

**H2020-INFRAEDI-2018-2020**



**Concerted action for the European HPC CoEs**  
**Project Number: 823964**

**D2.5 – Final Report on HPC3 meetings**  
**WP2 – The HPC CoE Council**



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## List of abbreviations

CASTIEL	CSA coordinating the HPC NCCs
CSA	Coordination and Support Action
DoA	Description of Action
CoE	Centre of Excellence
EC	European Commission
EHPCSW	EuroHPC Summit Week
EPI	European Processor Initiative
ETP4HPC	European Technology Platform for High-Performance Computing
EuroHPC JU	EuroHPC Joint Undertaking
GA	General Assembly (original term for HPC3)
HPC3	HPC CoE Council
INFRAG	Infrastructure Advisory Group of the EuroHPC JU
NCC	National Competence Centre in HPC
RIAG	Research and Innovation Advisory Group of the EuroHPC JU
SRA	Strategic Research Agenda
ToR	Terms of Reference
WG	Working Group

## Executive Summary

FocusCoE is a Coordination & Support Action (CSA) established in order to assist the European HPC Centres of Excellence (HPC CoEs) to fulfil their role in the European HPC ecosystem: Ensuring that extreme scale applications result in tangible benefits for addressing scientific, industrial or societal challenges in Europe. One of the core goals of FocusCoE was to “establish a CoE General Assembly (GA), which will be the focal point for collaborations among CoEs.” This is addressed by Work Package 2.

FocusCoE Task 2.1 developed an initial set of Terms of References (ToR) for the GA which were accepted during the inaugural meeting of the GA at the EuroHPC Summit week in Poznan in May 2019. During the inaugural meeting, the GA changed its name into “European HPC CoE Council”, or HPC3 for short. HPC3 elected the officers Edouard Audit (CEA / EoCoE) as Chair, Elisa Molinari (CNR / MaX) as Vice Chair and Erwin Laure (then KTH / BioExcel, now MPG / NOMAD) as General Secretary. Together with the FocusCoE coordinator, the HPC3 officers constitute the HPC3 office. The day-to-day operational support for HPC3 was provided by FocusCoE Task 2.2.

HPC3 continued to meet on a monthly basis since its foundation in Poznan. Five new CoEs (TREX, PerMedCoE, NOMAD, CoEC, RAISE) selected in call INFRAEDI-05-2020 were onboarded in the second half of 2020.

HPC3 invited relevant players from the European HPC ecosystem to its meetings in order to discuss directions of HPC application research, voice common needs of the CoEs, and explore opportunities for collaborations: Serge Bogaerts from PRACE, Jean-Pierre Panziera as RIAG and ETP4HPC chair, Michael Malms from ETP4HPC, and representatives from the EPI project in its first year (first reporting period of FocusCoE). In the second reporting period, meetings with representatives of the HPC ecosystem were mostly held with the HPC3 office only, for efficiency reasons: HPC3 was in exchange with EuroHPC director Anders Jansen, and – jointly with Task 2.3 - contacts with the Petascale and Pre-exascale consortia were established, and a series of meetings on potential collaboration took place with EuroCC/CASTIEL and the NCCs. Also, a series of bi-monthly meetings on specific technical HPC topics with CoEs and NCC has been initiated.

HPC3 and FocusCoE co-organised workshops at the EuroHPC Summit Weeks in 2021 and 2022. Prior to the 2021 summit week, a one-day CoE-only workshop on co-design aspects took place.

The Working Group on business and sustainability has published – jointly with a core team from FocusCoE work packages – a report on CoE business activities [11].

A brochure on the CoE impact for political decision makers and the general public was compiled, with FocusCoE WP2 and WP5 integrating contributions from the CoEs [10].

HPC3 supported the development of the FocusCoE sustainability strategies for continued operation of HPC3 (led by Task 2.4 and laid out in D2.4 [6]).

By March 2022, HPC3 has become a firmly established player in the European HPC ecosystem. The HPC3 members decided to continue operation as by the current Terms of Reference after the end of the extended FocusCoE term in March 2022, admitting new CoE members from upcoming EuroHPC JU calls for CoE proposals. In order to avoid disruption during a long gap before a potential renewed grant for current CoEs, it was decided to extend membership for the existing CoEs to up to one year after their termination. Also, to ensure continuity, the term of the currently elected HPC3 officers was extended by one year to May 2023.

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## 1 Introduction

FocusCoE is a Coordination & Support Action (CSA) established to assist the European HPC Centres of Excellence (HPC CoEs) to fulfil their role in the European HPC ecosystem, with a focus on ensuring that extreme scale applications result in tangible benefits for addressing scientific, industrial or societal challenges. One of the specific goals of FocusCoE was to “establish a CoE General Assembly (GA), which will be the focal point for collaborations among CoEs.” The General Assembly (which was subsequently renamed HPC CoE Council or HPC3 for short) is a body of representatives from the HPC CoEs serving to foster collaboration between the CoEs, coordinate activities and bundle the CoEs’ views, establishing a strong voice of the European HPC ecosystem “application pillar”.

The role of FocusCoE was to establish the HPC3 organisation (the process leading to this was covered by Task 2.1 and has been reported in D2.1 [3]) and to support its operation in Task 2.2, which is the topic of Deliverable D2.2 [4] (covering the first year from May 2019 until May 2020) and this deliverable, which briefly summarizes the developments until May 2020 and then provides a detailed account on the FocusCoE and HPC3 activities until the end of FocusCoE (March 2022), including a detailed meeting-by-meeting description.

