 11 community flagship codes to address 11 domain-specific Exascale Computational Challenges on, eg., computational seismology, physical volcanology, magnetohydrodynamics. Codes will be optimized in terms of performance on different types of accelerators, scalability, deployment, containerization, and portability. Codes and workflows will combine to form a new generation of 9 Pilot Demonstrators underpinned by concepts like multi-scale, multi-source, and multi-physics, that will materialise in 15 Simulation Cases representing capability and capacity use cases of relevance in terms of science, social relevance, or urgency.

These are the 11 Exascale Computational Challenges of ChEESE-2P:

- Full-waveform inversion and high-resolution tomography (capability computing)
- Near real-time seismic scenarios (capacity computing)
- Physics-based Probabilistic Seismic Hazard Assessment (capacity & urgent computing)
- Near real-time tsunami source inversion and characterization (capability computing)
- Faster Than Real Time tsunami scenarios (capacity & urgent computing)
- Probabilistic Tsunami Hazard Assessment (capacity computing)
- Volcanic Explosions and Interactions (capability computing)
- Probabilistic Volcanic Hazard Assessment (capacity computing)
- The dynamo model and the Earth's magnetic field evolution (capability computing)
- Landslide triggering (capability computing)
- Lithospheric stress states and induces seismicity (capability computing)

These are the 11 codes on which ChEESE-2P is working on:

- SeisSOL [28]: complex earthquake simulation
- SPECFEM3D [29]: linear seismic wave propagation
- ExaHyPE [30]: special emphasis on ExaSeis collection of seismic models
- Tandem [31]: linear elasticity + sequences of earthquakes and seismic slips
- XSHELLS [32]: flows, magnetic fields including Geodynamo simulations
- HySEA [33]: earthquake –induced Tsunamis
- FALL3D [34]: atmospheric transport & ground deposition
- OpenPDAC[35]: simulation of volcanic fluids
- LaMEM [36]: thermo-mechanical geodynamic modelling
- pTatin3D [37]: simulation of long time-scale geodynamics processes
- ELMER/ICE [38]: Multi-physics package

## 5.4 ESiWACE-3

ESiWACE-3 focuses on the community's support to reach a higher readiness level regarding Exascale supercomputing and knowledge transfer between the different Earth System modelling centres and teams across Europe. The project focuses on three main pillars: (i) the transfer and establishment of knowledge and technology for efficient and scalable simulations of weather and climate across the Earth system modelling community, (ii) closing common technology knowledge gaps and providing toolboxes for high-resolution Earth system modelling via joint developments and (iii) serve as a sustainable community hub for training, communication and dissemination for high-performance computing for weather and climate modelling in Europe. ESiWACE-3 will bring the various approaches to address these challenges from the different modelling groups together to transfer knowledge across the weather and climate domain, generate synergies between the local efforts, provide targeted support to modelling groups via customised high-performance computing services, and provide training to educate the next generation of researchers.

These are the 5 objectives of ESiWACE-3:

- Increase the efficiency of weather and climate simulations on state-of-the-art supercomputers.
- Design tools to close technology gaps for high-performance computing.
- Develop tools to tackle the data challenge of high-resolution weather and climate modelling.
- Support the wider weather and climate modelling community using state-of-the-art supercomputers via targeted services, training and capacity building.
- Build a well-connected and inclusive community for high-resolution Earth System modelling across Earth system science and HPC.

These are the 4 codes and 1 benchmarking tool on which ESiWACE-3 is working on:

- EC-Earth [39]: coupled Earth System Model for climate simulations
- NEMO [40]: ocean model for climate simulations
- ICON [41]: coupled Earth System Model for climate simulations
- IFS [42]: Atmospheric model for weather simulations
- HPCW [43]: Set of weather & climate benchmarks



## 5.5 EXCELLERAT P2

EXCELLERAT P2 spans the whole domain of engineering – ensuring that innovations produced are applicable to other engineering challenges, that co-design is handled properly, that success stories are created and distributed. EXCELLERAT P2 strives to show the contribution of HPC, HPDA and AI in engineering to a low carbon, more environmentally friendly and socially responsible product development and manufacturing as well as the mobility and energy sector. The holistic view of EXCELLERAT P2 to the usage of HPC (and HPDA and AI) is needed, if engineering applications shall be supported to increase the European competitiveness.

