D1.3 Collaboration plan with the other Centers of Excellence
Version 1.0

Document Information

Contract Number	101143931
Project Website	www.pop-coe.eu
Contractual Deadline	M6, June 2024
Dissemination Level	PU
Nature	R
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Keywords	Collaboration, dissemination, training, business development

This project has received funding from the European High-Performance Computing Joint Undertaking (JU) under grant agreement No 101143931. The JU receives support from the European Union's Horizon Europe research and innovation programme and Spain, Germany, France, Portugal, and the Czech Republic.

Change Log

Version	Author	Description of Change
V0.1	Elena Markocic	Initial Draft
V0.2	Marta Garcia Bernd Mohr Brian Wylie Samir Ben Chaabane	Contributions from WPs 2 and 3
V1.0	Elena Markocic	Final version for submission

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Executive Summary

This deliverable describes the planned collaboration of POP3 with the other EuroHPC Centres of Excellence and CASTIEL2. The present document lists the activities and other initiatives that support the collaboration and will be followed by deliverables that monitor the progress and update the collaboration plan in months 18 and 36. This is a complementary initiative to the one described in the CASTIEL 2 Deliverable 1.7 - Collaboration Plan with the CoEs.

1. Introduction

The collaboration with other Centres of Excellence in HPC is one of the main objectives of the POP3 project. This project will be built on the activities from the previous POP and POP2 initiatives. In addition to assessing the codes generated by other CoEs, there will be collaboration on initiatives to increase the visibility of all CoEs and their output. This includes joint efforts in dissemination, training, and business development activities. These efforts will be further supported by the activities planned by CASTIEL2, in which POP3 will also actively participate. The goal of this collaboration plan is to amplify the impact of POP3 activities on other CoEs and third parties, while contributing to EuroHPC's objectives of supporting research and innovation in developing and adapting HPC applications for the exascale and post-exascale era.

2. Collaboration with the other CoEs in POP and POP2

The objective of the initial POP project was to establish a Centre of Excellence in Computing Applications, focusing on Performance Optimization and Productivity. This involved providing services to the software community, and it also included applications from other CoEs (CompBioMed, BioExcel, EoCoE, ESiWACE and MaX CoEs). The initiative's success[1] led the consortium to extend its efforts under the umbrella of the POP2 project. The follow-up project aimed to boost the collaboration with other HPC Centers of Excellence[2], based on 6 tasks:

- TASK: Formally invite all CoEs to collaborate with POP.
- TASK: Establish network with CoEs, with a single point of contact at POP
- TASK: Identify which CoEs could benefit from POP services.
- TASK: Undertake Periodic Campaigns for all interested CoEs.
- TASK: Through our established network with CoEs, identify events where training or attendance would be beneficial.
- TASK: Through regular contact with CoEs, ensure that all possible collaborations are exploited.

By completing all these tasks, the POP2 consortium has established a network with other CoEs [3] [4] (BioExcel, ChEESE, CompBioMed, E-CAM, EoCoE,

ESiWACE, EXCELLERAT, HiDALGO, MaX and Focus CoE). All CoEs have been invited to collaborate with POP2 and they were informed about the possible avenues for collaboration.

This initiative resulted in:

- Implementing performance assessment services for other CoEs
- Engaging with the other CoEs in a range of dissemination and outreach activities including newsletters, webinars, conference talks and joint presence in events
- Organisation of joint training events.

3. POP3 Collaboration plan

3.1 CoE Assessment campaigns and services

As stated in Annex 1 of the Grant Agreement, the main impact of POP3 is achieved through collaboration with the HPC CoEs. During the preparation of the POP3 proposal, the consortium engaged with 14 CoEs that may coexist with POP3 to identify and quantify these collaborative efforts. As a transversal CoE, POP3 aims to enhance the scalability and efficiency of European lighthouse HPC applications, validating the results on EuroHPC platforms.

POP3 will assess the lighthouse codes selected by the CoEs listed in Table 1, using their preferred input, configuration, and platform. This assessment will include an evaluation of efficiency and recommendations for improvement. The CoEs have allocated resources to enhance their lighthouse codes, and input from POP3 will help improve the efficiency and scalability of these codes. Some CoEs have requested a second assessment campaign; in such cases, the initial assessments by POP3 will be valuable for validating and evaluating the impact of developments made during the CoEs' lifetimes.

The table below summarizes the information provided during the discussions with the listed CoEs. Although some CoEs have not yet identified specific applications, a total of 83 studies are planned, covering over 60 different codes.