The members of HPC3 have expressed their intent to continue HPC3 operations beyond March 2022 according to the current Terms of Reference, and to also include any new HPC CoEs resulting from upcoming calls for proposals issued by the EuroHPC JU. The current HPC3 officers will continue their service until May 2023. It is planned to adapt the meeting frequency to the situation and to hold quarterly meetings.



## 2 The HPC CoE Council (HPC3)

### 2.1 HPC3 Goals

The FocusCoE DoA describes the overarching objective of HPC3 as “to act as focal point for collaborations among CoEs”. It can establish working groups for topics of interest to all or several CoEs, collect consolidated input from CoEs to third parties (supported by Task 2.3, see D2.3 [5] and D2.6 [7]), help to develop a common point of view on an application-oriented research agenda for European HPC and serve as a common voice for the application pillar in the HPC ecosystem, thus strengthening the role of application-oriented research.

During the reporting period, HPC3 did undertake all these actions, as shown in Subsection 2.3 below.

### 2.2 Establishment & Structure

The establishment of HPC3 was one of the primary objectives of FocusCoE WP2. It was realised by the set of 10 CoEs active in May 2019<sup>1</sup> agreeing to the initial terms of reference (ToR) during a meeting on 17.5.2019 at the European HPC Summit week in Poznan. The meeting elected Edouard Audit (CEA / EoCoE) as Chair, Elisa Molinari (CNR / MaX) as Vice Chair, and Erwin Laure (then KTH / BioExCel, now MPG / NOMAD) as General Secretary. These three elected HPC3 officers, together with the FocusCoE representative and deputies, constitute the HPC3 office. Also, the name of the body was changed from “HPC CoE General Assembly” to “HPC CoE Council” or HPC3 for short. Full details are contained in D2.1 [3] and D2.2 [4].

In the current Terms of Reference, only active (funded) HPC CoEs and FocusCoE are members of HPC3, i.e. have voting rights (cf. Table 1). Guests (called observers) can be invited for individual meetings on a case-by-case basis. Newly funded CoEs will become members of HPC3 as soon as they accept the Terms of Reference. Working groups can be established by HPC3 and may have participants also from outside the member projects.

FocusCoE WP2 provided operational support to HPC3, including organising the meetings and maintaining a collaboration and communication infrastructure. In detail, this involved:

- Organising physical or online meetings (all meetings after Dec. 2019 were online meetings)
- Setting up meeting agendas, conducting online meetings, writing minutes and following up on action items
- Setting up and maintaining mailing lists for HPC3 member representatives, working groups and HPC3 office (the latter comprising elected Chair, Vice Chair and General Secretary as well as FocusCoE WP2 support staff), maintaining a directory of HPC3 member representatives and roles
- Setting up and maintaining a document repository for HPC3 representatives, to manage e.g. documents created by HPC3, presentations given to HPC3 by guests, materials provided by CoEs
- Communicating with external parties (e.g. invited observers)

### 2.3 HPC3 meetings and Activities

Since its establishment in May 2019, HPC3 held 28 monthly meetings and one all-hands meeting (“CoE workshop”).

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<sup>1</sup> See Table 1 for an overview over all CoEs with their start and end dates

In the first year (May 2019-May2020), HPC3 invited guests from key HPC ecosystem players (PRACE, EuroHPC JU RIAG, ETP4HPC, and EPI). A common position of the CoEs with respect to HPC application research was developed and then communicated & discussed with the RIAG chairman, Jean-Pierre Panziera (also ETP4HPC chairman), thus building support for the CoEs' point of view in these bodies. An overview presentation highlighting the scientific challenges tackled by the HPC3 members was published. HPC3 also established a working group on business and sustainability. The activities of HPC3 in this time period are described in more detail in D2.2 [4].

The second year of HPC3 started with the onboarding of 5 new CoEs which had been selected from the INFRAEDI-05-2020 CoE call: TREX, NOMAD-2, PerMedCoE, CoEC and RAISE<sup>2</sup>. For these new CoEs, welcome meetings were organised by FocusCoE and the HPC3 office, in order to introduce them to the work of FocusCoE and HPC3, and give HPC3 a first impression on their scope. They were invited to HPC3 as permanent observers at first. Once they officially started (October 2020 except RAISE which started in January 2021) and accepted the ToR, they became full members.

HPC3 and FocusCoE organised public workshops at the EuroHPC Summit Weeks (EHPCSW):

- EHPCSW 2021 (online, about 100 participants), “CoEs on the road to Exascale” with an introduction of FocusCoE, an overview over the CoEs and their applications, and a panel discussion [12]
- EHPCSW 2021 (online, about 100 participants) “HPC Education & Training – Perspectives from EU13 Member States”, chaired by Simon Wong (ICHEC and FocusCoE WP4), focused on the HPC education and training landscape among the EU13 Member States with individual talks on existing programmes, target communities and industries, and future perspectives [13].
- EHPCSW 2022 (in person), “European HPC CoEs: perspectives for a healthy HPC application eco-system and Exascale”, featuring an introductory talk and two round table discussions with participation of all active CoEs [14].