These are the 7 use cases of EXCELLERAT P2:

- External aircraft aerodynamics - DLR - CODA
- Hydrogen combustion for propulsion - CERFACS – AVBP
- Migration of aeroacoustic noise - RWTH Aachen - m-AIA
- Fully integrated aircraft simulations with emission models - BSC - Alya
- High-fidelity simulations of rotating parts KTH - NEK5000/Neko
- Active control for drag reduction of transonic air foils - CINECA - FLEW
- Engineering design of digital twin of the first wall of tokamak fusion reactor - University of Ljubljana - OpenFOAM/Raysect

These are the 8 codes on which EXCELLERAT P2 is working on:

- m-AIA [44]: CFD-related, multi-physics code in C++ with hybrid MPI/OpenMP parallelization and some solvers ported to NVIDIA GPUs
- AVBP [45]: 3D parallel Navier-Stokes solver for reactive multi-phase multi-physics problems using Large Eddy Simulation on unstructured grids (runs on any CPU and NVIDIA GPUs).
- Neko [46]: spectral element method code running on CPU and GPUs using native accelerator kernels (HIP, Cuda, OpenCL).
- Alya [47]: Navier-Stokes solver exploiting a Spectral Element discretization. Runs fully on GPUs (mostly tested on Nvidia V100 and A100 GPUs).
- CODA [48]: CFD software, Python frontend, C++ backend, supports hybrid MPI/GASPI + OpenMP + NVIDIA GPUs
- OpenFOAM [49]: free, open source CFD software
- Mitsuba2 [50]: Monte Carlo Ray tracing for optical and radiative heat transfer simulations (runs on GPUs)
- FLEW [51]: FVM solver for DNS of compressible flow, written in Fortran and OpenACC

## 5.6 HiDALGO2

HiDALGO2 explores synergies between modelling, data acquisition, simulation, data analysis and visualisation. It will also efficiently utilise current and future HPC and AI infrastructures to develop highly scalable solutions to global climate and social challenges (e.g. violent weather, floods, pollution). HiDALGO2 aims at bringing together advanced solutions (HPC-AI-HPDA) to provide decision makers and stakeholders tools that would mitigate tragic consequences of climate and civilization phenomena, by delivering necessary knowledge.

The 4 use cases of HiDALGO2 [52] are:

- Urban Air Project: evolution of air in urban areas considering pollution, wind, comfort and planning. The core is the Urban Air Flow (UAP.AF) computational model, based on two main software: OpenFOAM and Fluid-Solver. For both solvers, modelling of more physical properties will be developed including thermal convection, solar heat radiation, transport and reaction between several species.
- Urban Building: advanced building models for better integration with architecture and for pollutants and heat models.
- Renewable Energy Sources: Solutions for production of renewable energy accustomed to urban and rural areas. Multiscale weather prediction based on Fortran and MPI coupled energy production estimation (based on AI/HPDA)
- Wildfires: Simulations of wildfires and atmosphere interaction and smoke dispersion in forest and urban areas. Forecast of weather conditions from WRF and LES at very detailed scales, generating ensembles of weather scenarios over the landscape and coupling of CFD solutions for the detailed modelling of air flow at the settlement scale.