CoE	Codes identified in the support letter	Number of codes
bioExcel-3	GROMACS	1
CEEC	FLEXI, Alya, Nek5000/NekRS, Neko, waLBerla	5
ChEESE2	SeisSol, SPECFEM3D, pTatin3D, TANDEM, HxaHyPE, xSHELLS, HySEA, FALL3D, Open-PDAC, Elmer/ICE, LaMEM	11
EoCoE	not specified	5
ESiWACE	EC-Earth, IFS, NEMO, ICON	6

EXCELLERAT2	Neko, Alya, M-AIA,VISTLE	6
Hidalgo2	OpenFOAM, EULAG, waLBerla	3
BrainScoEPE	Arbor, NEST, ATLaS, ExTract, MiMiC	6
MAX	Quantum ESPRESSO, SIESTA, BigDFT, Fleur, Yambo	5
MultiXscale	ESPResSo	3
PermedCoE	PhysiBoSS	3
Plasma-PEPSC	BIT1 and BIT3, GENE-X, PIConGPU, Vlasiator	4
SPACE	OpenGADGET, PLUTO, RAMSES	3
TREX	not specified	2
	Total	**64 codes, 82 studies**

Table 3: Collaboration of POP3 with other CoEs

The assessements done for the other CoEs are organized under the so called “campaigns” the initial idea of a campaign is to assess all the codes of the CoE the during the same time span. However, due to the differences on the organization of the different CoEs and the different levels of maturity of the codes within each CoE we will be flexible and for some of the CoEs assess the different codes when requested without enforcing it to be during the same time span.

For each campaign we will have a POP3 responsible that will be the main contact point and in charge of following the progress of the different assessments. We will also ask each CoE to name a contact point for the campaign to ensure a fluid comunication between the two projects.

3.2 Dissemination

The POP3 dissemination team will work closely with the dissemination team of other CoEs, once a POP assessment campaign (see above) is successfully finished. Another collaboration case is an especially successful POP performance assessment or 2nd-level service for a CoE application code (“success story”). In both cases, we plan to publish a POP blog article about the successful collaboration and/or a blog/news article on the corresponding CoE website or ideally both. In some cases (depending on the topic), the success story could be further disseminated via an episode of our POP webinar series.

In addition, the POP dissemination team watches the social media and newsletter posts from the other CoEs, and by liking and re-tweeting their content, we help them increase their reach. We expect that the dissemination team of the other CoEs do the same.

3.3 Training

A variety of training in the use of POP3 assessment tools and methodology will be made available to all, mostly via the established Virtual Institute - High Productivity Supercomputing (VI-HPS). This will be complemented with bespoke training offered to individual CoEs (potentially in conjunction with an assessment campaign), groups of CoEs in related application areas or sharing the same codes, EuroHPC hosting entities and related projects for application support and training such as EPICURE and HPC SPECTRA. Hackathon-style workshops where participants (ideally in teams) apply our tools to assess their own application codes on EuroHPC computer systems (or similar systems) will be favoured. We plan to have at least four training events and more than 25 people trained in using our tools and methodology each calendar year.

3.4 Business development

The majority of services to be provided by POP3 will be to CoEs (80/120) and were planned before the start of the project. This represents almost 65% of the services to be provided by POP3.

We will extend this co-operation to other CoEs who are not already involved in making available the codes that they develop, and we will eventually use the Castiel Project to try to attract new CoEs.

4. POP3 Collaboration with CASTIEL2

The collaboration with CASTIEL2 CSA is detailed in the corresponding deliverable of this CSA. The Main Objectives of this Collaboration Agreement, signed also by POP3, are:

- Collaboration and Coordination: Facilitate collaboration and coordination among CoEs to advance research and development in high-performance computing (HPC).
- Resource Sharing: Share computational resources, expertise, and knowledge to enhance the efficiency and effectiveness of HPC applications.
- Innovation and Development: Promote innovation in HPC technologies and applications, focusing on areas like climate modelling, biomolecular research, materials design, and astrophysics.

The POP3 dissemination team participates in the regular online and (as much as possible) face-to-face meetings of the CASTIEL2 communication work package. We will also contribute with relevant input about our services, results, success stories and events to the CASTIEL2 dissemination channels (e.g. the regular CASTIEL2 Newsletter).

POP3 will actively participate in CASTIEL2 collaboration meetings, including those of its working groups.

- Training, Twinning, Mentoring: We will summarise the variety of POP3 training activities and engage in discussion and documentation of best practices for training. We will partner with CoEs and NCCs in organising joint training events, including the CASTIEL2 Training Sprint initiative. Our training events will be entered in the appropriate portals (initially the HPC in Europe portal until superceded by the CASTIEL2 C2ISS portal).
- Continuous Integration and Continuous Development: We will share our experience with our existing CI setups and code deployments on EuroHPC and related HPC systems, and contribute to the discussion, specification and evaluation of repositories and processes established within CASTIEL2.