Full details of these events are provided in D2.6 [7], and in D4.2 [8] for the training-related event.

Prior to the EHPCSW'21, a full-day workshop on co-design was organised with FocusCoE WP2 and WP4 (with over 80 attendees, but limited to the CoEs), in order to exchange experience and advance the understanding of this complex topic. Details are provided in D4.2 [8].

Through the HPC3 office, the CoEs were in contact with the EC and EuroHPC JU and its director Anders Jansen and voiced the specific needs and points of view of the CoEs, for instance in a meeting of the HPC3 office with A. Jensen in October 2020. A letter was submitted in December 2021 to the EuroHPC director regarding CoE concerns on the delay of the planned calls for new CoEs (HORIZON-EUROHPC-JU-2021-COE-01).

Further contacts to important players in the European HPC ecosystem were established, using assistance from T2.3: Meetings with the Petascale and pre-Exascale consortia funded by the EuroHPC JU were organised, in order to check options for development access for the CoEs to these systems on the one hand, and opportunities to support HPC application users on these

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<sup>2</sup> Originally named AISEE.

systems through the CoEs in the future. More details about these meetings and these consortia are given in D2.6 [7].

Close links were established to the National HPC Competence Centres (NCCs) and in particular their coordinating CSA CASTIEL. Jointly with CASTIEL, a series of thematic meetings was kicked off, facilitating matchmaking between NCCs in need of technology support and CoEs with the relevant competences (for details on the interactions with the NCCs, see D2.6 [7]).

The HPC3 office acted as coordination point for third parties wanting to work with the CoEs. For instance, a workshop on 2.3.2022 specifically for CoEs offered by Intel on oneAPI (with high relevance for the future uptake of EPI developments) was organised with support from Task 2.3 and FocusCoE WP5, and attended by about 20 participants from the CoEs [15]. Beyond the final reporting period, a workshop on co-design centred on the European flagship codes represented by the CoEs has been accepted for the ISC 2022 conference and will take place on June 2<sup>nd</sup>, 2022 [16]. The workshop organisers comprise representatives from Nvidia Ltd, ARM Ltd., SiPEARL and the FocusCoE coordinator, the programme committee will also include the HPC3 Chair and information about the event will be hosted on the [hpccoe.eu](http://hpccoe.eu) website.

HPC3 updated its overview presentation, in particular with information of the new CoEs [9]. General information on HPC3 is available on the HPC CoE web hub **Error! Reference source not found.** HPC3 initiated the creation of a “CoE impact brochure” aiming at political and executive-level HPC ecosystem stakeholders and also the general public [10]. For the production of this brochure, a significant contribution came from FocusCoE WP2 and WP5 with an editorial role ensuring the production of an engaging document accessible also by informed lay persons. See Figure 1 for a sample page.