## 5.7 MaX-3

MaX-3 targets lighthouse codes for material simulations aimed at understanding, predicting, and discovering the properties and performance of materials. The aim is: to upscale the MaX codes and their performance to multiple heterogeneous exascale architectures; to endow these codes with innovative capabilities enabled by such architectures; to co-design the hardware and software in collaboration with the relevant European stakeholders; to enable turn-key simulation capabilities that meet the power of exascale resources and deliver the resilience needed; to disseminate the entire ecosystem of codes, workflows, and data; and to train and engage developers and users in fully leveraging such powerful instruments for discovery and innovation.

These are the 5 lighthouse codes of MaX-3:

- Quantum ESPRESSO [53] is an integrated suite of open-source computer codes for electronic-structure calculations and materials modelling at the nanoscale. It is based on density-functional theory (DFT), plane waves, and pseudopotentials.
- SIESTA [54] is a code that performs efficient electronic structure calculations and ab initio molecular dynamics simulations of molecules and solids. SIESTA's efficiency stems from the use of a basis set of strictly localized atomic orbitals.
- YAMBO [55] is an open-source code implementing first-principles methods based on Green's function theory to describe excited-state properties of realistic materials.
- FLEUR [56] is a code family for calculating ground-state as well as excited-state properties of solids within the context of DFT. A key difference lies in the treatment of all electrons on the same footing.
- BigDFT [57] is an electronic structure pseudopotential code that employs Daubechies wavelets as a computational basis, designed for usage on massively parallel architectures.

## 5.8 MultiXscale

MultiXscale aims at increasing performance, productivity and portability in the domain of multiscale simulation. It couples the scientific expertise of the CECAM network, represented by leading experts in multiscale simulations from different European institutions, with the

technical expertise of the EESSI collaboration, and targets the computational laboratories of EuroHPC and beyond. It will shoulder much of the technical burden of developing and distributing domain-relevant applications for (pre-)exascale through application co-design for exascale technologies, and the provisioning of exascale-oriented libraries and services that nudge the community to adopt battle-tested, future-oriented, scalable workflows and portable technologies. These will allow application developers to pursue domain-relevant scientific innovation without being over-burdened by technical detail, and empower industrial and academic application users to painlessly adopt bleeding-edge technologies from the domain on whatever computational resource they may have access to

These are the 3 use cases of MultiXscale:

- Helicopter design and certification for civil transport.
- Battery applications to support the sustainable energy transition.
- Ultrasound for non-invasive diagnostics and biomedical applications.

This is the complete build and deployment environment on which MultiXscale is working on:

- EESSI [58] (European Environment for Scientific Software Installation): complete build and deployment environment for all MultiXscale applications and beyond. Provides a streaming service for scientific software, automatically distributing hardware-optimised applications and updates to all hardware types: supercomputers, servers and laptops.

Applications used and contributed to that enter the multiscale workflows:

- ESPResSo [59]: highly versatile software package for performing and analysing scientific Molecular Dynamics many-particle simulations of "coarse-grained" bead-spring models as they are used in soft-matter research in physics, chemistry and molecular biology.
- LAMMPS [60]: classical molecular dynamics code with a focus on materials modelling.
- WaLBerla [61]: Lattice Boltzmann based multiphysics framework.

## 5.9 Plasma-PEPSC

Plasma-PEPSC aims at reaching scientific breakthroughs in plasma science Grand Challenges through exascale computing and extreme-scale data analytics, by enabling unprecedented simulations on current pre-exascale and future exascale platforms to control plasma-material interfaces, optimize magnetically confined fusion plasmas, design next-generation plasma accelerators and predict space plasma dynamics in the Earth's magnetosphere. Plasma-PEPSC aims at achieving these goals by maximizing the parallel performance and efficiency of four European flagship plasma codes with a large user base: BIT, GENE, PICongPU, and Vlasiator, by building on algorithmic advances as well as on programming model and library developments (MPI, accelerator and data movement APIs and runtimes, in-situ data analysis). Plasma-PEPSC ensures an integrated HPC software engineering approach for deploying, verifying, and validating extreme-scale kinetic plasma simulations that can serve as a community standard