POP3 also attended the CASTIEL2 All-Hands-Meeting in Slovakia in April 2024. This was a real opportunity to initiate discussions with a number of CoEs and NCCs, to present the POP3 activities and service evolution compared to POP2, and to answer any questions related to these topics.

Some of these questions were:

- What are the overall objectives of the POP CoE?
- How to apply for these services?
- Who is affected by these services?
- What are the conditions for acceptance?
- What are the deadlines for the provision of the services?

The appropriate answers have been provided; moreover, additional meetings will be planned with CoEs and NCCs to present the POP3 activities in more detail and to explain the impact and possible benefits that users and the whole ecosystem can enjoy as a result of the POP3 services.

5. Expected impact of the Collaboration

5.1 Impact for POP3

The scale and significance of a successful collaboration with the CoEs is reflected by the POP3 KPIs. These include 120 POP services, out of which 82 for CoE codes, and more than 100 people in the POP methodology.

Collaboration with the CASTIEL2 and other CoE dissemination teams will increase the impact and reach of our dissemination work. This in turn will help us to maintain and improve the POP3 CoE reputation for expertise and excellence in HPC performance assessments and analysis.

The collaboration will also allow POP3 to better reach the HPC community in Europe and target training and services to their needs, along with associated development of our tools and methodology.

Moreover, by collaborating with the other CoEs, POP3 will benefit from:

- Work on high-level and highly complex scientific applications tailored to intensive computing.
- Challenge the analysis tools used by POP teams and prove their efficiency and value.
- The use cases provided by the CoEs can lead to excellent success stories.
- Very useful kernels can be produced and published from CoEs use cases.

5.2 Impact for other CoEs

POP3 aims to function as a horizontal CoE, primarily supporting other CoEs in enhancing the scalability and efficiency of their lighthouse codes. We believe this external perspective is highly valuable, a view supported by our previous experiences with POP and POP2. The commitment to collaboration of the other CoEs is evident in their letters of support during the preparation of the POP3 proposal.

Our assessments will accurately identify potential roadblocks to improving the efficiency and scaling of applications, providing code owners with insights and quantified expectations for performance improvements. CoEs utilizing our services will gain detailed insights into the efficiency and scaling issues of their specific application codes, along with advice on appropriate remedies. Additionally, CoEs receiving training on our tools and methodology will be equipped to conduct some assessments independently, integrating these practices into their development processes.

5.3 Impact for third parties

Academic and industrial parallel application developers who are not part of HPC CoEs can similarly request and benefit from our services and training activities. EuroHPC hosting entities (and specifically their application support personnel such as those within EPICURE), NCCs and other projects (such as HPC SPECTRA) will also be able to exploit our services and training to complement and expand their own offerings.

6. Conclusion

Collaboration with other CoEs is a major component of POP3 activities, serving as a natural continuation of the efforts from POP and POP2. The results of this collaboration will be reflected in the POP3 KPIs and outputs, thus significantly impacting the project. We anticipate that this impact will extend to the other CoEs and, more broadly, to the entire HPC community.

Acronyms and Abbreviations

POP3 Beneficiaries

- BSC: BARCELONA SUPERCOMPUTING CENTER - CENTRO NACIONAL DE SUPERCOMPUTACION
- FZJ: FORSCHUNGSZENTRUM JÜLICH GMBH
- RWTH: RHEINISCH-WESTFAELISCHE TECHNISCHE HOCHSCHULE AACHEN
- IT4I@VSB: TECHNICAL UNIVERSITY OF OSTRAVA
- INESC ID: INSTITUTO DE ENGENHARIA DE SISTEMAS E COMPUTADORES, INVESTIGACAO E DESENVOLVIMENTO EM LISBOA
- TERATEC: TERATEC
- UVSQ: UNIVERSITE DE VERSAILLES SAINT-QUENTIN-EN-YVELINES
- USTUTT: UNIVERSITY OF STUTTGART FOR ITS HIGH PERFORMANCE COMPUTING CENTER STUTTGART

References

[1] POP Deliverable D2.4 Final Customer Feedback Report (https://cordis.europa.eu/project/id/676553/results)
[2] POP2 Deliverable D2.1 Plan for targeting CoEs (https://cordis.europa.eu/project/id/824080/results)
[3] POP2 Deliverable D2.3 First Business Development and Sustainability Review (https://cordis.europa.eu/project/id/824080/results)
[4] POP2 Deliverable D2.4 Final Business Development and Sustainability Review (https://cordis.europa.eu/project/id/824080/results)