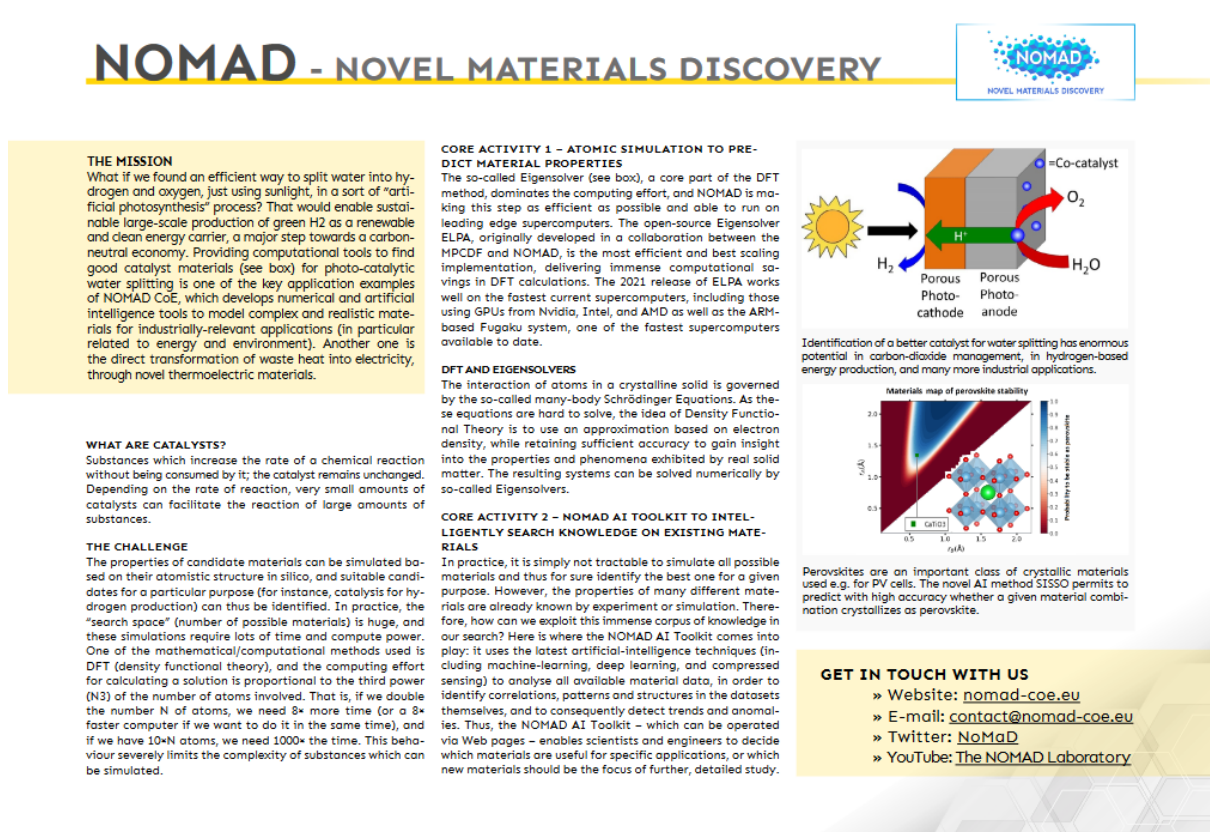


Figure 1: Sample page from the CoE impact brochure

HPC3 provided input to the ETP4HPC SRAs (see D2.6 [7] for more details).

The HPC3 WG on business and sustainability originally set out to outline in a white paper preferred options for achieving sustainability in the HPC applications research field covered by the CoEs focussing on achieving sustainability of CoEs as entities, by building on the sustainability plans of the CoEs and highlighting related international best practices. As the original intent of that paper became less relevant (in light of the prospect of upcoming calls for new CoEs), and many business-related joint activities led by FocusCoE were kicked off, the focus was changed to use the output of these activities, leverage the prior work within the group and augment this with additional information on CoE experience with business activities to summarise experience and findings on the topic of business activities, opportunities and challenges in a public document [11].

HPC3 also supported the development of sustainability options for its future operation after the end of FocusCoE, and feedback from HPC3 was fed into the related FocusCoE WP2 deliverable D2.4 [6]. Towards the end of FocusCoE, HPC3 decided to continue operation beyond March 2022, acknowledging the continued support offered by scapos (mailing lists and HPC3 operational support) and U. Stuttgart (website and social media) on a *pro-bono, best effort* basis and the willingness of the current HPC3 officers to serve for another year until May 2023. Current CoEs will, if desired, be able to remain members for up to one year after their contractual completion date (cf. Tor changes in Appendix 5), and new CoEs granted through upcoming calls will be accepted as members. It is planned to adapt the meeting frequency to the changed situation and to hold quarterly meetings.

<b>Acronym</b>	<b>Full Title</b>	<b>Runtime</b>	<b>Project web site</b>
BioExcel-2	BioExcel-2 Centre of Excellence for Biomolecular Research	01/2019-06/2022	<a href="https://bioexcel.eu/">https://bioexcel.eu/</a>
ChEese	Centre of Excellence for Exascale in Solid Earth	11/2018-03/2022	<a href="https://cheese-coe.eu/">https://cheese-coe.eu/</a>
CompBioMed	A Centre of Excellence in Computational Biomedicine	10/2019-09/2023	<a href="https://www.compbiomed.eu/">https://www.compbiomed.eu/</a>
EoCoE-II	Energy oriented Centre of Excellence for computer applications	01/2019-06/2022	<a href="https://www.eocoe.eu">https://www.eocoe.eu</a>
EsiWACE2	Excellence in Simulation of Weather and Climate in Europe, Phase 2	01/2019-12/2022	<a href="https://www.esiwace.eu/">https://www.esiwace.eu/</a>
E-CAM	An e-infrastructure for software, training and consultancy in simulation and modelling	10/2015-03/2021	<a href="https://www.e-cam2020.eu/">https://www.e-cam2020.eu/</a>
EXCELLERAT	The European Centre of Excellence for Engineering Applications	12/2018-05/2022	<a href="https://www.excellerat.eu">https://www.excellerat.eu</a>
HiDALGO	HPC and Big Data Technologies for Global Challenges	12/2018-02/2022	<a href="https://hidalgo-project.eu/">https://hidalgo-project.eu/</a>
MaX	Materials design at the Exascale	12/2018-05/2022	<a href="http://www.max-centre.eu/">http://www.max-centre.eu/</a>
POP2	Performance Optimisation and Productivity 2	12/2018-05/2022	<a href="https://pop-coe.eu/">https://pop-coe.eu/</a>

FocusCoE	Concerted action for the European HPC CoEs	12/2018-03/2022	<a href="https://www.hpccoe.eu/">https://www.hpccoe.eu/</a>
TREX	Targeting Real Chemical accuracy at the EXascale	10/2020-09/2023	<a href="https://trex-coe.eu/">https://trex-coe.eu/</a>
NOMAD-2	Novel materials for urgent energy, environmental and societal challenges	<u>10/2020-03/2024</u>	<a href="https://www.nomad-coe.eu/">https://www.nomad-coe.eu/</a>
CoEC	Advanced technology for combustion simulation	<u>10/2020-09/2023</u>	<a href="https://coec-project.eu/">https://coec-project.eu/</a>
PerMedCoE	High-performance computing to treat disease at individual level	<u>10/2020-09/2023</u>	<a href="https://permedcoe.eu/">https://permedcoe.eu/</a>
RAISE	Research on AI- and Simulation-Based Engineering at Exascale	<u>01/2021-12/2023</u>	<a href="https://www.coe-raise.eu/">https://www.coe-raise.eu/</a>

**Table 1: List of current and historic HPC3 members with runtimes (including planned or agreed extensions)**

From the HPC3 general presentation, we include a map showing the geographic distribution of the CoE partners. There are 13 partners from the EU13 countries.