These are the 4 use cases of Plasma-PEPSC [62]:

- Controlling Plasma-Material Interfaces - BIT1
- Optimizing Magnetically Confined Plasmas - GENE

- Enabling Next-Generation of Plasma Accelerators for Real World Applications - PIconGPU
- Predicting Near-Earth Space Dynamics - Vlasiator

These are the 4 codes on which Plasma-PEPSC is working on:

- GENE [63]: Plasma microturbulence based on Eulerian calculation and MPI domain decomposition.
- BIT1 [64]: full-size kinetic modelling of plasma edge.
- Vlasiator [65]: Semi-Lagrangian simulation of the Vlasov Equation and MPI domain decomposition. OpenMP/MPI hybrid parallelizations, sparse grids.
- PIconGPU[66]: plasma accelerators at full resolution and scale

## 5.10 SPACE

SPACE CoE aims to extensively re-engineer astronomy and cosmology (A&C) codes for exascale, adopting new computational solutions and innovative programming paradigms, software solutions, and libraries, to be able to extract information from the extremely complex and voluminous data that will be produced by the forthcoming missions/telescopes (e.g. SKA, Euclid). SPACE will address the high-performance data analysis of the data torrent produced by exascale A&C simulation applications, also with machine-learning and visualization tools.

These are the 8 codes on which SPACE is working on:

- PLUTO [67]: an Eulerian, finite-volume, shock-capturing code based on high-order Godunov methods providing several integration algorithms. It supports both classical and relativistic flows and it is equipped also with a particle module for hybrid MHD-PIC simulations.
- OpenGADGET [68]: one of the most used codes It is a N-body code that solves the gravitational and hydrodynamical equations in their Lagrangian form for a large ensemble of particles.
- CHANGA/GASOLINE [69]: Tree and Smoothed Particle Magnetohydrodynamics codes that are widely used for cosmological galaxy formation simulations. The two codes have the same implementation, but CHANGA features parallelisation design with Charm++ which enables scaling up to 128K cores for highly-clustered datasets.
- IPIC3D [70]: fully electromagnetic massively parallel particle in cell based on the semi-implicit approach to address multiple scale problems in plasma physics.
- RAMSES [71]: code to model astrophysical systems, featuring self-gravitating, magnetised, compressible, radiative fluid flow. Based on the Adaptive Mesh Refinement (AMR) technique.
- WhiskyTHC [72]: code aimed at solving the general-relativistic hydrodynamics equations on AMR grids by means of high-resolution shock capturing methods. It leverages a high-level C++ programming paradigm to achieve a high degree of efficiency.
- FIL [73]: it employs a fourth-order accurate finite differencing scheme to solve the equations of general-relativistic magnetohydrodynamics. It includes a framework for realistic microphysics through the use of temperature and composition dependent Equation of State tables.
- BHAC [74]: multidimensional general relativistic magnetohydrodynamics code based on the MPI-AMRVAC framework. BHAC solves the equations of ideal general

relativistic magnetohydrodynamics in one, two or three dimensions on arbitrary stationary spacetimes.

## 6 The WP2-WP4 Task Force “SME Assessment Tool”

During the EuroCC2/CASTIEL 2 Kick Off in Stuttgart in February 2023, Tomi Ilias from the Arctur computing centre, partner of NCC Slovenia, presented during a parallel session a tool developed by them for the assessment of the HPC maturity of SMEs. The feedback gathered from other NCCs on the utility of the tool developed by Arctur was positive and WP2 and WP4 decided to commonly support a Task Force focused on the upgrade of the tool, including the translation in different languages. Thus, WP2 launched a collection of volunteers to participate in the Task Force led by Arctur.

The Task Force started its activities in March 2023, and it was composed by the following NCCs: Belgium, Cyprus, Estonia, Greece, Hungary, Iceland, Montenegro, Netherlands, North Macedonia, Norway, Portugal, Romania, Slovenia, Sweden and Turkey, for a total of 15 NCCs. The Task Force completed the upgrade of the tool in August 2023.

WP2 and WP4 prepared an anonymized questionnaire dedicated to collect feedback on how the works of the Task Forces took place and on the uptake of the final product. The questionnaire was shared with Task Force members in September 2023 and 10 answers were collected. The following are the results of the questionnaire:

**Question 1:** What is your overall satisfaction with this task force outcomes? [ranking from 1 “Very dissatisfied” to 5 “Very satisfied”]

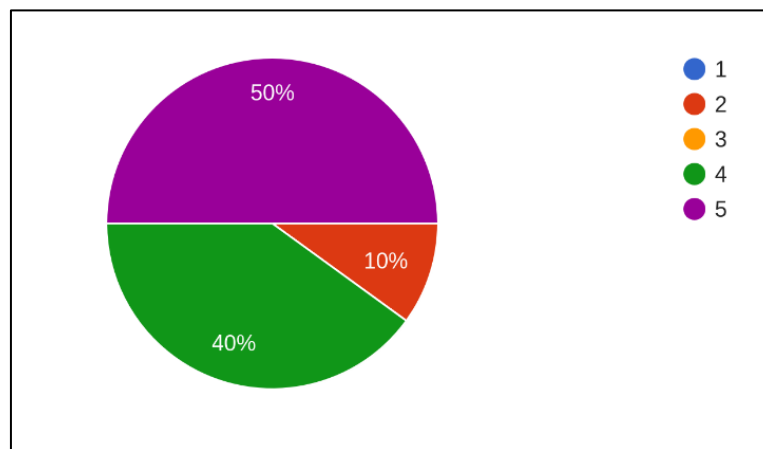
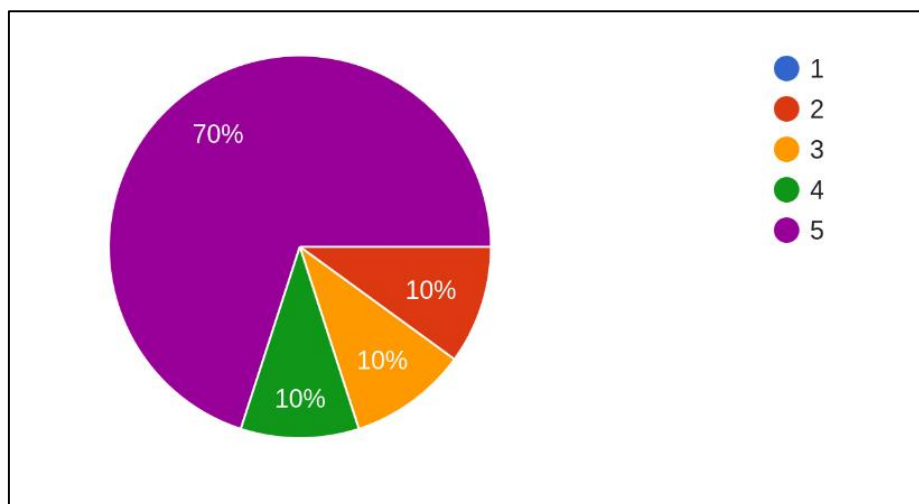


Figure 13: Answers to the question on the “SME Assessment Tool” Task Force outcomes.

The overall satisfaction with the outcomes of the Task Force is good, as 8 out of 10 people were “Very Satisfied” and “Satisfied”, as shown in Figure 13. Two Task Force members declared that they were “Dissatisfied” with the outcome.