## A pan-European network

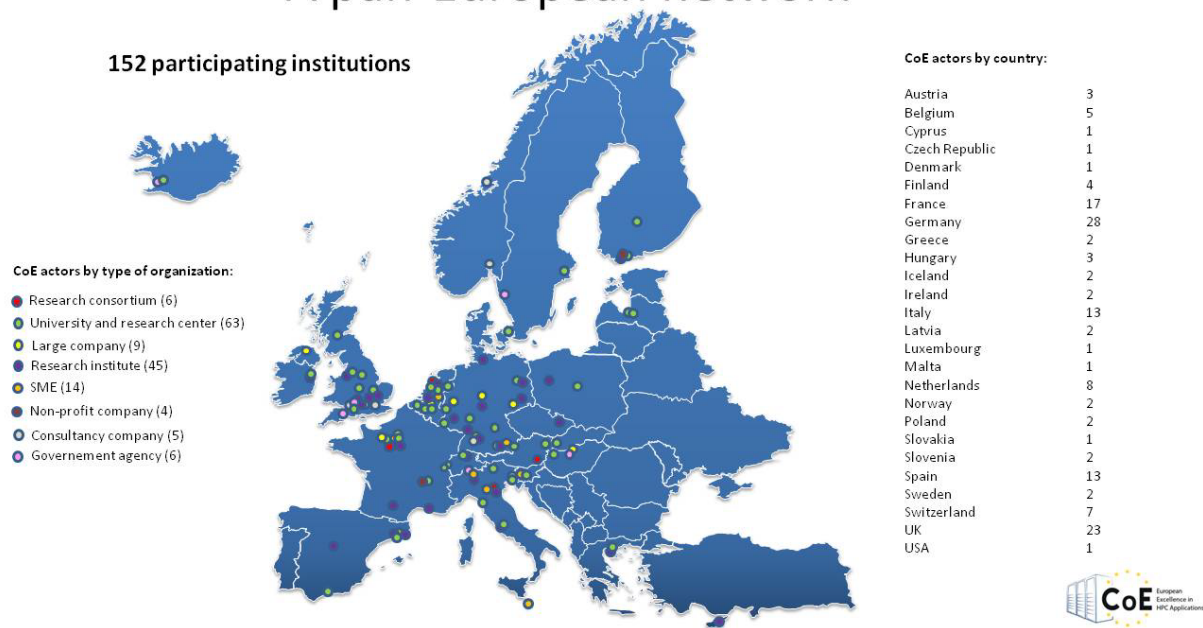


Figure 2: Map of CoE partners across all active CoEs

### 2.3.1 HPC3 Meeting Summaries

The summary of Meetings 1-10 is given in D2.2 [4].

#### Meeting 11, 10.6.2020

The main topic of this meeting was the “onboarding” of 3 new CoEs (which were selected but had not yet officially started): TREX, CoEC and NOMAD (PerMedCoE could not attend). Each new CoE gave presentations of about 15 minutes, plus a subsequent discussion on potential collaborations.

The presentations were subsequently collected and made available for all CoEs on the document repository.

The new CoEs would be invited as permanent observers to the HPC3 meetings until their official start, when they would become regular members.

A report on the ongoing work in the WG on business / sustainability was given.

Short reports from recent RIAG and INFRAG meetings were provided.

#### Meeting 12, 8.7.2020

Guests in the first part of this meeting were Estela Suarez (JSC), Etienne Walter (ATOS), and Daniele Cesarini (CINECA), who presented a proposal to the EuroHPC Call on “advanced pilots towards the European Exascale supercomputers”. The ways in which CoEs could collaborate with a project arising from a successful proposal to that call were discussed.

A first feedback from the FocusCoE midterm review was given, and first implications for the future work of HPC3 were discussed.

Progress from the WG Business was briefly presented.

#### Meeting 13, 9.9.2020

The new CoE PerMedCoE was presented & options for collaborations discussed.

Results of the FocusCoE review and their implications were discussed. One of the next steps would be a meeting of the elected HPC3 officers and the FocusCoE coordinator with the FocusCoE PO.

It was decided to open the October meeting and turn it into an all-hands CoE workshop, open to all persons from the CoEs responsible for contact with the FocusCoE work packages, and the representatives of the FocusCoE work package. Thus, any ideas, issues and developments pertaining to the specific working areas (industrial outreach, training, and dissemination) could be broadly discussed.

### **2<sup>nd</sup> CoE workshop 14.10.2020**

The half-day workshop (an “all-hands meeting”, open to all CoE representatives in contact with the FocusCoE work packages, not just the ones for HPC3) was centred on the topics of industrial outreach, training and dissemination and a final discussion round. The goal was to review the interactions of FocusCoE and the CoEs, and re-align goals and activities. Several adjustments to current processes were agreed upon, for instance a regular “news flash” on FocusCoE activities sent to all CoE representatives. Intensified collaboration between the CoEs on the topics of co-design and Exascale development was generally considered an area to be strengthened, a separate discussion channel on Slack was to be set up. Specific further activities were to be decided in the subsequent HPC3 meetings.

(Note: The 1<sup>st</sup> CoE workshop took place one day after the FocusCoE kickoff in Frankfurt in February 2019, before HPC3 was established.)

### **Meeting 14, 11.11.2020**

The 5<sup>th</sup> new CoE, AISEE (later renamed to RAISE) was welcomed.

HPC3 office gave a report of the meeting with the EuroHPC director Anders Jensen, on the future relationship of HPC3 and the EuroHPC JU, and the future of CoEs.

A meeting with 3 pre-exascale consortia took place earlier that morning and was reported on; and collaboration options for CoEs were discussed.

Following up the outcome of the CoE workshop, actions regarding co-design & Exascale topics were discussed.

Best options for interacting with the CASTIEL project and the European HPC NCCs were a topic of discussion (the large number of NCCs represents a real challenge, and not all of them are known yet).

A short report on the (1<sup>st</sup>) FocusCoE workshop on business & sustainability was presented, and feedback was generally positive.

### **Meeting 15, 16.12.2020**

RAISE gave a presentation introducing this new CoE to HPC3. In a subsequent discussion, collaboration options were considered.

The various ramifications of the co-design and Exascale development topics were discussed, and options to support common activities in these areas were considered. It was agreed to target two events: First a closed workshop for the CoEs, targeting co-design, and then an open event at the European HPC Summit Week 2021, targeting the contribution of the CoEs towards Exascale applications.

An *ad hoc* survey among the participants showed that first CoEs are considering plans for extension.



### **Meeting 16, 20.1.2021**

The planning for the two workshops on co-design and Exascale development continued, with the closed workshop having a more technical focus and the public workshop at European HPC Summit Week 2021 targeting a broader picture.

Information on the planned Call for an education programme targeting an “European Master of Science (MSc) in HPC” was shared.

### **Meeting 17, 17.2.2021**

Planning for the workshops on co-design (12.3.2021) and the European HPC Summit Week 2021 workshop (“CoEs on the road to Exascale”) was continued.

Information on how CoEs could obtain early access to pre-Exascale systems was discussed. A short presentation of the timeline of availability of EuroHPC JU Petascale and pre-Exascale systems was given. Reports on the past meetings with CASTIEL and EuroCC were given.

### **Meeting 18, 17.3.2021**

The internal workshop on co-design on 12.3.2021 was very successful, with approximately 60 participants. A recording will be published internally for the benefit of the CoEs.

Planning for the European HPC Summit Week 2021 workshop on 23.3. 2021 was continued.

The upcoming EU fitness check meeting on 22.4.2021 was briefly discussed. Reports on recent contacts with EuroCC / CASTIEL were given.

A meeting with the Petascale consortia<sup>3</sup> is planned for 13.4.2021.

### **Meeting 19, 20.4.2021**

The work of WP2 on options for a sustainable HPC3 operation after the end of FocusCoE was briefly presented, and options to include CoEs in these considerations were discussed. As the next step, a presentation by FocusCoE on the different options for HPC3 sustainability was agreed.

A refocus of the WG on business & sustainability is seen as necessary, as the intended focus of the “position paper” on the sustainability of the individual CoEs as entities has lost some relevance (in light of the upcoming call for new CoEs) and work has consequently lost momentum. Instead, it is seen as beneficial to leverage the recent joint activities initiated by FocusCoE and focus on what can be learned from the business plans and actual activities of the CoEs, eventually leading to a public report towards the end of FocusCoE. A core group from the WG and FocusCoE will be formed to lead this process.

A report was given on the meeting with the Petascale consortia on 13.4.2021; ideas were voiced on how CoEs could make a difference in this context (for instance by providing training and 3<sup>rd</sup> level application specific support), and on how CoEs could access the systems.

A retrospective on the European HPC Summit Week 2021 workshop was given, which was successful with about 100 participants. (See Reference [12] and the description in D2.6 [7]).

### **Meeting 20, 19.5.2021**

Approaches and options to gain access to large-scale systems for development purposes was a main topic. The background is that CoEs developing or optimising SW code for Exascale will require access to entire systems for SW development and benchmarking. This does not fit

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<sup>3</sup> PetaSC, Vega, Karolina, MeluXina, Deucalion

well to the standard policies for obtaining machine time. Best practices like “scaling days” at JSC were discussed. HPC3 will lobby for implementing best practices in the existing and upcoming EuroHPC JU systems.

A report of a meeting of FocusCoE with the CASTIEL management was given. A regular schedule for meetings on selected technical topics between interested CoEs and HPC NCCs was agreed, which would enable a matchmaking between NCCs in need of specific technical competence and CoEs offering matching expertise.

#### **Meeting 21, 16.6.2021**

The main topic of this meeting was a FocusCoE presentation on the various options for HPC3 sustainability and a subsequent discussion.

Short reports on the WG on business & sustainability meeting of the core group and next steps for NCC/CoE interactions were given. The first thematic meeting would take place on 8.7.2021 on the topic of quantum mechanical simulations in chemistry and materials science.<sup>4</sup>

#### **Meeting 22, 18.8.2021**

For the 2<sup>nd</sup> thematic meeting between the CoE and the HPC NCCs, the CFD topic was chosen, and several CoEs expressed interest to participate. A bi-monthly schedule for such thematic, technical meetings is anticipated.

FocusCoE prepared a survey to collect and analyse CoE preferences for HPC3 sustainability options; the structure of the survey and was presented to the CoEs.