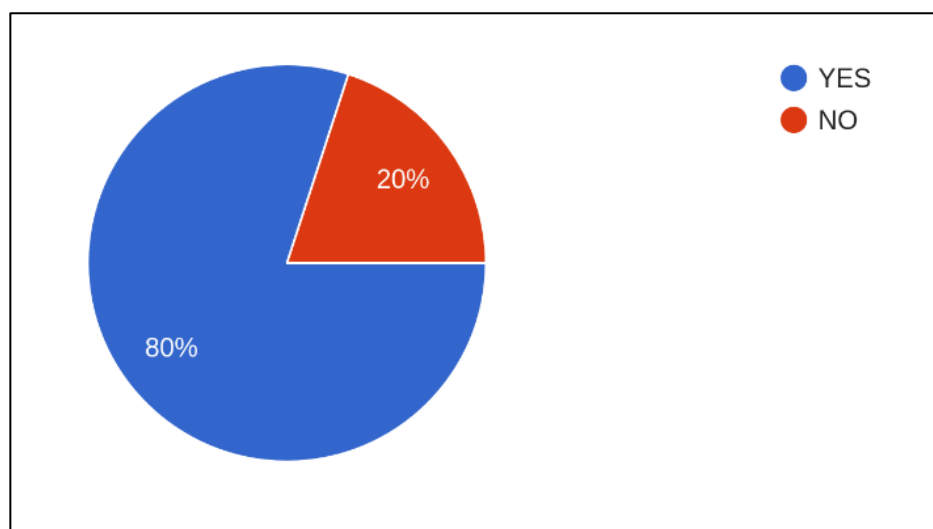
**Question 2:** Was the process used for this task force efficient in your opinion? [ranking from 1 “Very Inefficient” to 5 “Very efficient”]



**Figure 14: Answers to the question on the “SME Assessment Tool” Task Force efficiency.**

As shown in Figure 14, the process undergone by the Task Force members to upgrade the SMEs assessment tool was considered “Very Efficient” by 7 out of 10 people. Of the remaining three answers, 1 member voted for “Efficient”, 1 for “Neutral” and 1 for “Inefficient”.

**Question 3:** Are you using now (or planning in the next 6 months to) the SMEs assessment tool developed in this task force for your NCC and your national ecosystem?



**Figure 15: Answers to the question on the “SME Assessment Tool” uptake.**

The uptake of the upgraded tool by the NCCs who participated in the Task Force is very satisfactory, as 80% of the NCCs are already using or planning to use HPC4SME in the next 6 months (see Figure 15).

Overall, the Task Force “SMEs assessment tool” is considered very successful by the Task Force members, by CASTIEL 2 WP2 and WP4 and by NCC Slovenia who led the works. The way the Task Force operated was efficient and allowed to obtain a tangible result in a relatively short time. The upgraded tool will be presented to all NCCs on the 29<sup>th</sup> of November 2023 during a webinar led by Arctur that WP2 and WP4 helped to organise.

## 7 Major Achievements

The major achievements of the CASTIEL 2 WP2 are summarized below:



- The “NCCs-CoEs online meeting” that took place in April 2023 and was organised by WP2 was a great opportunity for:
  - the CoEs to better understand the structure of CASTIEL 2 and activities covered by the different WPs, to better get to know the NCCs, the nature of the activities they organise and examples of past NCC-CoE collaborations, as well as to better get to know the other CoEs, their area of work, their activities and plans for collaborations.
  - the NCCs to get to know all the CoEs, understand their area of work, their use cases and codes, as well as where the potential for collaboration lies.
  - CASTIEL 2 PMT and WPs to engage the NCCs and CoEs on the activities revolving around each WP and to get feedback on the planned activities during the breakout sessions.
- The milestone related to the Special Access Scheme for the CoEs was met and the collection of information resulted in a comprehensive list of details about the more than 60 codes managed by the CoEs.
- The summary document on CoEs that several NCCs asked for during the “NCCs-CoEs online meeting” was produced by WP2 and shared with NCCs and CoEs with information about the coordinator and PI, partners (name of institution and country), funding phase, type I or II of CoE, objectives and general description, use case/grand challenges, codes and contacts of the CASTIEL 2 champions and deputy for each WP.
- A common agreement was reached on the need to upgrade the NCCs Competence Map on EuroCC Access (and for the future C2ISS). A Task Force was created with the aim of working on such an upgrade. The upgrade is currently ongoing, and the new structure of the Competence Map is planned for the end of the year 2023.
- The answers provided by NCCs and CoEs to the questions prepared by WP2 for the C2ISS questionnaire gave important input on how NCCs and CoEs wish to have their codes and competences collected in the C2ISS database.
  - About codes, the answers provided by CoEs were taken into account when providing input to WP5 for designing the database that will collect all the information required to describe the CoEs’ codes.
  - About competences, NCCs and CoEs agreed that a Competence Map should also include practical examples for a given category, as well as links to success stories and/or training events where a given competence is/was used.
- Agreement with WP3 to use the upgraded Competence Map as an input for the Mentoring and Twinning program of WP3. This tool will be used to suggest combinations of NCCs (and in the future also CoEs) to conduct activities related to Mentoring and Twinning.
- Excluding the “NCCs-CoEs online meeting”, three other webinars organised by WP2 took place in the period January 2023 – October 2023:
  - “HiDALGO-2 in-depth introduction”;
  - “GVM Software by Arc Compute”;
  - “Large Language Models: a Challenge called scalability”;
  - “Introduction to Energy Efficient Computing and Thermal Control in today's HPC systems”.
- Other webinars are currently planned for Winter 2024. The topics of the organised webinars were suggested to WP2 by NCCs and CoEs when feedback on the same was requested:
  - “The EBRAINS Project: A Gateway to Collaborative Neuroscience”;
  - “Energy Efficient Monthly Webinars”.

- WP2 supports the organization of the “Code of the Month” webinars, during which each month a CoE presents one code potentially interesting for end-users. The organization of these webinars is a common effort of WP2, WP4 and WP5. In particular, WP2 oversees the organization by suggesting a code and finding the speakers for the webinars, a task that is possible thanks to the list of CoEs’ codes that was produced during the Special Access Scheme milestone activities.
- The Task Force “SMEs assessment tool” jointly supported by WP2 and WP4 was considered successful by the Task Force members, by CASTIEL 2 WP2 and WP4 and by NCC Slovenia who led the works. The way the Task Force operated was efficient and allowed to obtain a tangent result in a relatively short time.

## 8 Concluding Remarks

The activities undertaken by WP2 during the first year of the CASTIEL 2 project were essential for establishing the basis for a successful collaboration of NCCs and CoEs with WP2 and among them. Several activities are currently being planned for the second year of the project, including (but not limited to) the following points:

- The “Energy Efficient Computing” monthly webinars will take place regularly at least for the first part of 2024. WP2 plans to collect feedback from NCCs and CoEs on how they wish to continue the series of webinars.
- Organization of technical/development-oriented workshops and activities to address common issues of CoEs and NCCs related to code development and optimization, with a special focus on the inputs received by CoEs during the preparation of Deliverable 2.4 “Legacy Code Report” authored by WP2 and also due at M12.
- First collection of competences of NCCs and CoEs for the upgraded Competence Map. This activity, currently scheduled for winter 2024, will most likely involve 1-to-1 meetings with NCCs and CoEs.
- Regular monitoring of the improvement of competences of NCCs and CoEs using the upgraded Competence Map categories.

In general, WP2 will continue to focus on the mapping of competences and codes as inputs to C2ISS and EuroCC Access Portal and will act to foster collaboration between NCCs and CoEs, and with NCCs and CoEs with the whole European HPC Ecosystem.

## 9 References and Applicable Documents

- [1] CASTIEL 2 project, <https://www.eurocc-access.eu/about-us/the-projects/>
- [2] CASTIEL project, <https://cordis.europa.eu/project/id/951740>
- [3] HPC3, <https://www.hpccoe.eu/hpc-coe-council/>
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