#### **Meeting 23, 15.9.2021**

At the 2<sup>nd</sup> thematic NCC/CoE meeting on 22.9.2021 input was gathered from the CoEs RAISE, EXCELLERAT, CompBioMed, EoCoE and CoEC. Potential topics for the next such meetings are discussed; options of interest are AI and code optimisation.

First experience of some CoEs in accessing new EuroHPC JU systems for code development and optimisation were discussed.

WG business & sustainability reported on a new survey regarding the status of actual CoE sustainability and business plans and activities. It was agreed to feed that information into a public report on business activities of the CoEs (ultimately leading to the report [11]).

#### **Meeting 24, 20.10.2021**

The next thematic NCC/CoE meeting was set to take place on 23.11.2021 and discuss the topic of code optimisation.

The plans of the EuroHPC JU for the upcoming CoE call were discussed.

Details on the next ETP4HPC SRA were presented and CoEs were encouraged to provide input.

Results of the FocusCoE survey on HPC3 sustainability were presented. Most CoEs preferred an informal body like the current one (either supported by a CSA or self-sustained) over a more formal approach involving a legal entity funded by e.g. membership fees.

#### **Meeting 25, 17.11.2021**

HPC3 decided to publish a “CoE impact brochure” at the end of March 2022 targeting political and executive-level HPC ecosystem stakeholders and also the general public, and promoting the CoE approach and results in an engaging style [10].

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<sup>4</sup> Full details on these thematic meetings are provided by D2.6 [7]

A CoE workshop entitled “European CoEs in HPC: achievements and perspective for applications towards Exascale” was accepted by the European HPC Summit Week 2022 [14]. The structure of this workshop was discussed and agreed upon to be based on a presentation followed by 2 thematic round tables).

FocusCoE presented Deliverable D2.4 which discusses the options on HPC3 sustainability in light of the CoE survey results. Specific questions on the continuation of HPC3 after the end of FocusCoE were discussed.

#### **Meeting 26, 15.12.2021**

The severe implications on the delayed CoE calls for those CoE seeking continuation were discussed. It was agreed that the HPC3 office would write a letter to the EuroHPC JU director highlighting the need to reduce the time gap between the end of a CoE and the start of a possible continuation, in order to avoid disruption in terms of staff and expertise.

As many CoEs will terminate in the 1<sup>st</sup> half of 2022 and will apply in the upcoming calls for CoEs for a continuation, HPC3 would encounter a situation with many of its current members being in an ill-defined membership state according to the current ToR. Changes of the ToR are discussed to find a pragmatic solution.

Next steps for the impact brochure were discussed. Planning for the European HPC Summit Week workshop was continued, and the topic for the next NCC/CoE thematic meeting was discussed

#### **Meeting 27, 19.1.2022**

An update of the HPC3 terms of reference (ToR) was agreed, permitting CoEs to stay members for up to one year after their end.

Updates on the steps for the impact brochure were provided.

Details for the European HPC Summit Week 2022 CoE session were discussed and the topics for the 2 round tables agreed.

A refinement of the topics for the next NCC/CoE thematic meeting were discussed, providing more focus than the very broad topic of “tools” originally suggested.

A table of current CoE extension plans was compiled. FocusCoE partners SCAPOS and HLRS would offer to continue maintenance of current infrastructure after the end of FocusCoE without being reimbursed.

#### **Meeting 28, 16.2.2022**

Given the current HPC3 ToR, the term of the current HPC3 officers would end in May 2022. Because of the unavoidable gap between that point in time and the start of the next wave of CoEs, the current HPC3 officers offered to serve for another year, after which new officers would be elected from a full set of CoEs. This offer was accepted unanimously by HPC3.

As FocusCoE ends in March 2022, details on continuation of HPC3 operation were discussed, backed by the offer of scapos to provide continued operational support and the continuity in the HPC3 office (extension of the term of the three officers).

The planning for the European HPC Summit Week 2022 CoE workshop progressed, and the participant lists for the two round tables were filling up. There was however considerable uncertainty on the status of travel restrictions at the time of the event – many organisations impose their own limitations on travel. According to the European HPC Summit Week 2022 organisers, there was no plan to hold that event in a virtual or a hybrid way.

Status and next steps for the production of the impact brochure were presented.

The future process for setting up thematic meetings with the NCCs was agreed, which now shifts the responsibility for setting the topics to the HPC NCCs (coordinated via CASTIEL). In the discussion, a desire for an inverse flow of information from NCCs to CoEs was brought up, for instance to gain insight in the industrial outreach approaches used by the NCCs. FocusCoE WP2 will discuss options for such an exchange with CASTIEL (the sheer number of NCCs and their diverse nature presenting a challenge here).

Interest and logistic details of CoE participation in a workshop on the oneAPI programming methodology and environment offered by Intel were discussed, and FocusCoE WP2 was tasked to follow up with Intel, with the goal to organise a 1-2 day workshop at the beginning of March (this finally took place on the 2<sup>nd</sup> of March 2022, [15])

The meeting in March 2022 was split into preparatory meetings for the round tables at European HPC Summit Week and an informal in-person meeting at that event in Paris.

## **2.4 Outlook**

The goals and objectives of HPC3 remain valid after the end of FocusCoE. With continuing the support offered *pro bono* by scapos and the HPC3 officers, the current HPC3 members intend to continue the operation of HPC3 for the foreseeable future, leveraging and maintaining the established structures and the position of HPC3 in the European HPC ecosystem.

### **3 Conclusion & Lessons learned**

After close to 3 years of operation, HPC3 is firmly established as a significant player in the European HPC ecosystem and a recognized voice for the HPC application layer of the European HPC arena. It has made good progress to discuss, formulate and advocate the common interests of the HPC CoEs, and acts as a hub for collaborating with the EuroHPC hosting activities and key elements of the EuroHPC ecosystem, in particular EuroCC/CASTIEL and the HPC NCCs, and FocusCoE's Objective 1 on establishing the HPC CoE Council has been reached in full – HPC3 will continue after the end of FocusCoE. The important question of how to put HPC application research and development activities on a sustainable footing was investigated, and valuable technical information was made available across all CoEs.

The request by the CoE members to continue operation of HPC3 after the end of the FocusCoE term bears witness to them perceiving HPC3 as useful and worthwhile, and the offer to future CoEs to join ensures that HPC3 can stay relevant in the times ahead, which will see the first Exascale systems coming online.

Yet, it has been our experience that activities which go beyond simple coordination of actions, and which do entail a certain and continuous level of extra work, cannot be expected to be covered completely by the individual CoEs. Such endeavours – like planning and running joint events, creating larger common documents, managing infrastructure like a website and executing a cohesive common communication strategy - will require dedicated, funded effort; that is, a dedicated CSA like FocusCoE is instrumental for implementing such actions.

## 4 References

- [1] FocusCoE project – Web site of the European HPC CoEs <http://www.hpccoe.eu/>
- [2] FocusCoE project – web page on HPC3, <https://www.hpccoe.eu/hpc-coe-council/>
- [3] FocusCoE Deliverable D2.1, “Report on agreed GA Procedures and Terms of Reference”, Project Month 6 (May 2019)
- [4] FocusCoE Deliverable D2.2, “First Report on HPC3 meetings”, Project Month 18 (May 2020)
- [5] FocusCoE Deliverable D2.3, “First summary of consolidated CoE input provided to the EU HPC ecosystem”, Project Month 18 (May 2020)
- [6] FocusCoE Deliverable D2.4, “Report on propositions for a sustainable HPC CoE Council”, Project Months 36 (November 2020)
- [7] FocusCoE Deliverable D2.6, “Final summary of consolidated CoE input provided to the EU HPC ecosystem”, Project Month 40 (March 2022)
- [8] FocusCoE Deliverable D4.2, “Final Training Report”, Project Month 40 (March 2022)
- [9] HPC3 general presentation, [https://www.hpccoe.eu/wp-content/uploads/2021/11/CoE\\_General\\_Presentation\\_V2.1.pdf](https://www.hpccoe.eu/wp-content/uploads/2021/11/CoE_General_Presentation_V2.1.pdf)
- [10] CoE impact brochure, March 2022, available from <https://www.hpccoe.eu/impact>
- [11] HPC3 WG on business and sustainability: Report on CoE business activities: opportunities, challenges and lessons learned. Available at <https://www.hpccoe.eu/hpc-coe-council/>
- [12] CoE workshop “CoEs on the road to Exascale” at EHPCSW’21: FocusCoE news entry with link to recordings. <https://www.hpccoe.eu/2021/04/30/focuscoe-organizes-two-workshops-at-ehpcsw21>
- [13] CoE workshop “HPC Education & Training – Perspectives from EU13 Member States” at EHPCSW’21, Online recording available at <https://www.hpccoe.eu/2021/04/30/focuscoe-organizes-two-workshops-at-ehpcsw21/>
- [14] CoE workshop “European HPC CoEs: perspectives for a healthy HPC application ecosystem and Exascale” at EHPCSW’22, Paris. <https://www.hpccoe.eu/2022/03/24/focuscoe-at-eurohpc-summit-week-2022>
- [15] “FocusCoE Hosts Intel OneAPI Workshop for the EU HPC CoEs“, 4.3.2022, <https://www.hpccoe.eu/2022/03/04/focuscoe-hosts-intel-and-eu-hpc-coes-for-oneapi-workshop>
- [16] ISC 2022 Workshop on “Software Co-Design Actions in European Flagship HPC Codes”, 2.6.2022, <https://www.isc-hpc.com/agenda.html>

## 5 Appendix: Changes to the HPC3 Terms of Reference

The full text of the Terms of Reference (ToR) as of November 2020 is contained in D2.1 [3].

The only change in the reporting period was the pragmatic extension of membership of CoEs planning to apply for a continuation project, as discussed above and agreed by HPC3 in January 2022, in Section “HPC3 members” of the ToR:

Original text:

*CoEs with a “pending continuation contract” (that is, CoEs that have reached the termination date of an existing EC contract but which are waiting of the signature of a Grant Agreement for a follow-up or continuation) may remain an HPC3 member as long as there is no significant gap between the termination of the prior contract and expected commencement of the new contract. HPC3 will take a decision on the precise understanding of “significant gap” once informed by the CoE about the details of the pending continuation contract.*

Replacement text:

*CoEs and CSAs targeting a continuation may stay HPC3 members for up to one year after termination by simply declaring so. The membership of the terminated project ceases when a continuation project becomes member.*